XLiFE++

# Developer documentation

Nicolas KIELBASIEWICZ, Eric LUNÉVILLE, Manh Ha NGUYEN, Yvon LAFRANCHE

April 8, 2022

# Contents

# 1 General organization

## 1.1 Licence

XLIFE++ is copyright (C) 2010-2022 by E. Lunéville and N. Kielbasiewicz and is distributed under the terms of the GNU General Public License (GPL) (Version 3 or later, see https://www.gnu.org/licenses/gpl-3.0.en.html). This means that everyone is free to use XLIFE++ and to redistribute it on a free basis. XLIFE++ is not in the public domain; it is copyrighted and there are restrictions on its distribution. You cannot integrate XLIFE++ (in full or in parts) in any closed-source software you plan to distribute (commercially or not). If you want to integrate parts of XLIFE++ into a closed-source software, or want to sell a modified closed-source version of XLIFE++, you will need to obtain a different license. Please contact us directly for more information.

The developers do not assume any responsibility in the numerical results obtained using the XLIFE++ library and are not responsible of bugs.

## 1.2 Credits

The XLIFE++ library has been mainly developped by E. Lunéville and N. Kielbasiewicz of POEMS lab (UMR 7231, CNRS-ENSTA Paris-INRIA). Some parts are inherited from MELINA++ library developped by D. Martin (IRMAR lab, Rennes University, now retired) and E. Lunéville. Other contributors are :

- Y. Lafranche (IRMAR lab), mesh tools using subdivision algorithms, wrapper to ARPACK
- C. Chambeyron (POEMS lab), iterative solvers, unitary tests, PhD students' support
- M.H N'Guyen (POEMS lab), eigen solvers and OpenMP implementation
- N. Salles (POEMS lab), boundary element methods
- L. Pesudo (POEMS lab), boundary element methods and HF coupling
- P. Navaro (IRMAR lab), continuous integration
- E. Darrigrand-Lacarrieu (IRMAR lab), fast multipole methods
- E. Peillon (POEMS lab), evolution of (bi)linear forms

## 1.3 Installation

XLIFE++ is under an open git repository on the INRIA Gitlab instance. So developer access to source code needs to log to the gitlab and to define a ssh-key for authentication. The first part is to be registered to INRIA Gitlab and to be accepted as member of XLIFE++ project. To do so, please do as follows:

1. Please go to `https://gitlab.inria.fr/xlifepp/xlifepp/`.
2. If you have already had a user account, please go to step #4
3. If you don't have a user account, please create it.
4. If you have already been member of the XLIFE++ project on INRIA Gitlab, please go to step #6

5. If you are not member of the XLIFE++ project on INRIA Gitlab, please contact one of the XLIFE++ administrators to join the XLIFE++ development team and wait until your registration to XLIFE++ project on INRIA Gitlab is done to go to next section.

6. For further documentation, you may go to the XLIFE++ main page:

   `http://uma.ensta-paris.fr/soft/XLiFE++/`

### 1.3.1 Under MacOS and Linux

To install XLIFE++ in order to take part to its development, you may use the following steps:

1. Please install GIT (`http://www.git-scm.com`) and CMAKE (`http://cmake.org`).

2. If you have already generated a ssh key and want to use it for XLIFE++ project, please go to step #4

3. If you don't have generated a ssh key, please use the command `ssh-keygen` to generate one.

4. To add the public ssh key you want to use, please go to your account settings on INRIA GForge and add the key by clicking on "Edit keys" at the bottom. Copy the public key where it is needed, validate and register changes to your account. This may take some time so that the key is truly activated.

5. On `https://gforge.inria.fr/projects/xlifepp/`, please go to the "Sources" tab to see the `git clone ...` command-line you have to run in a terminal to create your local XLIFE++ repository.

6. In the root directory of XLIFE++, you have a shell script *pre-commit.sh* and a hidden directory *.git*. Copy the script to *.git/hooks/pre-commit* (without extension) and make the copy executable. When done, you will update file VERSION.txt automatically.

7. You can now compile and develop. See next section.

### 1.3.2 Under Windows

To install XLIFE++ in order to take part to its development, you may use the following steps:

1. Please install GIT (`http://www.git-scm.com`) and CMAKE (`http://cmake.org`). On Windows, git is usable with the contextual menu showed with clicks on the right mouse button.

2. Please open Git GUI in the contextual menu.

3. Please click on "Cloning existing repository". A window opens.

4. Please open the "Help" tab and select "Show SSH key"

5. Click on "Generate key". The public key will be shown. Copy it.

6. To add the public ssh key, please go to your account settings on INRIA GForge and add the key by clicking on "Edit keys" at the bottom. Copy the public key where it is needed, validate and register changes to your account. This may take some time so that the key is truly activated.

7. To set the "Source location" in the Git GUI window, please go to the "Sources" tab on `https://gforge.inria.fr/projects/xlifepp/` to see the `git clone ...` command-line. Copy the url (beginning by git+ssh//). Define a non-existing directory for the "Target' Directory'. And click on "Clone" to create your local repository.

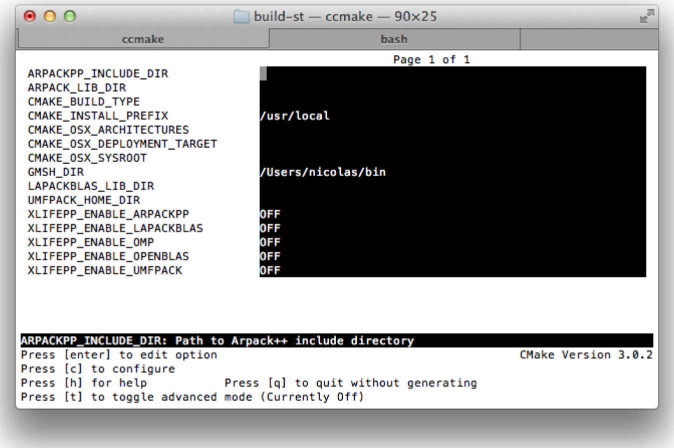
8. In the root directory of XLIFE++, you have a shell script *pre-commit.sh* and a hidden directory *.git*. Copy the script to *.git/hooks/pre-commit* (without extension) and make the copy executable. When done, you will update file VERSION.txt automatically.

9. You can now compile and develop. See next section.

## 1.4 Compilation

Compilation of XLIFE++ is managed by CMAKE, a high-level cross-platform compilation tool, running on MacOS, Windows, and Linux. This application only needs a configuration file named CMakeLists.txt, at the root directory of the XLIFE++ archive. Whatever the OS, cmake also asks for another directory where to put generated files for compilation, called build directory hereafter. This directory can be everywhere. It will contains compilation files (objects files, ...), a Makefile or an IDE project file named XLiFE++ (for Eclipse, CodeBlocks, Visual Studio, XCode, ...). So we suggest you to set this directory as a subdirectory of XLIFE++ install directory, with the name "build" for instance.

### 1.4.1 Under MacOS and Linux



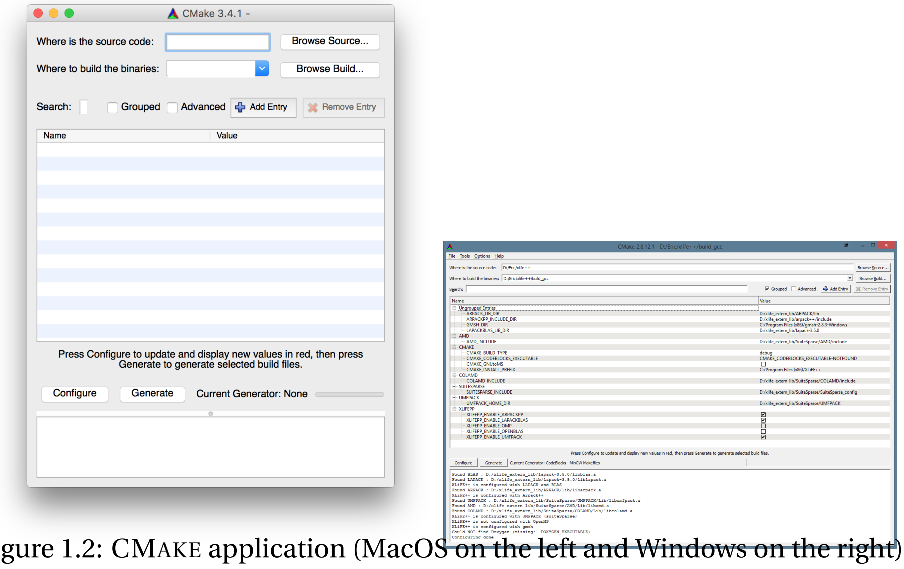
```
                                  Page 1 of 1
ARPACKPP_INCLUDE_DIR
ARPACK_LIB_DIR
CMAKE_BUILD_TYPE
CMAKE_INSTALL_PREFIX             /usr/local
CMAKE_OSX_ARCHITECTURES
CMAKE_OSX_DEPLOYMENT_TARGET
CMAKE_OSX_SYSROOT
GMSH_DIR                         /Users/nicolas/bin
LAPACKBLAS_LIB_DIR
UMFPACK_HOME_DIR
XLIFEPP_ENABLE_ARPACKPP          OFF
XLIFEPP_ENABLE_LAPACKBLAS        OFF
XLIFEPP_ENABLE_OMP               OFF
XLIFEPP_ENABLE_OPENBLAS          OFF
XLIFEPP_ENABLE_UMFPACK           OFF



ARPACKPP_INCLUDE_DIR: Path to Arpack++ include directory
Press [enter] to edit option                                     CMake Version 3.0.2
Press [c] to configure
Press [h] for help           Press [q] to quit without generating
Press [t] to toggle advanced mode (Currently Off)
```

Figure 1.1: ccmake (MacOS, Unix)

When running ccmake, the default CMAKE GUI under MacOS or Linux, the build directory is given in argument.

```
ccmake [options] path/to/CMakeLists.txt path/to/buildDirectory
```

When running CMAKE GUI application, you have to set the directory “Where is the source code” containing CMakeLists.txt you want to run CMAKE on, and to set the build directory: “Where to build the binaries”. Then, you click the “Configure” button. It will ask ou the generator you want. Then, you click the “Generate” button, to generate your IDE project file or your Makefile.



CMake 3.4.1 -
Where is the source code:
Browse Source...
Where to build the binaries:
Browse Build...
Search:
Grouped
Advanced
Add Entry
Remove Entry
Name
Value
Press Configure to update and display new values in red, then press Generate to generate selected build files.
Configure
Generate
Current Generator: None
CMake 2.8.12.1 - D:/Eric/xlife++/build_gcc
File
Tools
Options
Help
Browse Source...
Browse Build...
Search:
☑ Grouped
□ Advanced
Add Entry
Remove Entry
Press Configure to update and display new values in red, then press Generate to generate selected build files.
Configure
Generate

Where is the source code: D:/Eric/xlife++

Where to build the binaries: D:/Eric/xlife++/build_gcc

| Name | Value |
|---|---|
| ⊟ Ungrouped Entries | |
| ARPACK_LIB_DIR | D:/xlife_extern_lib/ARPACK/lib |
| ARPACKPP_INCLUDE_DIR | D:/xlife_extern_lib/arpack++/include |
| GMSH_DIR | C:/Program Files (x86)/gmsh-2.8.3-Windows |
| LAPACKBLAS_LIB_DIR | D:/xlife_extern_lib/lapack-3.5.0 |
| ⊟ AMD | |
| AMD_INCLUDE | D:/xlife_extern_lib/SuiteSparse/AMD/include |
| ⊟ CMAKE | |
| CMAKE_BUILD_TYPE | debug |
| CMAKE_CODEBLOCKS_EXECUTABLE | CMAKE_CODEBLOCKS_EXECUTABLE-NOTFOUND |
| CMAKE_GNUtoMS | □ |
| CMAKE_INSTALL_PREFIX | C:/Program Files (x86)/XLiFE++ |
| ⊟ COLAMD | |
| COLAMD_INCLUDE | D:/xlife_extern_lib/SuiteSparse/COLAMD/include |
| ⊟ SUITESPARSE | |
| SUITESPARSE_INCLUDE | D:/xlife_extern_lib/SuiteSparse/SuiteSparse_config |
| ⊟ UMFPACK | |
| UMFPACK_HOME_DIR | D:/xlife_extern_lib/SuiteSparse/UMFPACK |
| ⊟ XLIFEPP | |
| XLIFEPP_ENABLE_ARPACKPP | ☑ |
| XLIFEPP_ENABLE_LAPACKBLAS | ☑ |
| XLIFEPP_ENABLE_OMP | □ |
| XLIFEPP_ENABLE_OPENBLAS | □ |
| XLIFEPP_ENABLE_UMFPACK | ☑ |

Current Generator: CodeBlocks - MinGW Makefiles

```
Found BLAS : D:/xlife_extern_lib/lapack-3.5.0/libblas.a
Found LAPACK : D:/xlife_extern_lib/lapack-3.5.0/liblapack.a
XLiFE++ is configured with LAPACK and BLAS
Found ARPACK : D:/xlife_extern_lib/ARPACK/lib/libarpack.a
XLiFE++ is configured with Arpack++
Found UMFPACK : D:/xlife_extern_lib/SuiteSparse/UMFPACK/Lib/libumfpack.a
Found AMD : D:/xlife_extern_lib/SuiteSparse/AMD/Lib/libamd.a
Found COLAMD : D:/xlife_extern_lib/SuiteSparse/COLAMD/Lib/libcolamd.a
XLiFE++ is configured with UMFPACK (suiteSparse)
XLiFE++ is not configured with OpenMP
XLiFE++ is configured with gmsh
Could NOT find Doxygen (missing:  DOXYGEN_EXECUTABLE)
Configuring done
```

Figure 1.2: CMAKE application (MacOS on the left and Windows on the right)

When running CMAKE in command-line mode, the build directory is generally the directory in which you are when calling the CMAKE command. If you want to know the general case, please take a look at CMAKE option -b.

To compile XLIFE++, you just have to run CMAKE on the CMakeLists.txt file:

```
cmake path/to/CMakeLists.txt
```

If you generated a project file, you launch your IDE on this file and can compile and run tests. The following command chooses for instance to use codeblocks on unix platform:

```
cmake path/to/CMakeLists.txt -G "CodeBlocks - Unix Makefiles"
```

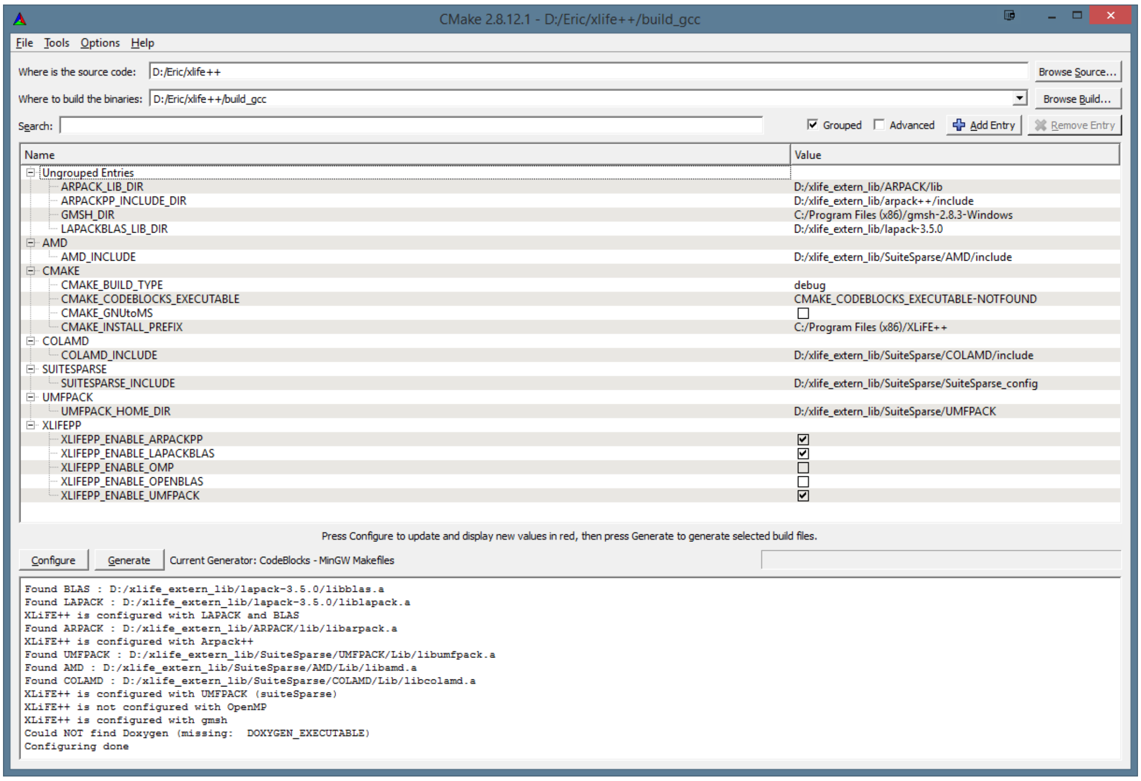
If you generated a Makefile, you have to run the `make` command, to compile XLIFE++ sources and tests. If you want to compile XLIFE++ sources only, the target is "libs":

```
make libs
make
```

If you generated an IDE project file, you have to open it and compile target all to compile everything, sources and tests, or target libs, to compile sources only.

### 1.4.2 Under Windows

When running CMAKE GUI application, you have to set the directory “Where is the source code” containing CMakeLists.txt you want to run CMAKE on, and to set the build directory: “Where to build the binaries”. Then, you click the “Configure” button. It will ask ou the generator you want. Then, you click the “Generate” button, to generate your IDE project file or your Makefile.



Where is the source code: D:/Eric/xlife++

Where to build the binaries: D:/Eric/xlife++/build_gcc

Search:

☑ Grouped ☐ Advanced

| Name | Value |
|---|---|
| Ungrouped Entries | |
| ARPACK_LIB_DIR | D:/xlife_extern_lib/ARPACK/lib |
| ARPACKPP_INCLUDE_DIR | D:/xlife_extern_lib/arpack++/include |
| GMSH_DIR | C:/Program Files (x86)/gmsh-2.8.3-Windows |
| LAPACKBLAS_LIB_DIR | D:/xlife_extern_lib/lapack-3.5.0 |
| AMD | |
| AMD_INCLUDE | D:/xlife_extern_lib/SuiteSparse/AMD/include |
| CMAKE | |
| CMAKE_BUILD_TYPE | debug |
| CMAKE_CODEBLOCKS_EXECUTABLE | CMAKE_CODEBLOCKS_EXECUTABLE-NOTFOUND |
| CMAKE_GNUtoMS | ☐ |
| CMAKE_INSTALL_PREFIX | C:/Program Files (x86)/XLiFE++ |
| COLAMD | |
| COLAMD_INCLUDE | D:/xlife_extern_lib/SuiteSparse/COLAMD/include |
| SUITESPARSE | |
| SUITESPARSE_INCLUDE | D:/xlife_extern_lib/SuiteSparse/SuiteSparse_config |
| UMFPACK | |
| UMFPACK_HOME_DIR | D:/xlife_extern_lib/SuiteSparse/UMFPACK |
| XLIFEPP | |
| XLIFEPP_ENABLE_ARPACKPP | ☑ |
| XLIFEPP_ENABLE_LAPACKBLAS | ☑ |
| XLIFEPP_ENABLE_OMP | ☐ |
| XLIFEPP_ENABLE_OPENBLAS | ☐ |
| XLIFEPP_ENABLE_UMFPACK | ☑ |

Press Configure to update and display new values in red, then press Generate to generate selected build files.

Current Generator: CodeBlocks - MinGW Makefiles

```
Found BLAS : D:/xlife_extern_lib/lapack-3.5.0/libblas.a
Found LAPACK : D:/xlife_extern_lib/lapack-3.5.0/liblapack.a
XLiFE++ is configured with LAPACK and BLAS
Found ARPACK : D:/xlife_extern_lib/ARPACK/lib/libarpack.a
XLiFE++ is configured with Arpack++
Found UMFPACK : D:/xlife_extern_lib/SuiteSparse/UMFPACK/Lib/libumfpack.a
Found AMD : D:/xlife_extern_lib/SuiteSparse/AMD/Lib/libamd.a
Found COLAMD : D:/xlife_extern_lib/SuiteSparse/COLAMD/Lib/libcolamd.a
XLiFE++ is configured with UMFPACK (suiteSparse)
XLiFE++ is not configured with OpenMP
XLiFE++ is configured with gmsh
Could NOT find Doxygen (missing:  DOXYGEN_EXECUTABLE)
Configuring done
```

Figure 1.3: `cmake` (Windows), after you clicked the configure button.

You can have the list of available generators inside CMAKE help. It does not tell that eclipse, codeblocks, ... are installed, but it tells that they can be installed on your computer and how you can tell CMAKE to use them as generators.

### 1.4.3 Useful general options to CMake

Four options may be very useful:

**CMAKE_CXX_COMPILER** This option is used to set the compiler CMake will use to compile your code:

```
cmake path/to/CMakeLists.txt -DCMAKE_CXX_COMPILER=g++-48
```

**CMAKE_BUILD_TYPE** This option is used to set the type of build (debug, release, . . . ). Possible values are essentially Debug and Release. The default value is Release.

```
cmake path/to/CMakeLists.txt -DCMAKE_BUILD_TYPE=Debug
```

**XLIFEPP_PRECISION** This option is used to set the precision of numerical types (int, . . . ). Possible values are STD, LONG and LONGLONG. The default value is LONG.

```
cmake path/to/CMakeLists.txt -DXLIFEPP_PRECISION=LONG
```

Except if you have a very good reason, you are not supposed to use this option.

**XLIFEPP_STRING_TYPE** This option is used to set string type: STD (for std::string) and WIDE (for std::wstring). The default value is STD.

```
cmake path/to/CMakeLists.txt -DXLIFEPP_STRING_TYPE=STD
```

Except if you have a very good reason, you are not supposed to use this option.

### 1.4.4 Configuring XLiFE++ with Gmsh and/or Paraview

**XLIFEPP_GMSH_EXECUTABLE** To specify the Gmsh binary with full path. If Gmsh is in your PATH, it will be automatically detected, else you can use this option:

```
cmake path/to/CMakeLists.txt -DXLIFEPP_GMSH_EXECUTABLE=gmsh/exe/with/full/path
```

**XLIFEPP_PARAVIEW_EXECUTABLE** To specify the Paraview binary with full path. If Paraview is in your PATH, it will be automatically detected, else you can use this option:

```
cmake path/to/CMakeLists.txt -DXLIFEPP_PARAVIEW_EXECUTABLE=paraview/exe/with/full/path
```

### 1.4.5 Configuring XLiFE++ with OpenMP

**XLIFEPP_ENABLE_OMP** Activates/Deactivates use of OpenMP

```
cmake path/to/CMakeLists.txt -DXLIFEPP_ENABLE_OMP=ON
```

### 1.4.6 Configuring XLiFE++ with Arpack

Configuring with Arpack also means configuring with Blas and Lapack. When asked, these 3 libraries are automatically searched in standard paths. If these libraries are installed in other paths, you can give it directly. Otherwise, sources files of Arpack inside XLiFE++ sources will be compiled and used.

**XLIFEPP_ENABLE_ARPACK** Activates/Deactivates configuration with Arpack. Default is OFF.

**XLIFEPP_SYSTEM_ARPACK** To use a system distribution of Arpack (ON) or the provided one (OFF). Default is OFF.

**XLIFEPP_BLAS_LIB_DIR** To specify the directory containing Blas library

**XLIFEPP_LAPACK_LIB_DIR** To specify the directory containing Lapack library

**XLIFEPP_ARPACK_LIB_DIR** To specify the directory containing Arpack library

See section A.3 for more details

### 1.4.7 Configuring XLIFE++ with UMFPACK

Configuring with UMFPACK also means configuring with BLAS and LAPACK. It can also mean configuring with other libraries provided by SUITESPARSE, insofar as UMFPACK is now distributed inside SUITESPARSE.

**XLIFEPP_ENABLE_UMFPACK** Activates/Deactivates configuration with UMFPACK. Default is OFF.

**XLIFEPP_BLAS_LIB_DIR** To specify the directory containing BLAS library

**XLIFEPP_LAPACK_LIB_DIR** To specify the directory containing LAPACK library

**XLIFEPP_UMFPACK_INCLUDE_DIR** To specify the directory containing UMFPACK header

**XLIFEPP_UMFPACK_LIB_DIR** To specify the directory containing UMFPACK header

**XLIFEPP_SUITESPARSE_HOME_DIR** To specify the home directory of SUITESPARSE, including UMFPACK. This option is to be used if you compiled SUITESPARSE by yourself. In this case, UMFPACK will be searched in the UMFPACK subdirectory.

There are specific options to each library provided by SUITESPARSEUMFPACK may depend on. See section A.2 for more details.

> Using CMAKE generates a cache file (CMakeCache.txt) containing value of every option defined during execution of CMAKE, so that when reusing cmake on the same file resuses CMakeCache.txt, unless you change some options. This is why XLIFEPP_ENABLE_XXX options can take the value OFF.

## 1.5 Folder organisation

The XLIFE++ main directory is organised as follows :

**bin** the binary directory containing the test executable and the output files for test execution

**CMakeLists.txt** this is the parameters file for CMAKE

**doc** the documentation directory with the source documentation (the **api** subdirectory), generated by DOXYGEN, and the TeX/pdf documentation (the **tex** subdirectory)

**etc** this directory contains templates files for installation, parameters files for DOXYGEN, dictionaries and messages formats

**include** this directory contains the header aliases for each sublibrary of XLIFE++ and config files

**lib** this directory contains the static sublibraries of XLIFE++

**README** the README file

**src** this directory contains all source and header files. Each subdirectory represents a sublibrary of XLIFE++

**tests** this directory contains source files for unitary and non-regressive tests

**usr** this directory contains all files needed by the user to write a program using XLIFE++ and compile it.

## 1.6 Namespace

The whole XLIFE++ library is defined in the namespace ***xlifepp***. Then, the developers have to encapsulate all their developments in this namespace either in the header files (.hpp) or in the implementation files (.cpp). For instance, a header file looks like :

```
#ifndef FILE_HPP
#define FILE_HPP

#include "otherfile.hpp"
#include <sysinclude>

namespace xlifepp{
  ...

} //end of namespace
#endif
```

## 1.7 Headers

All the header files of the library end by *.hpp* and are located in the folder related to the topics of the header file. There are four particular header files located in the *init* folder :

- *setup.hpp* defining the pre-compiler macro related to the install path, the operating system, the precision type, the string type, the language and debug feature. Be cautious, changing one of this macro implies the recompilation of all the library.
- *config.hpp* declaring all the general stuff : scalar definitions, string definition, enumeration, numerical constants and global variables used by general tools. It includes the header *setup.hpp*. Note that this file may be (and must be) included everywhere.
- *globalScopeData.hpp* initializing global variables declared in *config.hpp*. This file has to be included once.

Some header interface files are defined in the *include* folder, their name end with *.h*. The header interface files are

- lib*.h* for each library folder (e.g *init.h, utils.h, ...*). This header file included all the header files (.hpp) of the library folder and is used by other libraries that require objects of this library folder.
- *config.h* is an alias to the *config.hpp* located in the *init* folder.
- *globalScopeData.h* is an alias to the *globalScopeData.hpp* located in the *init* folder.
- *xlife++.h* is the global header file. As this file includes the *globalScopeData.hpp* initializing all the global variables it must be included only in the main program.

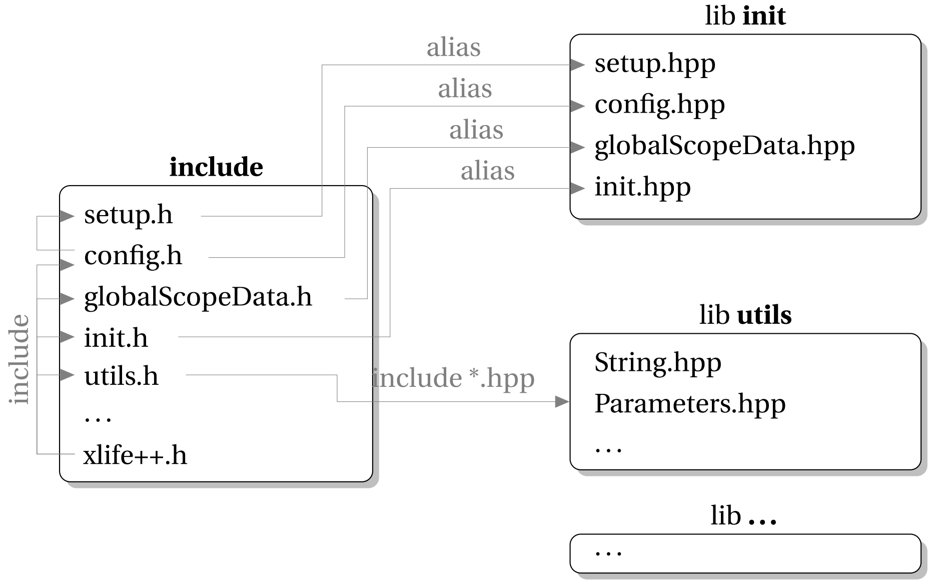


Figure 1.4: Headers organisation

From a practical point of view :

- when you develop a new class or utilities in the *mystuff.cpp* file in the library *lib*, create the header file *mystuff.hpp* and add the alias *#include "../src/lib/mystuff.hpp"* in the *lib.h* located in the *include* folder.
- include the *config.h* in your files to access to all general definitions, local header files (.hpp) if you refer to some stuff of the library and global header files (.h) if you refer to some stuff of other libraries
- when you develop a new library (*mylib*), you have to create the *mylib.h* header file in the *include* folder and add *#include "mylib.h"* in the *xlife++.h*.

## 1.8 Development principles

This section gives some "philosophical" principles to developp the library XLiFE++. These principles can be sum up in the following commandments :

- **Code has to be efficient**

  It means that time consuming functions and memory consuming object has to be designed to be the most efficient as possible. It is not required else.

- **Be friendly with end users**

  no templated and not too much end user's classes, no pointers, friendly syntaxes, ...

- **Be friendly with not advanced developers**

  it means that the intermediate code has to be not too intricate

- **Make code documentation**

  Write inline documentation along Doxygen syntax and outline documentation in Latex: the developer documentation gives principles, useful comments and a description of classes and functions, user documentation describes how to use the end user's classes and functions.

- **Write test functions**

  It is mandatory to perform low level tests and to archive it (see chapter Test Policy)

As usual, there may be exceptions to the rules but they have to be approved.

### Dealing with multithreading

Up to now, XLiFE++ supports OMP if library is compiled with the OMP flag. It is up to the developer to use it or not but when heavy computation it is advised to. As XLiFE++ already uses OMP in all FE computations or matrix computations, be care when using it at a high level of the code.

### How to encapsulate a class hierarchy in an end user class

The problem is to propose to end user a single class (`User`) masking a class hierarchy (`Child1`,`Child2`,... that inherits from `User`):

```
class Child1 : public User {...};
class Child2 : public User {...};
```

There are at least three solutions :

- using child pointers of child classes inherited from `BaseChild` base class :

```
class BaseChild {...}
class Child1 : public BaseChild {...};
class Child2 : public BaseChild {...};

class User
{ChildType childType;        //type of child
 Child1 * ch1_p;             //pointer to Child1 object
 Child2 * ch2_p;             //pointer to Child2 object
 ...                         //common attributes and functions
};
```

All the member functions of `User` class analyse the child type to adress the right child functions.

- using pointer to `BaseChild` base class :

```
class BaseChild {...}
class Child1 : public BaseChild {...};
class Child2 : public BaseChild {...};

class User
{BasicChild * bch_p;         //pointer to BaseChild object
 ...
};
```

All the member functions of `User` class call their equivalent `BaseChild` member functions.

- using a contraction of the previous model named "abstact/non abstract pattern" :

```
class User
{User* us_p;    //pointer to child or itself if it is a child
 virtual Child1* child1()
   {if(us_p!=this) us_p->child1();
    return 0;}
};

class Child1 : public User
{Child1* child1(){return this;}
 ...
};
class Child2 : public User
{Child2* child2(){return this;}
 ...
};
```

This model is named "abstract/non abstract" because `User` class is a non abstract class but is used as an abstract class. In this model, `User` class attributes are duplicated. If they take a large amount of memory, encapsulate it in a structure and use a pointer to this structure :

```
class Attributes
{...
};

class User
{User* us_p;       //pointer to child or itself if it is a child
 Attributes* at_p; //pointer to User attributes
};
```

Each of them has their advantages and defaults. Use the one you prefer.

# 2 Initialization and global definitions

## 2.1 About the init function

Initialization is the aim of the *init* library and more precisely the *init.cpp* and *init.hpp* files and the definition of the init functions.
Each user program needing XLiFE++ has to begin with a call to the init routinewith up to 4 key/value arguments:

**_lang** enum to set the language for print and log messages. Possible values are $en$, $fr$, or $de$. Default value is $en$.

**_verbose** integer to set the verbose level. Default value is 1.

**_trackingMode** boolean to set if in the log file, you have a backtrace of every call to a XLiFE++ routine. Default value is false.

**_isLogged** boolean to activate log. Default value is false.

Available languages are English, French and German, but XLiFE++ is easily extendible for other languages.

```
init(_lang=en)
```

What is the init function doing ?

1. If the init function was previously called, it stops, or does the following steps otherwise.
2. It builds the global Environment object to initializes dictionary and paths to messages formats, according to the given language.
   The path to the english dictionary file is XLIFEPP_DIR/etc/Messages/en/dictionary.txt, the path to the french messages file is XLIFEPP_DIR/etc/Messages/fr/messages.txt, ...
3. It builds the global Trace object to initialize logs
4. It prints the execution header (logo + execution date, host machine ...)
5. It opens the print file and write the header in it.
6. It builds the global Messages object to load messages formats
7. It initializes RTI names for Function and Value objects.

Global objects are declared in *config.hpp* and defined in *globalScopeData.hpp*. In the next section, we will see what is the content of these two files and of *setup.hpp*

## 2.2 Global declarations and definitions

### 2.2.1 *setup.hpp*

This file is automatically generated when you execute CMake. Its aim is to set compilation macros :

- **OS_IS_UNIX**, **OS_IS_WIN**, to set the OS. It is useful for instance to load specific source code for time management (*Timer.*pp*)

- **XLIFEPP_WITH_GMSH** and **XLIFEPP_WITHOUT_GMSH**, to activate/deactivate compilation of XLIFE++ routines using a system call to GMSH
- **XLIFEPP_WITH_PARAVIEW** and **XLIFEPP_WITHOUT_PARAVIEW**, to activate/deactivate compilation of XLIFE++ routines using a system call to PARAVIEW
- **XLIFEPP_WITH_ARPACKPP** and **XLIFEPP_WITHOUT_ARPACKPP**, to activate/deactivate compilation of XLIFE++ interface of ARPACK++ library.
- **XLIFEPP_WITH_UMFPACK** and **XLIFEPP_WITHOUT_UMFPACK**, to activate/deactivate compilation of XLIFE++ interface of UMFPACK library.
- **XLIFEPP_WITH_OMP** and **XLIFEPP_WITHOUT_OMP**, to activate/deactivate compilation of XLIFE++ using OPENMP library.
- **XLIFEPP_WITH_EIGEN** and **XLIFEPP_WITHOUT_EIGEN**, to activate/deactivate compilation of XLIFE++ using EIGEN library.
- **XLIFEPP_WITH_AMOS** and **XLIFEPP_WITHOUT_AMOS**, to activate/deactivate compilation of XLIFE++ using AMOS library.
- **XLIFEPP_WITH_MAGMA** and **XLIFEPP_WITHOUT_MAGMA**, to activate/deactivate compilation of XLIFE++ using MAGMA library.
- **INSTALL_PATH**, to set the install path of XLIFE++ and build paths for dictionary or messages formats.
- **GMSH_EXECUTABLE**, to set the executable of GMSH with full path.
- **PARAVIEW_EXECUTABLE**, to set the executable of PARAVIEW with full path.
- **VISUTERMVECM_PATH**, to set the path to visuTermVec.m MATLAB script that can be used in post-processing.
- **STD_TYPES**, **LONG_TYPES**, **LONGLONG_TYPES** to set the precision of scalar non integer values. The default is **LONG_TYPES**
- **STD_STRING**, **WIDE_STRING**, to set the encoding of strings, by loading either the STL string classes, or . The default is **STD_STRING**.
- **COMPILER_IS_32_BITS**, **COMPILER_IS_64_BITS** to set the precision od integer values

The last five macros are used in *config.hpp* to define some typedefs.

### 2.2.2 *config.hpp*

This file defines some scalar types, objects and parameters, and also enums.

- **Scalar types :** XLIFE++ uses scalar types that depend on the precision given in *setup.hpp* : `int_t` , `real_t`, `complex_t` are typedefs for respectively `int`, `float`, `complex<float>` and their families (`long int`, `double`,...) according to the corresponding macro. Two additional typedefs are `number_t` and `dimen_t` respectively for `size_t` and `short unsigned int`, independent on precision. These scalar types can be called by users. According to the XLIFE++ code convention, they have user typedefs : `Int`, `Real`, `Complex`, `Number`, `Dimen`. For the same reason, there is the `String` typedef for STL classes `string` or `wstring` according to the corresponding macro, and the `Strings` typedef for `std::vector<String>`
- **Global parameters :** This is about output format parameters and extremal values :

```
extern const number_t entriesPerRow;
extern const number_t entryWidth;
extern const number_t entryPrec;
extern const number_t addrPerRow;
extern const number_t addrWidth;
extern const number_t numberPerRow;
extern const number_t numberWidth;
extern const number_t theNumberMax;
extern const size_t theSizeMax;
extern const dimen_t theDimMax;
extern const real_t theRealMax;
extern const real_t theEpsilon;
extern const real_t theTolerance;
extern const real_t theZeroThreshold;
extern const number_t theLanguage;
extern unsigned int theGlobalVerboseLevel;
extern unsigned int theVerboseLevel;
```

There is also some mathematical constants :

```
extern const real_t over3;
extern const real_t over6;
extern const real_t pi;
extern const real_t overpi;
extern const real_t over2pi;
extern const real_t over4pi;
extern const real_t sqrtOf2_;
extern const real_t sqrtOf3_;
extern const real_t logOf2_;
extern const real_t theEulerConst;
```

- **Global objects :** Global Trace, Messages, Parameters and Environment are also declared here
- **enums :** This is the list of enums defined here. For convenience, we give only their declaration :

```
enum Language;
enum ShapeType;
enum ShapesType;
enum StrucType;
enum SymType;
enum ValueType;
enum FunctType;
enum FuncFormType;
enum SobolevType;
enum SpaceType;
enum DofType;
enum SupportType;
enum UnknownType;
enum FEType;
enum FESubType;
enum PolynomType;
enum QolynomType;
enum LinearFormType;
enum QuadRule

//for matrix storages
enum StorageType;
enum AccessType;
enum MatrixPart;

// for solver purpose
enum FactorizationType;
enum PreconditionerType;
enum EigenComputationalMode;
enum EigenSolverMode;
enum MsgEigenType;

enum ComputationInfo;
enum IOFormat;
enum TestStatus;
enum DataAccess;
```

Each enum has a dictionary counter-part for output.

### 2.2.3 *globalScopeData.hpp*

This file is the last file include by main programs. Its aim is to define the global parameters and objects declared in *config.hpp*, and also the static class attributes :

```
std::vector<Interpolation*> Interpolation::theInterpolations;
std::vector<Space*>  Space::theSpaces;
Number FeSpace::lastEltIndex = 0;
std::vector<Unknown*> Unknown::theUnknowns;
std::vector<DifferentialOperator*> DifferentialOperator::theDifferentialOperators;
std::map<String, std::pair<ValueType, StrucType> > Function::returnTypes;
std::map<String, std::pair<ValueType, StrucType> > Function::returnArgs;
std::map<String, std::pair<ValueType, StrucType> > Value::theValueTypeRTInames;
std::vector<const GeomDomain*> GeomDomain::theDomains;
std::vector<GeomRefElement*> GeomRefElement::theGeomRefElements;
std::vector<RefElement*> RefElement::theRefElements;
std::vector<Quadrature*> Quadrature::theQuadratures;
std::vector<Term*> Term::theTerms;
std::vector<MatrixStorage*> MatrixStorage::theMatrixStorages;
```

You may read their function in the chapter dedicated to the corresponding classes.

## 2.3 About the `finalize` function

The `finalize` function is defined in the *finalize* library. Its aim is to clean every global static list defined in globalScopeData.hpp. Why a library with a single external function ? For dependencies purpose. As the *init* library and *utils* library depend on each other through headers, the `finalize function` depends on libraries concerned by those global static lists, namely *finiteElements*, *operator*, *space*, *geometry*, *largeMatrix* and *term*. To preserve independence of the *utils* library, the `finalize` function cannot be placed in the *init* library.
Here is the implementation of this function :

```
void finalize()
{
  // clean all non user run-time lists
  Interpolation::clearGlobalVector();
  GeomRefElement::clearGlobalVector();
  RefElement::clearGlobalVector();
  DifferentialOperator::clearGlobalVector();
  Domain::clearGlobalVector();
  Space::clearGlobalVector();
  Unknown::clearGlobalVector();
  Quadrature::clearGlobalVector();
  MatrixStorage::clearGlobalVector();
  Term::clearGlobalVector();
}
```

It is used to preserve independence of tests when running all tests.

# 3 The *utils* library

The *utils* library collects all the general useful classes and functionalities of the XLiFE++ library. It is an independent library. It addresses:

`String` capabilities (mainly additional functions to the `std::string` class),

`AngleUnit` class to deal with angle unit,

`Point` class to deal with point of any dimension,

`Vector` class to deal with numerical vectors (say real or complex vectors),

`Matrix` class to deal with numerical matrices with dense storage (small matrices),

`Value` class to handle any real/complex scalar/vector/matrix value,

`VectorEntry` class to deal with any scalar/vector real/complex vector,

`Collection` class to deal with collection of anything, inheriting from std::vector,

`Parameter` classes to deal with general set of user parameters,

`Tabular` classes to deal with tabulated values

`Function` class encapsulating user functions,

`SymbolicFunction` class handling symbolic functions,

`Kernel` class encapsulating user kernels,

`ThreadData` class handling FE data computation (normal vectors, ...),

`Transformation` class to handle geometric transformations,

`Messages` classes to handle error, warning and info messages,

`Trace` class to handle log messages,

`Timer` class to handle timer utilities,

`Memory` class to handle memory utilities,

`PrintStream` class that handles the output stream in multi-thread environment

`Environment` class to handle XLiFE++ runtime variables,

`Graph` class to deal with graph,

`KdTree` class to handle kdtree (binary separation of kd points with a fast search of nearest point),

`EigenInterface` class that handles the interface to Eigen library

## 3.1 The `Environment` class

The `Environment` class collects all stuff related to the XLiFE++ execution context: machine, operating system, processors-thread, some paths, message language, . . .

```
class Environment
{
private:
Language theLanguage_;           // language as an int
string_t theXlifeppVersion_;     // version number of XLiFE++
string_t theXlifeppDate_;         // version date of XLiFE++
string_t theOS_;                  // OS name
string_t theProcessor_;           // processor or machine type
string_t theMachineName_;         // machine name
string_t thePathToMessageFiles_;  // path to error files
string_t thePathToGeoMacroFile_;  // path to geo macro file

static const string_t theInstallPath_;          // xlife++ installation path
static const string_t theGmshPath_;             // gmsh binary path
static const string_t theParaviewPath_;         // paraview binary path
static bool running_;                           // true when running
static bool parallelOn_;                        // parallel flag (default on)
static std::map<string_t, std::vector<string_t> > enumWords_; // global enums
static std::map<string_t, string_t> words_;     // global words
```

At initialization (see init.cpp), the `Environment` pointer `theEnvironment_p` is allocated and initialized.

Only one constructor from language is allowed :

```
Environment(int lang = _en );
```

Copy constructor and assign operator are not available.

As all member data are private, there exists their corresponding accessors:

```
static bool running();
static bool parallelOn();
static string_t installPath();
static string_t gmshPath();
static string_t paraviewPath();
static int numberOfLanguages();
int language() const;
void language(Language);
string_t osName() const;
string_t processorName() const;
string_t machineName() const;
string_t msgFilePath() const;
string_t geoMacroFilePath() const;
bool known() const;
static void parallel(bool);
void names();
void processor();
void setMsgFilePath();
void setGeoMacroFilePath();
void localizedStrings();
void version();
string_t languageString() const;
```

Besides some utilities are provided:

```
int returnedFunctionType(const string_t& s);
int returnedKernelType(const string_t& s);
void printHeader(const Timer&);
void printHeader(std::ofstream&);
void printDictionary(std::ostream&);
```

Other utilities are provided as non member functions:

```
bool is32bits();
bool is64bits();
bool parallelOn();
void parallel(bool);
```

```
number_t numberOfThreads(int n=-1);  //if omp is available
number_t currentThread();            //if omp is available
```

### 3.1.1 Using the dictionary

The Environment class provides 4 external functions to deal with localized strings:

```
String words(const String&);
String words(const char*);
String words(const bool b);
String words(const String&, const int);
```

The last function deals with enumeration items. You give the family and the enum item and you get the localized string. The two first functions deals with dictionary words. You give the dictionary keyword :

```
std::cout << words("shape",_segment) << std::endl;
std::cout << words("access type",_sym) << std::endl;
std::cout << words("constructors for real matrix") << std::endl;
```

| | |
|---:|---|
| library : | **utils** |
| header : | **Environment.hpp** |
| implementation : | **Environment.cpp** |
| unitary tests : | |
| header dependences : | **config.h, String.hpp, Timer.hpp, Messages.hpp, logo.hpp** |

## 3.2 Messages management

Handling error, warning and info messages is a essential part of a code. In C++, a choice could be using exceptions. As XLIFE++ is a very large code, with a high number of levels (routines called by routines themselves called by routines ...), using exceptions has a lot of constraints. The other way is to develop our own classes. The message machinery works as follows:

- A message is a string of characters including free text and particular codes (as much as you want) of the form %s, %i, %r, %c and %b which will be substituted respectively by a string, an integer, a real, a complex and a boolean.
- For each message is defined a unique string identifier, a type (ERROR,WARNING or INFO), a runtime behaviour (STOP or CONT) and an output console flag (STDOUT or NOSTDOUT).
- All the messages are listed in a file named *messages.txt* in the directory *etc/Messages/lang* where *lang* is the language code; for instance *en* for the English, *fr* for the French, ...
- By translating the English reference *messages.txt* file in an other language it is easy to internationalize the XLIFE++ code.

For instance, the beginning of the English *messages.txt* is

```
#/
============================ internal messages =================================

# logon INFO CONT STDOUT Log file "%s" activated.
# logoff INFO CONT STDOUT Log file "%s" deactivated.
# errorundef ERROR STOP STDOUT Error message of type %s and id %i undefined (%s)!
This might occur with a double string message Id in a message.txt file
or the forgetting of the message type, the behaviour type or the output type
...
```

Note that a message format may be defined on several lines (the next character # is the end delimiter of a message) and a comment begins by #/.

The message management is based on three classes: MsgData (storage of the values to be included), MsgFormat (multilingual message format) and Messages, the main class collecting all formats and methods to produce and output the formatted messages.

### 3.2.1 The MsgData class

The aim of the MsgData class is to store in the same structure, all sorts of variables to use to build a message, of various types: integer, real, complex, string and bool. Thus, this class proposes as private members:

```
class MsgData {
  private :
    std::vector<int> i_;          // to store int type data
    std::vector<real_t> r_;       // to store real_t type data
    std::vector<complex_t c_;     // to store complex_t type data
    std::vector<String> s_;       // to store string data
    std::vector<bool> b_;         // to store boolean data
    bool read_;                   // flag to specify that the structure has been read
  ...
};
```

It offers:

- a default constructor:

```
MsgData() : i_(0), r_(0), c_(0), s_(0), b_(0), read_(true) {}
```

- some public access functions to data

```
yyy xxxParameter(const unsigned int n);
// where (xxx,yyy)=(int,int), (real,real_t), (complex,complex_t), (string,string), (boolean,bool)
bool read();
```

- a public method to specify data was read

```
void readData();
```

- some public append methods for each managed data type or variant (unsigned int or char* for example)

```
void push(const T t); // T is int, real_t, string, ...
```

- some public streaming operators, appending data of various types

```
MsgData& operator<<(const T i) // T is int, real_t, string, ...
```

- a private reset method, to reset every list of data

```
void reset_();
```

### 3.2.2 The MsgFormat class

The MsgFormat Object contains a message format for output. In addition, it contains information on message such as the message type, the message behaviour, the message output and the message id. Thus, the MsgFormat class proposes as private members:

```
enum MsgType {_error=0,_warning,_info};

class MsgFormat {
  private :
    String format_;          // format of message
    MsgType type_;           // flag for warning/error
    bool stop_;              // flag for stop/continue
    bool consoleOut_;        // flag for output to console
    String ids_;             // string id of format
  ...
};
```

It offers:

- two constructors, the default one and the full one:

```
MsgFormat(const String &ms, const String &ids, MsgType t, bool s, bool c);
```

- some accessors, one for each attribute:

```
String format() const {return format_;}
MsgType type() const {return type_;}
bool stop() const {return stop_;}
bool console() const {return consoleOut_;}
String stringId() const {return ids_;}
```

### 3.2.3 The Messages class

The Messages class manages the list of messages format and the display of every message. Thus, this class proposes as private members:

```
class Messages {
  private :
    String msgType_;                              // message type
    std::map<String,MsgFormat*> stringIndex_;    // index of messages by string id
    std::ofstream* msgStream_p;                   // file stream where are sent messages
    String msgFile_;                              // file where are sent messages
  ...
};
```

It offers:

- two constructors, the default one and the full one:

```
Messages(const std::string& file, std::ofstream& out, const std::string& msgFile, const
    std::string& msgType = std::string("XLiFE++"));
```

- some accessors:

```
String msgType() const;
String msgFile();
std::ofstream* msgStream() const;
```

- some utilities:

```
int numberOfMessages() const;
void loadFormat(const String&);      // load format from a file
void printList(std::ofstream&);      // print the list of all messages
MsgFormat* find(const String&);      // find an error format
void append(MsgFormat&);             // append a new message format in list
void appendFromFile(const String&); // append a new message format in list
```

### 3.2.4 External functions

To throw messages, some external functions with useful aliases and shorcuts functions are provided. The general functions are:

```
String message(const String& msgIds, MsgData& msgData=theMessageData,
               Messages* msgSrc=theMessages_p);
void msg(const String& msgIds, MsgData& msgData, MsgType& msgType, Messages* msgSrc);
```

The first one (*message*) reads the message format and replaces the strings %i,%r,%c,%s and %b by their values given by the `MsgData` object. It produces a `String` containing the formatted message. This function is called by the *msg* function which outputs the formatted message to the console or to a print file. Note that this function may be also called by any function to retrieve the formatted message without output.
The *msg* function is called by the three useful functions:

```
void error(const String& msgIds, MsgData& msgData=theMessageData,
           Messages* msgSrc=theMessages_p);
void info(const String& msgIds, MsgData& msgData=theMessageData,
          Messages* msgSrc=theMessages_p);
void warning(const String& msgIds, MsgData& msgData=theMessageData,
             Messages* msgSrc=theMessages_p);
```

which are aliases for the *msg* function, giving the value of the `msgType` argument. These are the functions to be used when you need to throw messages in other classes of XLIFE++ library.

Besides, for sake of simplicity, some shorcut functions are also provided. They avoid to manage explicitely the `MsgData` object storing the message values.These shorcut functions are templated functions (one, two or three templated parameters), so they only work up to three message values!

```
String message(const String& msgIds, const T& v, Messages* msgSrc=theMessages_p);
String message(const String& msgIds, const T1& v1,const T2& v2,
               Messages* msgSrc=theMessages_p);
String message(const String& msgIds, const T1& v1,const T2& v2, const T3& v3,
               Messages* msgSrc=theMessages_p);
void error(const String& msgIds, const T& v, Messages* msgSrc=theMessages_p);
void error(const String& msgIds, const T1& v1,const T2& v2,
           Messages* msgSrc=theMessages_p);
void error(const String& msgIds, const T1& v1,const T2& v2,const T3& v3,
           Messages* msgSrc=theMessages_p);
//the same for warning and info functions
```

### 3.2.5 Throwing messages

There is one global `MsgData` object: *theMessageData* which is used as default argument of message functions. Using it, it is very easy to throw messages. For instance, these lines show how to throw an error message:

```
 if(x.size()!=y.size())
    {theMessageData<<name()<<x.size()<<y.size();   //store the message values
     error("ker_bad_dim");                          //throw the error message ker_bad_dim
    }
```

The message format *ker_bad_dim* has the following definition:

```
# ker_bad_dim ERROR STOP STDOUT Call of kernel \%s
with vectors of incompatible dimensions : (\%i,\%i)
```

If you want to use international messages in your own output stream, you cannot use the function *info* because it outputs the message on the default print stream. You have to use the function *message* which returns the message as a `String` without printing output. For instance:

```
std::ostream& operator<<(std::ostream& out, const Space & sp)
{   theMessageData<<sp.name()<<sp.typeOfSpace()<<sp.domain().name();
    out<<message("space_def");
    return out;
}
```

with the message format *space_def*:

```
# space_def INFO CONT STDOUT space %s of type %s on the geometrical domain %s
```

Using shortcut functions, the previous example reads:

```
std::ostream& operator<<(std::ostream& out, const Space & sp)
{   out<<message("space_def",sp.name(),sp.typeOfSpace(),sp.domain().name());
    return out;
}
```

| | |
|---:|:---|
| library : | **utils** |
| header : | **Messages.hpp** |
| implementation : | **Messages.cpp** |
| unitary tests : | **test_Messages.cpp** |
| header dependences : | **config.h, String.hpp** |

## 3.3 Managing traces

### 3.3.1 The `Trace` class

The `Trace` class is devoted to keep trace of runtime of the hierarchy of function calls. Thus, we can have access to a stack of called functions, the next position to be used and the last one. Thus, this class proposes as members:

```
class Trace {
  private:
    number_t pos_;                     //!< next position in trace object list member
    static const number_t maxPos_=36;  //!< last position in trace object list member
    String fList[maxPos_];             //!< stack of called functions

    static const String theLogFile_;   //!< name of log file
    static bool isLogged_;

  public:
    static std::ofstream theLogStream_;
  ...
};
```

It offers:

- a default constructor that initializes pos_ to 0, and private copy constructor and assignment operator

- some public access functions to data:

```
static const String logFile() { return theLogFile_; }
static bool isLogged() { return isLogged_; }
static void logOn() { isLogged_ = true; }
static void logOff() { isLogged_ = false; }
number_t length() const; //!< function length returns the number of items of f_list
```

- some public utilities methods for adding trace or having info on current position:

```
void push(const String&);          //!< "pushes" name into Trace function list member
void pop();                        //!< "pops" current input out of a Trace function list member
String current(const number_t);    //!< returns string of last l to current inputs of a Trace object
    list
String current();                  //!< returns last input string of a Trace object list
String list();                     //!< returns function list of a Trace object list
```

- some public display management methods:

```
void indent();                     //!< function indent prints context-depending indentation to log
    file
void print(std::ofstream&);        //!< prints function list to opened ofstream or to default print
    file
void print();
```

- some public methods to build log messages:

```
void log(); //!< outputs indentation to log file
template<typename T_0> void log(const T_0& s);
template<typename T_0, typename T_1>  void log(const T_0& s, const T_1& t1)
template<typename T_0, typename T_1, typename T_2> void log(const T_0& s, const T_1& t1, const
    T_2& t2);
template<typename T_0, typename T_1, typename T_2, typename T_3> void log(const T_0& s, const
    T_1& t1, const T_2& t2, const T_3& t3);
template<typename T_0, typename T_1, typename T_2, typename T_3, typename T_4> void log(const
    T_0& s, const T_1& t1, const T_2& t2, const T_3& t3, const T_4& t4);
```

- some external functions to manage trace errors:

```
void incompleteFunction(const String& s = "");
void invalidFunction(const String& s = "");
void constructorError();
set setNewHandler();
```

- some external functions to manage verbose level:

```
void setGlobalVerboseLevel(const unsigned int);
unsigned int verboseLevel(const unsigned int);
```

- one external functions to manage the message location :

```
String & where(const String& s);
```

### 3.3.2 How to use the verbose level ?

The verbose level is managed through 2 global variables : `theVerboseLevel` and `theGlobalVerboseLevel`, and 2 functions. The behavior is the following :

- To set globally the maximum verbose level to an int value $i$, you can use the following syntax : **setGlobalVerboseLevel**(i); This sets the variable `theGlobaVerboseLevel` and overrides every local definition of the verbose level to higher values. This function is to be used once at the beginning of a main program.
- To set locally the maximum verbose level to a value $i$, you can use the following syntax :

```
int j=verboseLevel(i);
if (i < theGlobalVerboseLevel) {
  j=theVerboseLevel}=i;
} else {
  j=theGlobaVerboseLevel;
}
```

- To get the current maximum verbose level, you can use directly the variable `theVerboseLevel`

### 3.3.3 How to know where does messages come ?

To see how to throw messages, please read the previous section about it. Here, we will discuss how a message knows where it is and how to give is more information about it.

The main mechanism is to use the functions `push` and `pop` respectively at the beginning and the end of whatever function. This piece of information is dealt with by messages handlers automatically. But we cannot do it for every function in the code. We have to reserve it for the top-level functions in order not to slow execution.

For the deepest functions, there is another way : using the `where` function. This function is to be used just before a message call where `push` and `pop` are not used. Messages will deal with this additional information automatically. As a result, there is no need to define message format with the routine name as message data.

| | |
|---:|:---|
| library : | **utils** |
| header : | **Trace.hpp** |
| implementation : | **Trace.cpp** |
| unitary tests : | |
| header dependences : | **config.h, String.hpp** |

## 3.4 The `Timer` class

The `Timer` class is a utility class to perform computational time analysis (cpu time and elapsed time) and manage dates. It uses the following data members which store time, cpu time and system time in various format.

```
class Timer
{private:
    time_t t;                         //time type provided by ctime
    tm localt;                        //time structure provided by ctime
    long int sec_, microSec_;         //time in seconds and microseconds
                                      // since 01/01/1970 00:00:00
    long int usrSec_, usrMicroSec_; // cputime in seconds and microseconds
                                      // since beginning of current process
    long int sysSec_, sysMicroSec_; // system time in seconds and microseconds
                                      // since beginning of current process
 ...
};
```

The Timer class has only one constructor (no argument) which initializes the start time. It provides a few basic functionalities:

```
void update()                    // converts time to tm struct
int year()                       // year as an int
unsigned short int month()       // month as an int [0-11]
unsigned short int day()         // day of month as an int [0-31]
unsigned short int hour()        // hour of day (24h clock)
unsigned short int minutes()     // minutes of hour [0-59]
unsigned short int seconds()     // seconds of minute [0-59]
void getCpuTime()                // update cputime interval since beginning of process
double deltaCpuTime(Timer*)      // returns elapsed time interval since "ot" time
void getTime()                   // update time in s and ms since 01/01/1970 00:00:00
double deltaTime(Timer*)         // returns elapsed time interval since "ot" time
```

Associated to these member functions, there are the following external functions (user functions):

```
String theTime()            // returns current time
String theDate()            // returns current date as dd.mm.yyyy
String theShortDate()       // returns current date as mm/dd/yyyy or dd/mm/yyyy
String theLongDate()        // returns current date as Month Day,Year or Day Month Year
String theIsoDate()         // returns ISO8601 format of current date (yyyy-mm-dd)
String theIsoTime()         // returns ISO8601 format of current time (hh-mi-ss)

double cpuTime()                        // returns cputime in sec.since last call
double cpuTime(const String&)           // same and prints it with comment
double totalCpuTime()                   // returns cputime in sec.since first call
double totalCpuTime(const String&)      //same and prints it with comment
double elapsedTime()                    // returns elapsed time  in sec. since last call
double elapsedTime(const String&)       // same and prints it with comment
double totalElapsedTime()               // returns elapsed time in sec. since first call
double totalElapsedTime(const String&)  // returns elapsed time interval in sec.
                                        // same and prints it with comment
```

Note that this class is OS dependant because Unix and Windows do not provide the same system time functions. The macro OS_IS_WIN32 set in *setup.hpp* is used to select the right version. In particular, for Unix platform the class uses some functions provided by the header *sys/time.h* and for Windows platform, some functions provided by the header *sys/timeb.h,*, this header requiring the headers *windef.h, stdio.h, cstdarg, winbase.h.*

The function *timerInit()* in the *init.cpp* file creates two Timer objects (*theStartTime_p* and *theLastTime_p*) at the beginning of the execution. These objects have a global scope and are used by the Timer class to make easier the time computation analysis for the user. There is no reason to create other instances of Timer.

So, it is easy to the user to perform time computation analysis. For instance:

```
#include "xlife++.h"
using namespace xlifepp;
int main()
{
  init(fr);  //initializes timers
  //task 1
  ...
  cpuTime("cpu time for task 1");
  elapsedTime("ellapsed time for task 1");
  //task 2
  ...
  cpuTime("cpu time for task 2");
  elapsedTime("ellapsed time for task 2");
  //end of tasks
  totalCpuTime("total cpu time");
  totalElapsedTime("total ellapsed time");
}
```

| | |
|---|---|
| library : | **utils** |
| header : | **Timer.hpp** |
| implementation : | **Timer.cpp** |
| unitary tests : | |
| header dependences : | **config.h** |

## 3.5 The `Memory` class

The `Memory` class is a small utility class giving some informations about the memory usage in different format.

```
enum MemoryUnit {_byte,_kilobyte,_megabyte,_gigabyte,_terabyte};
class Memory
{
public:
static real_t physicalMem(MemoryUnit mu=_megabyte);
static real_t physicalFreeMem(MemoryUnit mu=_megabyte);
static real_t virtualMem(MemoryUnit mu=_megabyte);
static real_t virtualFreeMem(MemoryUnit mu=_megabyte);
static real_t processPhysicalMem(MemoryUnit mu=_megabyte);
static real_t processVirtualMem(MemoryUnit mu=_megabyte);
};

real_t byteTo(number_t mem, MemoryUnit mu=_megabyte);
```

All the member functions are static. Default unit is the MegaByte. Note that virtual memory is not available for unix/linux systems!

| | |
|---|---|
| library : | **utils** |
| header : | **Memory.hpp** |
| implementation : | **Memory.cpp** |
| unitary tests : | |
| header dependences : | **config.h** |

## 3.6 The `String` class

String is no more than an alias (typedef) to the String class of the STL. By using a macro variable it is possible to choose either standard string (utf8) or wide string (utf16):

```
#ifdef WIDE_STRING
  typedef std::wstring String;
#else
  typedef std::string String;
#endif
```

The *WIDE_STRING* macro variable is currently set in the *Config.hpp* header file.

As a the string or wstring class of STL, String proposes all the functionalities of std::string (see the STL documentation) and new additional ones:

```
//conversion utilities
```

```
template<typename T_> String tostring(const T_& t);   //'anything' to String
template<typename T_> T_ stringto(const String& s);   //String to 'anything'

//transformation utilities
String lowercase(const String&);    // String converted to lowercase
String uppercase(const String&);    // String converted to uppercase
String capitalize(const String&);   // String with initial converted to uppercase
String trimLeading(const String& s, const char* delim = " \t\n\f\r");  // trims leading white
    spaces
String trimTrailing(const String& s, const char* delim = " \t\n\f\r"); // trims trailing white
    spaces
String trim(const String& s, const char* delim = " \t\n\f\r"); // trims leading and trailing
    white spaces
String delSpace(const String& s);  //delete all white space
String& replaceString(String& s, const String& s1, const String& s2); // replace string s1 by
    string s2 in string s
String& replaceChar(String& s, char c1, char c2); // replace char c1 by char c2 in string s
String fileExtension(const String& f); // return file name extension using last point as delimiter
std::pair<String, String> fileRootExtension(const String& f); // return rootname and extension of
    a file
void blanks(String&,int n);   // add or remove n blanks at end of string

//search capabilities
int findString(const String, const std::vector<String>&); //!<returns index
```

Be cautious with templated conversion functions. The function *tostring* (resp. *stringto*) works when the operator << (resp. >>) on stringstream is defined for the template type *T_*. The function *tostring* is more flexible than *stringto*. Note that the template *T_* type has to be clarified when invoking *stringto*.

```
//examples of conversion stringto
    String s="1 2 3";
    int i=stringto<int>(s);             //i=1
    real_t r=stringto<real_t>(s);       //r=1.
    complex_t c=stringto<complex_t>(s); //c=(1.,0)
    void * p=stringto<void*>(s);        //p=0x1
    String ss=stringto<String>(s);      //ss="1"
    s="(0,1)";
    c=stringto<complex_t>(s);           //c=(0.,1.)
```

| | |
|---:|:---|
| library : | **utils** |
| header : | **String.hpp** |
| implementation : | **String.cpp** |
| unitary tests : | **test_String.cpp** |
| header dependences : | |

## 3.7 The AngleUnit class

The purpose of the small AngleUnit class is to deal with angle unit. More precisely, it allows to specify angles either in radian or in degree by processing the desired unit conversion. The default angle unit defined in the file *GlobalScopeData.hpp* is the radian:

```
AngleUnitType defaultAngleUnit=_rad;
```

where AngleUnitType is the enumeration of angle units available (up to now, only two!) :

```
enum AngleUnitType {_deg, _rad};
```

This class handles the unit converter and provides only one constructor relating two angle units:

```
class AngleUnit
{public:
   ConvAngleType type;   // type of conversion
   real_t eps;           // eps in rounding process
   AngleUnit(AngleUnitType ts, AngleUnitType td, real_t tol=0.);
};
```

Available unit converters are enumerated as following:

```
enum ConvAngleType{_noAngleConversion,_degToRad,_radToDeg};
```

`eps` is an additional data used, if not zero (default value), to control rounding error conversion (`eps*round(a/eps)`).

Angle conversion is processed by the `*` operator between a real scalar and a `AngleUnit` object :

```
inline real_t operator*(real_t, const AngleUnit&);
```

XLiFE++ declares in *GlobalScopeData.hpp* two `AngleUnit` objects:

- `deg_` to handle the conversion from degree to the default angle unit (radian)
- `rad_` to handle the conversion from radian to the default angle unit (radian), that has no real interest

Finally, it allows users to deal either with radian or degree:

```
Real angle1 = pi_/4;       // default in radian
Real angle2 = 45*deg_;     // convert degree to radian, angle2 value is pi/4
Real angle3 = pi_/4*rad_; // do nothing, angle3 value is still pi/4
```

| | |
|---:|---|
| library : | **utils** |
| header : | **AngleUnit.hpp** |
| implementation : | |
| unitary tests : | |
| header dependences : | **config.h** |

## 3.8 The `Point` class

The purpose of the `Point` class is to deal with point in any dimension. It is derived from the *std:vector<Real>*.

```
typedef std::vector<Real>::iterator ivr_t;
typedef std::vector<Real>::const_iterator civr_t;

class Point : public std::vector<Real>
{public:
 static Real tolerance;
 ...
}
```

The static member *tolerance* is used in comparison operations. By default, its value is 0; As a child class of `std::vector`, the Point class does not have copy constructor and assignment = operator.
It offers some basic constructors:

```
Point(const int, const Real v = 0.); // dimension and constant value
Point(const Dimen, const Real v = 0.); // dimension and constant value
Point(const Real x1); // 1D constructor by coordinate
Point(const Real x1, const Real x2); // 2D constructor by coordinates
Point(const Real x1, const Real x2, const Real x3); // 3D constructor by coordinates
Point(const Dimen d, Real* pt); // constructor by dimension and Real array
Point(const std::vector<Real>& pt); // constructor by stl vector
Point(const std::vector<Real>::const_iterator, Dimen); // constructor by stl vector iterator
~Point(); // destructor
```

One can access (both read and read/write access) to the coordinates either by index (from 1 to dim) or by explicit name x(), y() and z() (restricted to 3D point):

```
Real operator()(const Dimen d) const; //the d-th coordinates (r)
Real& operator()(const Dimen d);      //d-th coordinates (r/w)
Real  x() const; //the first coordinate  (r)
Real& x();       //the first coordinate  (r/w)
Real  y() const; //the second coordinate (r)
Real& y();       //the second coordinate (r/w)
Real  z() const; //the third coordinate  (r)
Real& z();       //the third coordinate  (r/w)
std::vector<Real> toVect(const Point &)  //!<convert to a std::vector
```

Through overloaded operator, the Point class provides some algebraic operations and distance computation functions:

```
Point& operator+=(const Point &); //add a point to the current point
Point& operator-=(const Point &); //subtract a point to the current point
Point& operator+=(const Real);  //add a constant point to the current point
Point& operator-=(const Real);  //subtract a constant point to the current point
Point& operator*=(const Real ); //scale the current point
Point& operator/=(const Real ); //scale the current point
Real squareDistance(const Point&) const; //square distance to an other point
Real distance(const Point&) const; //distance to an other point
```

Note that size compatibility tests are performed on such computations.

Algebraic operations on points may be also be processed by external function to the class:

```
Point operator+(const Point &);                 //same point (completeness)
Point operator-(const Point &);                 //opposite point
Point operator+(const Point &,const Point &);   //sum of two points
Point operator-(const Point &,const Point &);   //difference of two points
Point operator+(const Point &,const Real );     //sum of two points
Point operator-(const Point &,const Real );     //difference of two points
Point operator+(const Real,const Point & );     //sum of two points
Point operator-(const Real,const Point & );     //difference of two points
Point operator*(const Real ,const Point &);     //scale a point
Point operator*(const Point &,const Real );     //scale a point
Point operator/(const Point &,const Real );     //scale a point
Real pointDistance(const Point&,const Point&);  //distance between two points
Real squareDistance(const Point&,const Point&); //square distance between two points
```

`distance()` is a function of the *std::iterator* class, it is the reason why the distance between two points is named `pointDistance`.

Finally, to order (partially) a couple of points, the comparison operators (==, !=, <, >, <= and >=) are overloaded:

```
bool operator==(const Point &,const Point &); //equality of two points
bool operator!=(const Point &,const Point &); //not equality of two points
bool operator< (const Point &,const Point &); //leather than
bool operator<=(const Point &,const Point &); //leather than or equal
bool operator> (const Point &,const Point &); //greater than
bool operator>=(const Point &,const Point &); //greater between or equal
```

The comparison between points are performed using the tolerance value $\tau$ (`Point::tolerance`) which means for points $p$ and $q$ in $\mathbb{R}^n$:

$$p == q \text{ if } |p-q| \le \tau$$
$$p < q \text{ if } \exists i \le n,\ \forall j < i,\ |p_j - q_j| \le \tau \text{ and } p_j < q_j - \tau.$$

| | |
|---|---|
| library : | **utils** |
| header : | **Point.hpp** |
| implementation : | **Point.cpp** |
| unitary tests : | **test_Point.cpp** |
| header dependences : | **config.h** |

## 3.9 The `Vector` class

The purpose of the `Vector` class is mainly to deal with complex or real vector. It is derived from the `std:vector<K>` and templated by the vector type:

```
template<typename K>
class Vector : public std::vector<K>
{
public:
    typedef K type_t;
    typedef typename std::vector<K>::iterator ivk_t;
    typedef typename std::vector<K>::const_iterator civk_t;
    ...
```

As it is templated, it is also possible to deal with vector of vectors and generally vector of anything. But some algebraic functions no longer work.

It offers some basic constructors and assignment function:

```
Vector();                          //default constructor
Vector(const dimen_t);             //constructor by length
Vector(const dimen_t, const K&);   //constructor by length for constant vector
void assign(const K&);             //assign const scalar value to all entries
Vector<K>& operator=(const K&);    //assign const scalar value to all entries
```

The default constructor initializes a vector of lengh 1 with a "0" value (*K()*).

One can access (both read and read/write access) to the component either by iterators (`begin()` and `end()`) or by index from 1 to the length:

```
size_t size() const;          //overloaded size
ivk_t begin();                //overloaded iterator begin()
civk_t begin() const;         //overloaded const iterator begin()
ivk_t end();                  //overloaded iterator end()
civk_t end() const;           //overloaded const iterator end()
K  operator()(int i) const;   //i-th component (i=1..n) (r)
K& operator()(int i);         //i-th component (i=1..n) (r/w)
```

There are also generalized accessors that allow to get or set a part of vector, indices being given either by lower and upper indices or by a vector of indices:

```
Vector<K> get(Number i1, Number i2) const;          //get i1->i2 components
Vector<K> get(const std::vector<Number>& is) const; //get 'is' components
void set(Number i1, Number i2, const std::vector<K>& vec);   //set i1->i2 components
void set(const std::vector<Number>& is, const std::vector<K>& vec); //set 'is' components
Vector<K> operator()(const std::vector<Number>& is) const;   //get 'is' components
Vector<K> operator()(Number i1, Number i2) const;      //get i1->i2 components
```

Through overloaded operators, the `Vector` class provides the following (internal) algebraic operations:

```
Vector<K>& operator+=(const K&); //add a scalar to current vector
Vector<K>& operator-=(const K&); //substract a scalar to current vector
Vector<K>& operator*=(const K&); //multiply the current vector by a scalar
Vector<K>& operator/=(const K&); //divide the current vector by a scalar
Vector<K>& operator+=(const Vector<K>&); //add a vector to current vector
Vector<K>& operator-=(const Vector<K>&); //substract a vector to current vector
```

Note that compatibility tests are performed on such computations:

```
void mismatchSize(const String&, const size_t) const;
void divideByZero(const String&) const;
void complexCastWarning(const String&, const dimen_t) const;
```

The class also provides norm computations:

```
Real norminfty() const;      //sup norm
Real norm2squared() const;   //squared quadratic norm
Real norm2() const;          //<quadratic norm
```

and output facilities (templated ostream <<):

```
void print(std::ostream& ) const;
template<typename K>
  std::ostream& operator<<(std::ostream&,const Vector<K>&);
```

Algebraic operations are defined as external templated functions (*template <typename K>* is omitted):

```
Vector<K> operator+(const Vector<K>&);                  //+U
Vector<K> operator-(const Vector<K>&);                  //-U
Vector<K> operator+(const Vector<K>&,const Vector<K>&); //U+V
Vector<K> operator+(const K&, const Vector<K>&);        //x+U
Vector<K> operator+(const Vector<K>&,const K&);         //U+x
Vector<K> operator-(const Vector<K>&,const Vector<K>&); //U-V
Vector<K> operator-(const K&, const Vector<K>&);        //x-U
Vector<K> operator-(const Vector<K>&,const K&);         //U-x
Vector<K> operator*(const K&, const Vector<K>&);        //x*U
Vector<K> operator*(const Vector<K>&, const K&);        //U*x
Vector<K> operator/(const Vector<K>&, const K&);        //U/x
Vector<K> conj(const Vector<K>&);                       //conjugate(U)
```

Not that the conjugate function is defined for every vector of type *K*; it assumes that the *conj* function is also defined for *K* value and returns a *K* value.

To insure automatic cast from real to complex (not the contrary) and particular functions related to complex, some template specializations are provided:

```
std::ostream& operator<<(std::ostream&, const Vector<Real>&);     // real vector flux insertion
std::ostream& operator<<(std::ostream&, const Vector<Complex>&); //complex vector flux insertion
Vector<Complex> operator+(const Vector<Real>&, const Vector<Complex>&); //rU+cV
```

```
Vector<Complex> operator+(const Vector<Complex>&, const Vector<Real>&); //cV+rU
Vector<Complex> operator-(const Vector<Real>&, const Vector<Complex>&); //rU-cV
Vector<Complex> operator-(const Vector<Complex>&, const Vector<Real>&); //cV-rU
Vector<Complex> operator+(const Vector<Real>&, const Complex&);          //rU+cx
Vector<Complex> operator+(const Complex&, const Vector<Real>&);          //cx+rU
Vector<Complex> operator+(const Vector<Complex>&, const Real&);          //cU+rx
Vector<Complex> operator+(const Real&, const Vector<Complex>&);          //rx+cU
Vector<Complex> operator-(const Vector<Real>&, const Complex&);          //rU-cx
Vector<Complex> operator-(const Complex&, const Vector<Real>&);          //cx-rU
Vector<Complex> operator-(const Vector<Complex>&, const Real&);          //cU-rx
Vector<Complex> operator-(const Real&, const Vector<Complex>&);          //rx-cU
Vector<Complex> operator*(const Complex&, const Vector<Real>&);          //cx*rU
Vector<Complex> operator*(const Vector<Real>&, const Complex&);          //rU*cx
Vector<Complex> operator*(const Real&, const Vector<Complex>&);          //rx*cU
Vector<Complex> operator*(const Vector<Complex>&, const Real&);          //cU*rx
Vector<Complex> operator/(const Vector<Real>&, const Complex&);          //rU/cx
Vector<Complex> operator/(const Vector<Complex>&, const Real&);          //cU/rx
Vector<Real> real(const Vector<Complex>&);                                 //real(U)
Vector<Real> imag(const Vector<Complex>&);                                 //imag(U)
Vector<Complex> cmplx(const Vector<Real>&);
Vector<Complex> cmplx(const Vector<Complex>&);
```

Note that the operations and their specializations allow all standard operations a user can wait from a real or complex vector. In particular, operations involving a casting from real to complex. On the other hand, be cautious when using a *Vector<Vector<K>> V* , all algebraic operations involving *V* and a scalar (of type K) are not supported, only those involving *V* and a *vector<K>* are working. Besides, automatic casting from real to complex of vector of vectors is not supported, use the *cmplx* function to convert to complex type.

```
Vector<Vector<Complex> > cmplx(const Vector<Vector<Real> >&);
```

Although the Point class also inherits from std::vector and offers similar algebraic computations facilities to the Vector class, it is not linked to the Vector class because it deals only with real vector and offers other functionalities, in particular comparison capabilities.

Useful aliases hiding template syntax, are available for end users:

```
typedef Vector<Real> Reals;
typedef Vector<Complex> Complexes;
typedef Vector<Real> RealVector;
typedef Vector<Complex> ComplexVector;
typedef Vector<Vector<Real> > RealVectors;
typedef Vector<Vector<Complex> > ComplexVectors;
```

They are defined in *users_typedef.hpp* (*init* library).

| | |
|---:|---|
| library : | **utils** |
| header : | **Vector.hpp** |
| implementation : | **Vector.cpp** |
| unitary tests : | **test_Vector.cpp** |
| header dependences : | **config.h** |

## 3.10 The Matrix class

The purpose of the Matrix class is to deal with complex or real dense matrices. It is derived from the *std:vector<K>* and templated by the coefficient type; the coefficients are stored row by row.

```
template<typename K>
class Matrix : public std::vector<K>
{private:
   dimen_t rows_;        //!<number of rows
 public:
   typedef K type_t;     //!<alias on matrix coefficient type
   typedef typename std::vector<K>::iterator itvk_t;
   typedef typename std::vector<K>::const_iterator citvk_t;
   ...
```

As it is templated, it is also possible to deal with matrix of matrices. But all functions are not supported, in particular those involving autocast.

It offers some basic constructors and assignment function:

```
Matrix();                                         //by default
Matrix(const dimen_t, const dimen_t);             //by dimensions
Matrix(const dimen_t r, const dimen_t, const K&); //by dimensions and constant
Matrix(const Matrix<K>&);                         //by copy
Matrix(const vector<K>&);                         //diagonal square matrix from vector
Matrix(const vector<vector<K> >&);                //from a vector of vectors
Matrix(const vector<Vector<K> >&);                //from a vector of Vectors
Matrix(const dimen_t, const SpecialMatrix);       //for special square matrix
Matrix(const String&);                            //from file
Matrix(const char *);                             //from file
```

As the `Vector` class inherited from `std::vector`, the constructor from std::vector of `std::vector` works also for `Vector` of `std::vector`, for `std::vector` of  `Vector` and for `Vector` of `Vector`. The special matrices are enumerated by the *enum*:

```
enum SpecialMatrix{ _zeroMatrix=0, _idMatrix, _onesMatrix, _hilbertMatrix };
```

Besides the constructors, the following assignment operators are allowed:

```
Matrix<K>& operator=(const Matrix<K>&);
Matrix<K>& operator=(const Matrix<KK>&);
Matrix<K>& operator=(const vector<vector<K> >&);
Matrix<K>& operator=(const vector<Vector<K> >&);
private: void assign(const KK&);
```

Be cautious with the generalized templated version **Matrix**<K>\& **operator**=(**const** **Matrix**<KK>\&).

One can access to the dimensions, to the coefficients (both read and read/write access) either by iterators (`begin()` and `end()`) or by index from 1 to the length, to the rows or the columns (both read and read/write access), to the main diagonal:

```
size_t  size() const;                 //overloaded size()
size_t  vsize() const;                //column length (number of rows)
dimen_t numberOfRows() const;         //number of rows
size_t hsize() const;                 //row length (number of columns)
dimen_t numberOfColumns() const;      //number of columns
itvk_t  begin();                      //overloaded iterator begin
citvk_t begin() const;                //overloaded const_iterator begin
itvk_t  end();                        //overloaded iterator end
citvk_t end() const;                  //overloaded const_iterator begin
const K& operator()(const dimen_t, const dimen_t) const; //protected access
K& operator()(const dimen_t, const dimen_t);             //read/write access
Vector<K> row(const dimen_t) const;            //return r-th row (r > 0) as Vector
void row(const dimen_t, const vector<K>&):     //set r-th row from a stl vector
```

```
Vector<K> column(const dimen_t) const;          //return c-th  column as a Vector
void column(const dimen_t, const vector<K>&);  //set c-th column from a stl vector
Vector<K> diag() const;                         //return diagonal as a Vector
Matrix<K>& diag(const K);                       //reset matrix as a diag. matrix
Matrix<K>& diag(constvector<K>&);               //reset matrix as a diag. matrix
```

Be care with functions on the diagonal, they change the current matrix to a diagonal matrix.

There are also generalized accesors that allow to extract or set a part of matrix. The row indices and column indices may be given either by lower and upper indices or by vector of indices:

```
Matrix<K> get(const std::vector<Dimen>&, const std::vector<Dimen>&) const;
Matrix<K> get(const std::pair<Dimen,Dimen>&, const std::pair<Dimen, Dimen>&) const;
Matrix<K> get(Dimen, const std::pair<Dimen, Dimen>&) const;
Matrix<K> get(const std::pair<Dimen,Dimen>&, Dimen) const;
Matrix<K> get(Dimen, const std::vector<Dimen>&) const;
Matrix<K> get(const std::vector<Dimen>&, Dimen) const;
Matrix<K> get(Dimen, Dimen, Dimen, Dimen) const;
Matrix<K> operator()(const std::vector<Dimen>&, const std::vector<Dimen>&) const;
Matrix<K> operator()(const std::pair<Dimen,Dimen>&, const std::pair<Dimen, Dimen>&) const;
Matrix<K> operator()(Dimen, const std::pair<Dimen, Dimen>&) const;
Matrix<K> operator()(const std::pair<Dimen,Dimen>&, Dimen) const;
Matrix<K> operator()(Dimen, const std::vector<Dimen>&) const;
Matrix<K> operator()(const std::vector<Dimen>&, Dimen) const;
Matrix<K> operator()(Dimen, Dimen, Dimen, Dimen) const;
void set(const std::vector<Dimen>&, const std::vector<Dimen>&, const std::vector<K>&);
void set(const std::pair<Dimen,Dimen>&, const std::pair<Dimen, Dimen>&, const std::vector<K>&);
void set(Dimen, const std::pair<Dimen, Dimen>&, const std::vector<K>&);
void set(const std::pair<Dimen,Dimen>&, Dimen, const std::vector<K>&);
void set(Dimen, const std::vector<Dimen>&, const std::vector<K>&);
void set(const std::vector<Dimen>&, Dimen, const std::vector<K>&);
void set(Dimen, Dimen, Dimen, Dimen, const std::vector<K>&);
```

Through overloaded operators, the `Matrix` class provides the following (internal) algebraic operations:

```
Matrix<K>& operator+=(const Matrix<KK>&); //add a matrix to the matrix
Matrix<K>& operator+=(const K&);          //add a scalar to the matrix
Matrix<K>& operator-=(const Matrix<KK>&); //substract a matrix to the matrix
Matrix<K>& operator-=(const K&);          //substract a scalar to the matrix
Matrix<K>& operator*=(const KK&);         //multiply by a scalar the matrix
Matrix<K>& operator/=(const KK&);         //divide by a scalar the matrix
```

Be careful, the operations such as `Matrix<Matrix<K> > += Matrix<K>` does not work.

Moreover, the `Matrix` class provide a lot of functionalities:

```
bool shareDims(const Matrix<KK>&) const; //true if matrices bear same dimensions
bool isSymmetric() const;                //symmetric matrix test
bool isSkewSymmetric() const;            //skew-symmetric matrix test
bool isSelfAdjoint() const;              //self adjoint matrix test
bool isSkewAdjoint() const;              //skew adjoint matrix test
Matrix<K>& transpose();                  //matrix self-transpostion
Matrix<K>& adjoint();                    //matrix self-adjoint
Matrix<Real> real() const;               //real part of a matrix
Matrix<Real> imag() const;               //imaginary part of a matrix
```

and input/output and error utilities:

```
void loadFromFile(const char*);
void saveToFile(const char*);
```

```
istream& operator >> (istream&, Matrix<K>&);
ostream& operator<<(ostream&, const Matrix<Real>&);
ostream& operator<<(ostream&, const Matrix<Complex>&);
void print(ofstream&);
void print() const;

void nonSquare(const String&, const size_t, const size_t) const;
void mismatchDims(const String& ,const size_t, const size_t) const;
void divideByZero(const String&) const;
void isSingular() const;
void complexCastWarning(const String&, const size_t, const size_t) const;
```

Finally, this class provides almost algebraic operations as external functions, with specialized versions allowing automatic cast from real to complex type:

```
bool operator==(const Matrix<K>&,const Matrix<K>&);      //matrix comparison
bool operator!=(const Matrix<K>&,const Matrix<K>&);      //matrix comparison

Matrix<K> operator+(const Matrix<K> &);                  //unary operator+
Matrix<K> operator-(const Matrix<K> &);                  //unary operator-

Matrix<K> operator+(const Matrix<K>&, const Matrix<K>&); //matrix + matrix
Matrix<K> operator+(const KK&, const Matrix<K>&);        //scalar + matrix
Matrix<K> operator+(const Matrix<K>&, const KK&)         //matrix + scalar
Matrix<Complex> operator+(const Complex&, const Matrix<Real>&);
Matrix<Complex> operator+(const Matrix<Real>&, const Complex&);
Matrix<Complex> operator+(const Matrix<Real>&, const Matrix<Complex>&);
Matrix<Complex> operator+(const Matrix<Complex>&, const Matrix<Real>&);

Matrix<K> operator-(const Matrix<K>&, const Matrix<K>&);   //matrix - matrix
Matrix<K> operator-(const KK&, const Matrix<K>&);          //scalar - matrix
Matrix<K> operator-(const Matrix<K>&, const KK&)           //matrix - scalar
Matrix<Complex> operator-(const Complex&, const Matrix<Real>&);
Matrix<Complex> operator-(const Matrix<Real>&, const Complex&);
Matrix<Complex> operator-(const Matrix<Real>&, const Matrix<Complex>&);
Matrix<Complex> operator-(const Matrix<Complex>&, const Matrix<Real>&);

Matrix<K> operator*(const KK&, const Matrix<K>&);        //scalar * matrix
Matrix<K> operator*(const Matrix<K>& ,const KK&);        //matrix * scalar
Matrix<Complex> operator*(const Complex&, const Matrix<Real>&);
Matrix<Complex> operator*(const Matrix<Real>&, const Complex&);
Matrix<K> operator/(const Matrix<K>&, const KK&);        //matrix / scalar
Matrix<Complex> operator/(const Matrix<Real>&, const Complex&);

Vector<K> operator*(const Matrix<K>&, const Vector<V>&);   //matrix * vector
Vector<Complex> operator*(const Matrix<Real>&, const Vector<Complex>&);
Vector<Complex> operator*(const Matrix<Complex>&, const Vector<Real>&);

Matrix<K> operator*(const Matrix<K>&, const Matrix<K>&);   //matrix * matrix
Matrix<Complex> operator*(const Matrix<Real>&, const Matrix<Complex>&);
Matrix<Complex> operator*(const Matrix<Complex>&, const Matrix<Real>&);

Matrix<K> transpose(const Matrix<K>&);         //transpose matrix
void diag(Matrix<K>&);                         //change matrix into its diagonal
Matrix<Real> real(const Matrix<Complex>&);     //real part
Matrix<Real> imag(const Matrix<Complex>&);     //imaginary part
Matrix<Real> conj(const Matrix<Real>&);        //conjugate complex matrix
Matrix<Complex> cmplx(const Matrix<Real>&);    //cast a real matrix to complex one
Matrix<Complex> conj(const Matrix<Complex>&);  //conjugate complex matrix
```

Some of algebraic operations are based on general templated functions using iterators on vector or matrix:

```
void transpose(const dimen_t, const dimen_t, M_it, MM_it); //transposition
void adjoint(const dimen_t, const dimen_t, M_it, MM_it);    //adjoint
void matvec(M_it, const V1_it, const V1_it, V2_it, V2_it); //matrix * vector
V2_it matvec(const Matrix<K>&, const V1_it, const V2_it);  //matrix * vector
void vecmat(M_it, const V1_it, const V1_it, V2_it, V2_it); //vector * matrix
V2_it vecmat(const Matrix<K>&, const V1_it, const V2_it);  //vector * matrix
void matmat(A_it, const dimen_t, B_it, const dimen_t, const dimen_t, R_it); //matrix * matrix
```

*Use these algebraic operations only with* Matrix<real_t> *and* Matrix<complex_t>. *They do not all work for more complicated structure such that* Matrix<Matrix<K> >.

If the Eigen library is available (it should be), QR and SVD decomposition are available:

```
void qr(const Matrix<T>&, Matrix<T>&, Matrix<T>&);
void svdMat(const Matrix<T>&, Matrix<T>&, Vector<T>&, Matrix<T>&, real_t eps=0);
```

Useful aliases hiding template syntax, are available for end users:

```
typedef Matrix<Real> RealMatrix,
typedef Matrix<Complex> ComplexMatrix;
typedef Matrix<Matrix<Real> > RealMatrices;
typedef Matrix<Matrix<Complex> > ComplexMatrices;
```

They are defined in *users_typedef.hpp* (*init* library).

| | |
|---|---|
| library : | **utils** |
| header : | **Matrix.hpp** |
| implementation : | **Matrix.cpp** |
| unitary tests : | **test_Matrix.cpp** |
| header dependences : | **config.h, Vector.hpp, Trace.hpp, Messages.hpp, String.hpp, Algorithms.hpp, complexUtils.hpp** |

## 3.11 The `Transformation` class

The `Transformation` class is related to 1D-2D-3D transformation given, either by a matrix $A$ and a vector $b$ (general linear transformation $x \rightarrow Ax+b$) or by some canonical transformations (may be chained).Up to now, only linear transformations are handled. They are listed in the following enumeration :

```
enum TransformType
{ _noTransform, _translation, _rotation2d, _rotation3d, _homothety, _scaling, _ptReflection,
   _reflection2d, _reflection3d, _composition, _explicitTf };
```

When the transformation is a chain of some transformations, each of them are listed in a vector :

```
class Transformation
{
 protected:
  string_t name_;                  //name of the transformation
  TransformType transformType_;    //geometrical transformation
  Matrix<real_t> mat_;             //matrix of the transformation (when linear), default Id in R3
  Vector<real_t> vec_;             //vector of the transformation (when linear), default (0,0,0)
  bool is3D_;                      //true if a 3D transformation (set by buildMat)
 private:
  vector<const Transformation*> components_;    //chain rule Transformation if not empty
 ...
};
```

It offers 3 constructors, a clone function and the destructor:

```
Transformation(const string_t& nam = "", TransformType trt=_noTransform); //basic constructor
Transformation(real_t a11,real_t a12, real_t a13, real_t a21,real_t a22, real_t a23,
               real_t a31,real_t a32, real_t a33, real_t b1=0, real_t b2=0, real_t b3=0);
               //explicit constructor from matrix and vector coefficients
Transformation(const Transformation& t);     //copy constructor
virtual Transformation* clone() const;       //virtual clone constructor
virtual ~Transformation();                   //destructor
```

some accessors to private or protected member data. Besides, some useful functions are provided:

```
void buildMat();                             //build mat_ and vec_ related to the transformation
virtual void print(std::ostream&) const;     //print Transformation
virtual void print(PrintStream&)  const;
friend ostream& operator<<(ostream&, const Transformation&);
```

To deal with chain of transformation the following function are available, in particular the operators *= and *:

```
friend Transformation toComposite(const Transformation&);
friend Transformation composeCompositeAndComposite(const Transformation&, const Transformation&);
friend Transformation composeCompositeAndCanonical(const Transformation&, const Transformation&);
friend Transformation composeCanonicalAndComposite(const Transformation&, const Transformation&);
friend Transformation composeCanonicalAndCanonical(const Transformation&, const Transformation&);
Transformation& operator*=(const Transformation&);     //to chain transformation
friend Transformation operator*(const Transformation&, const Transformation&);
```

To get the action of the transformation on a `Point`, the following member function has to be called:

```
virtual Point apply(const Point&) const;     //apply the transformation
```

All the canonical transformations (translation, rotation 2D, rotation 3D, ... see previous enumeration) are managed thru inheriting classes from the `Transformation` class. For instance, translations are handled by the `Translation` class:

```
class Translation : public Transformation
{
 protected:
  vector<real_t> u_; //vector of the translation
 public:
  Translation(vector<real_t> u = vector<real_t>(3,0.));
  Translation(real_t ux, real_t uy = 0., real_t uz = 0.);
  virtual Transformation* clone() const;
  virtual ~Translation() {}
  const vector<real_t>& u() const;
  virtual const Translation* translation() const;
  virtual Translation* translation();
  virtual Point apply(const Point&) const;
  virtual void print(std::ostream&) const;
  virtual void print(PrintStream& ) const;
};
```

that proposes some specific constructors and accessors and provides the virtual member functions of the `Transformation` class.

| | |
|---|---|
| library : | **utils** |
| header : | **Transformation.hpp** |
| implementation : | **Transformation.cpp** |
| unitary tests : | **unit_Transmission.cpp** |
| header dependences : | **config.h, Point.hpp, Matrix.hpp, Messages.hpp, Environnement.hpp** |

## 3.12 The collection classes

The Collection and PCollection are simple template classes to deal with with collection of objects or pointers to object. Inheriting from vector<T> or vector<T*>, they propose constructors with one, two, three, ... objects that are useful when users want to pass several numbers, several strings, ... to Parameter object.

### 3.12.1 The Collection class

The Collection class deals with some collections of objects. It has the following constructors :

```
template <typename T>
class Collection : public std::vector<T>
{
 public:
 Collection () : std::vector<T>() {}
 Collection (const std::vector<T>& ts);
 explicit Collection (int n);
 explicit Collection (int n, const T& s)
 Collection(const T& s1);
 Collection(const T& s1, const T& s2);
 ...  //constructors up to 48 arguments !
}
```

Besides, it has one accessor to the i-th item and some print stuff

```
const T& operator()(number_t n) const;
T& operator()(number_t n);
void print(std::ostream& out) const;
void print(PrintStream& os);
template<typename S>
ostream& operator<<(ostream& out, const Collection<S>& ns);
```

and the operator << is overloaded to mimic the insertion of an object in the collection :

```
template<typename T>
Collection<T>& operator<<(Collection<T>& ns, const T& n)
```

Two important collections are predefined in XLiFE++: the Numbers (Collection<Number>) and the Strings (Collection<String>):

```
Numbers ns(2,34,12);
Strings ss("Omega","Gamma","Sigma");
```

### 3.12.2 The PCollection class

the PCollection class is similar to the Collection class but it deals with collection of pointers to avoid copy of large objects. In order to be user friendly, it hides the pointers and its use is the same as the Collection class:

```
template <typename T>
class PCollection : public std::vector<T*>
{
 public:
 explicit PCollection (number_t n=0) : std::vector<T*>(n,0) {}
 explicit PCollection (int n) : std::vector<T*>(n,0) {}
 PCollection (const std::vector<T*>& ts) : std::vector<T*>(ts) {}
 PCollection(const T& t1);
 PCollection(const T& t1, const T& t2);
 ...  //constructors up to 10 arguments !
 const T & operator()(number_t n) const;
 PCollectionItem<T> operator()(number_t n);
 void clearPointers()
 void print(std::ostream& out) const;
 void print(PrintStream& os) const ;
 template <typename S>
 ostream& operator<<(ostream& out, const PCollection<S>& ts)
 template <typename S>
 PCollection<T>& operator<<(PCollection<T>& ts, const T& t)
}
```

PCollectionItem class is a small class that interfaces one item of the collection. Its purpose is to move from reference to pointer when inserting an item in the collection using the access operator ():

```
template<typename T> class PCollectionItem
{ public:
 typename std::vector<T*>::iterator itp;
 PCollectionItem(typename std::vector<T*>::iterator);
 T& operator = (const T& t);
 operator T&(); // //autocast PCollectionItem -> T&
}
```

As said before, this class may be used in a same way as the Collection class is used, keeping in mind that there is no copy of objects and therefore the pointers are shared!

```
PCollection<String> ss(3);
String s1="Omega";
ss(1)=s1;       // OK while s1 is not deleted
ss(2)="Gamma"; // FORBIDEN because "Gamma" is temporary
```

This class is designed for large objects of XLIFE++, such as GeomDomain, Space that will be presented later.

| | |
|---|---|
| library : | **utils** |
| header : | **Collection.hpp** |
| implementation : | **Collection.hpp** |
| unitary tests : | **test_Parameters.cpp** |
| header dependences : | **config.h** |

## 3.13 Parameters management

It may be useful to have a data structure to store freely any kind of parameters (values, string, ...) with a very simple interface for the end user. In particular, such structure could be attached to user functions (see chap. 3.15). This is achieved with two classes : the Parameter class which define one parameter and the Parameters class which manages a list of Parameter objects.

### 3.13.1 The Parameter class

The aim of the Parameter class is to encapsulate in the same structure, a data of integer type, of real type, of complex type, of string type, of real vector/complex vector type, of real vector/complex matrix type or of pointer type (void pointer) with the capability to name the parameter. Thus, this class proposes as private members:

```
class Parameter
{private :
  int i_;                //!<to store int type data
  real_t r_;             //!<to store real_t type data
  complex_t c_;          //!<to store complex_t type data
  String s_;             //!<to store string data
  void * p_;             //!<to store pointer
  String name_;          //!<parameter name
  number_t type_;        //!<type of value
  ...
  }
```

It offers
- a copy constructor and constructors associated to each managed type T (*int, real_t, complex_t, string, char*, void *, real vector, complex vector, real matrix, complex matrix*), with optional naming:

```
Parameter(const T, const String& nm = String(""));
Parameter(const Parameter&, const String& nm = String(""));
```

- assignment operator = with specialized cases

```
Parameter& operator=(const Parameter& p);
Parameter& operator=(const T&);
```

The real/complex vector and real/complex matrix are managed using the void pointer p_. More precisely, when a parameter is defined from a vector (or a matrix), for instance :

```
Parameter par(std::vector<Real>(5,1.);
```

a copy of the given vector is allocated and its pointer is stored as a void pointer in member p_. In assignment operator, the *deletePointer()* member function is used to free memory previously allocated.

The class provides
- some access functions to data

```
T get_s() const; //(T,s)=(int,i),(real_t,r),(complex_t,c),(String,s),(void *,p)
                 //(T,s)=(std::vector<real_t>&,rv),(std::vector<complex_t>&,cv)
                 //(T,s)=(Matrix<real_t>&,rm), (Matrix<complex_t>&,cm)
number_t get_value_type(const String&);
```

- access to the parameter name and its type

```
string name();              //acces to name
void name(const String &);  //to change the name
number_t type() const;      //access to type
string_t typeName() const ; //access to type name
```

- some print and read facilities

```
ostream& operator<<(ostream&, const Parameter&);
void print(const Parameter&);
istream& operator>>(istream&, Parameter&);
```

- some control functions

```
void illegalOperation(const String& t1, const String& op, const String& t2) const;
void illegalOperation2(const String& op, const String& t) const;
void undefinedParameter(const String& t) const ;
void illegalDivision() const;
```

When it has meaning, the operator +=, -=, *=, /=,+ , -, *, /, ==, !=, >, >=, <, <= are overloaded for parameters and it is possible to call standard mathematical functions (*abs, conj, log, ...*) with a *Parameter* object as argument.

Obviously, these operations are not allowed for pointer or string type parameter.
The pointer type parameter has been introduced to give to the user the possibility to store anything in a parameter (useful in the context of user functions). **It is the responsibility of the users to well manage their void pointers !**

There are casting operators associated to the `Parameter` class. Some are explicit:

```
real_t real(const Parameter& p);
complex_t cmplx(const Parameter& p);
String str(const Parameter& p);
void * pointer(const Parameter& p);
```

and the others are implicit (cast operator):

```
operator int();                         //!<cast to int
operator real_t();                      //!<cast to real_t
operator complex_t();                   //!<cast to complex_t
operator String();                      //!<cast to String
operator void*();                       //!<cast to void*
operator std::vector<real_t>();         //!< cast to real vector
operator std::vector<complex_t>();      //!< cast to complex vector
operator Matrix<real_t>();              //!< cast to real matrix
operator Matrix<complex_t>();           //!< cast  to complex matrix
```

These cast operators allow to write such syntax:

```
Parameter pi(Real(3.1415926), "the real pi");
real_t x=pi;  //autocast
```

Unfortunately, casting a parameter to complex does not fully work:

```
Parameter i(complex_t(0,1)); //i is a complex parameter
complex_t j=i;               //is working
j=i;                         //does not work !!!
```

The compiler cannot resolve an ambiguity on the operator = : *complex_t=real_t* or *complex_t=complex_t*. The reason is that the autocast of the Parameter can produce either a *complex_t* or *real_t* ! It is not possible to omit the *complex_t* autocast version because then the form *complex_t j=i;* no longer works. There is probably a solution but we did not find it !

The Parameter class is very simple to use, for instance:

```
Parameter k(3.1415926,"k");                    //named real parameter
Parameter i(complex(0.,1.),"i");               //named complex parameter
Parameter s("my string");                      //no named string parameter
Parameter pv(RealVector(5,0.5),"vec 5");
Parameter pam(Matrix<Real>(3,_hilbertMatrix),"hilbert matrix");
Vector<String> mat_names(3);
mat_names(1)="iron";mat_names(2)="aluminium";mat_names(1)="air";
Parameter names(&mat_names,"mat_names"); //named pointer parameter
real_t vk=get_r();
Parameter ik=i*k;                              //operation on parameters
ik.name("i*k");                                //rename parameter
```

### 3.13.2 The `Parameters` class: list of parameters

The `Parameters` class manages a list of `Parameter` objects. Using stream operator >>, it offers a friendly way to add a parameter in the list and an index or string index to access to the parameters of the list. It is based on the *map* structure of the STL:

```
class Parameters
{private :
  std::map<String,int> index_;      //!<associative list to manage string index
  std::vector<Parameter*> list_;    //!<list of parameter's pointers
}
```

The list of parameters pointers is stored in a vector thus providing a direct access to a parameter of the list. The associative map *index_* also provides a direct access to a parameter using a string index.

This classes proposes constructors with a single parameter initialization with an optional name:

```
Parameters();
Parameters(Parameter&);
Parameters(const void*, const string_t& nm = string_t(""));
template<typename T>
  Parameters(const T& t, const string_t& nm = string_t(""));
```

some list insertion facilities:

```
void push(Parameter&);                      //!< append a parameter into list
Parameters& operator<<(Parameter*);         //!< insert a parameter into list
Parameters& operator<<(Parameter&);         //!< insert a parameter into list
Parameters& operator<<(const Parameter&);   //!< insert a parameter into list
Parameters& operator<<(const void*);        //!< insert a void pointer into list
template<typename T>
  Parameters& operator<<(const T& t)      // insert a T value in list
```

some direct access operators (by index, string index or parameter):

```
Parameter& operator()(unsigned int);
Parameter& operator()(const String&);
Parameter& operator()(const char *);
Parameter& operator()(const Parameter&);
```

and some print utilities:

```
void print(std::ostream&) const ;
void print() const ;
friend void print(const Parameters&);
friend std::ostream& operator<<(std::ostream&, const Parameters&);
```

This parameter list is easy to use:

```
Parameter k(3.1415926,"k");   //named real parameter
RealVector v(10,0.);          //a real vector
Parameter pv(v,"v1");         //associate vector v to a parameter pv
Parameters params;            //new list of parameters
params<<k<<"a string"<<pv;    //insert parameters or explicit data
RealVector x=params("v1");    //retrieve vector v1
```

When you retrieve a parameter from the list, you have to know the type of the parameter to cast it in the right type. Note that the member function *type()* of the Parameter class gives the parameter type.

There exists a *defaultParameters* global variable declared in the header *config.h* and initialized as an empty list in the header *globalScopeData.h*.
There exists an alias of `Parameters`: `Options` for the management of user options.
What is an option ? An option has:

- A name, that will be used to get the value of an option, as for a `Parameter`.

> ⚠ An option name cannot start with a sequence of "-" characters.

- One or several keys used to define an option (key in a file or command line option). A key cannot be used twice and some keys are forbidden, due to some keys dedicated to system options.
- A value, that can be scalar (`Int`, `Number`, `Real`, `Complex` or `String`) or vector (`Ints`, `Numbers`, `Reals`, `Complexes` or `Strings`). This is the defautl value of the option and determines its data type. For vector types, size is not relevant.

This class provides a default constructor. In order to define a user option, you can use the function `addOption`:

```
Options opts;
opts.addOption("t1", 1.2);
opts.addOption("t2", "tata");
opts.addOption("t3", "-t", Complex(0.,1.));
opts.addOption("t4", Strings("-tu","-tv"), Reals(1.1, -2.4, 0.7));
opts.addOption("t5", Strings("tata","titi"));
```

To parse options from file and or command line arguments, you may use one of the following line:

```
opts.parse(argc, argv);
String filename="param.txt";
opts.parse(filename);
opts.parse(filename, argc, argv);
```

where `argv` and `argv` are the arguments of the `main` function dedicated to command line arguments of the executable. When using both filename and command line arguments, the latter are given priority.

Let's now talk about how use options in a file or command-line.
First option is named "t1". So it can be used through the key "t1", "-t1" or "–t1". Fourth option is named "t4" and has 2 aliases: "-tu" et "-tv". So it can be used through the key "t4", "-t4", "–t4", "-tu" or "-tv".

```
./exec --t1 2.5 -t2 tutu -t3 2.5 -0.1 -t4 2.2 -4.8 1.4  -t5 "tutu" toto "ta ta" titi
```

When passing options from command line, you consider a `Complex` value as 2 `Real` values. Furthermore, quotes are not necessary for `String` values, unless the value contains special characters such as blank spaces, escape characters, ... Here is an example of ascii file used to define options:

```
t1 3.7
t2 "ti ti"
t3 (2.5,-0.2)
t4 2.5 -2 3.4 4.7
t5 "titi" tutu "ta ta" toto
```

When passing options from a file, a `Complex` value is now written as a complex, namely real part and imaginary part are delimited by a comma and inside parentheses. As for command-line case, quotes are not necessary for `String` values, unless the value contains special characters such as blank spaces, escape characters, ...

| | |
|---|---|
| library : | **utils** |
| header : | **Parameters.hpp** |
| implementation : | **Parameters.cpp** |
| unitary tests : | **test_Parameters.cpp** |
| header dependences : | **config.h, String.hpp** |

## 3.14 The `Tabular` class

The `Tabular` class allows to manage tabulated values of a function. More precisely, it handles the values of a function on a uniform grid of any dimension, mainly providing some tools to create the table, to save the table to a file, to load a table from a file, and to evaluate the values of the function at some points by interpolation. More precisely, `Tabular` is a template class inherited from the `std::vector<T>` class:

```
template <typename T>
class Tabular : public std::vector<T>
{
public:
number_t dim;                 // grid dimension
std::vector<real_t> start;    // starting coordinates
std::vector<real_t> step;     // coordinate steps
std::vector<number_t> nbstep; // number of  steps
std::vector<string_t> name;   // coordinate names
std::vector<number_t> bs;     // block sizes (interna)
...
```

It handles the standard C++ functions with the following prototypes

```
typedef T(*funT1) (real_t);
typedef T(*funTP1)(real_t, Parameters&);
typedef T(*funT2) (real_t, real_t);
typedef T(*funTP2)(real_t, real_t, Parameters&);
typedef T(*funT3) (real_t, real_t, real_t);
typedef T(*funTP3)(real_t, real_t,real_t, Parameters&);
```

There are few ways to construct a `Tabular` object, either passing a function or not:

```
Tabular(real_t x0,real_t dx,number_t nx,const string_t& nax="x1");
Tabular(real_t x0,real_t dx,number_t nx,real_t y0,real_t dy,number_t ny,
        const string_t& nax="x1",const string_t& nay="x2");
Tabular(real_t x0,real_t dx,number_t nx,real_t y0,real_t dy,number_t ny,
        real_t z0, real_t dz, number_t nz, const string_t& nax="x1",
        const string_t& nay="x2", const string_t& naz="x3");
void addCoordinate(real_t c,real_t dc,number_t nc,const string_t& nac="");
Tabular(real_t x0, real_t dx,number_t nx,funT1 f,const string_t& nax="x1");
Tabular(real_t x0,real_t dx,number_t nx,funTP1 f,Parameters& pars,
        const string_t& nax="x1");
Tabular(real_t x0,real_t dx,number_t nx,real_t y0,real_t dy,number_t ny,funT1 f,
        const string_t& nax="x1", const string_t& nay="x2")   ;
Tabular(real_t x0,real_t dx,number_t nx,real_t y0,real_t dy,number_t ny,funT1 f,
        Parameters& pars, const string_t& nax="x1", const string_t& nay="x2");
Tabular(real_t x0,real_t dx,number_t nx,real_t y0,real_t dy,number_t ny,
        real_t z0, real_t dz, number_t nz, funT3 f, const string_t& nax="x1",
        const string_t& nay="x2", const string_t& naz="x3");
Tabular(real_t x0,real_t dx,number_t nx,real_t y0,real_t dy,number_t ny,
        real_t z0, real_t dz, number_t nz, funT3 f, Parameters& pars,
        const string_t& nax="x1", const string_t& nay="x2", const string_t& naz="x3");
Tabular(const string_t& filename);
```

The first functions where no function is passed, construct only a 1D, 2D, 3D grid, the function values will be set using the member functions `createTable`:

```
void createTable(funT1 f);
void createTable(funTP1 f, Parameters& pars);
void createTable(funT2 f);
void createTable(funTP2 f, Parameters& pars);
void createTable(funT3 f);
void createTable(funTP3 f, Parameters& pars);
```

The function `addCoordinate` allows to add more directions in the uniform grid, and then to build grids of any dimension. The function involved in some constructors or in functions `createTable` must be consistent with the grid (same number of arguments than the grid dimension).

The values of the function are stored in a contiguous vector:

```
[ v0.00 v0.01 ... v0.0n v0.10 v0.11 ... v0.1n ...]
```

So, the access to the $i_1, i_2, ..., i_d$ values is given by $k = i_1(s_2\, s_3 \dots s_d) + i_2(s_3 \dots s_d) + \dots i_d$ where $s_n$ is the size of the $n^{th}$ grid coordinate.

Saving the table of values to a file is done by the function:

```
void saveToFile(const string_t& filename,  const string_t& comment="Tabular") const;
```

using the following ascii format:

```
dim
comment
name1 x1 dx1 nx1 name2 x2 dx2 nx2 ... named xd dxd nxd
...
x1_i1 x2_i2 ... xd_id v_i1i2...id
...
```

and load from a file by using

```
void loadFromFile(const string_t& filename);
```

or straightforward from the constructor.

The main operation consists in evaluating the function at any point using the tabulated values. It is done by using $Q^k$ interpolation (linear in 1D) and the operator `()`:

```
T& operator()(real_t x) const;
T& operator()(real_t x, real_t y) const;
T& operator()(real_t x, real_t y, real_t z) const;
T& operator()const std::vector<real_t>& z) const;
T valrec(number_t d, number_t k, const std::vector<number_t>& is,
        const std::vector<number_t>& bs,const std::vector<real_t>& as) const;
```

The `valrec` function does a recursive evaluation and it is called by the operator `()` when the grid dimension is greater than 2.

Finally, the `Tabular` class provides some internal tools and some print stuff:

```
void clear();  //reset the object
void globalToIndex(number_t k, number_t bs, number_t d,
     std::vector<number_t>::iterator ijk) const;
void print(std::ostream&)  const;
std::ostream& operator<<(std::ostream&,const Tabular<T>&);
```

| | |
|---|---|
| library : | **utils** |
| header : | **Tabular.hpp** |
| implementation : | **Tabular.hpp** |
| unitary tests : | **test_Tabular.cpp** |
| header dependences : | **config.h, utils.h** |

## 3.15 The `Function` class

The object function aims to encapsulate the user functions with an additional information, says parameter data. This encapsulation are concerned with functions of a point or a couple of points, required by finite element computations at a low level. These functions are typically some physical parameters involved in integrals or source data functions. They may require other constant parameters. It is the reason why it is necessary to attach to the function a list of parameters (constant values of real type, complex type, ...). This class is designed to deal with standard functions involved in a finite element software (24 types):

```
    r          function(const Point&, Parameters&)
    Vector<r>  function(const Vector<Point>&, Parameters&)
    r          function(const Point&, const Point&, Parameters&)
    Vector<r>  function(const Vector<Point>&, const Vector<Point>&, Parameters&)
```

with r of type:

```
real_t, complex_t, Vector<real_t>, Vector<complex_t>, Matrix<real_t>, Matrix<complex_t>
```

The functions (resp. kernels) taking a point or a couple of points as input argument are called "scalar" functions (resp. kernel) whereas those taking a vector of points or a couple of vector of points are called "vector" functions (resp. kernels). Do not confuse a "vector" function with a function returning a vector and taking a point as input argument. For a such function, its vector form returns a vector of vectors.

The object function is based on the non templated class `Function`:

```
template<typename T_> class Function
{class Function
 protected:
 ValueType type_returned_;     // type of returned value ( _real, _complex)
 StrucType struct_returned_;   // struct of returned value (_scalar,_vector,_matrix)
 FunctType type_function_;     // type of the function (_function or _kernel}
 ArgType argType_;             // type of the argument (_point,_vector_point)
 mutable Parameters* params_;  // pointer to parameter list
 dimPair dims_;                // dimension of returned values
 String name_;                 // name of function and comments
 void * fun_;                  // store pointer to function in a void *
 void* table_;                 // Tabular pointer as void*  (default 0)
 Function* pointToTabx_;       // Function to associate Point or Point pair to variables
 //flag in OperatorOnUnknown construction (see operator lib)
 mutable bool check_type_;     // to activate a checking of arguments
 mutable bool conjugate_;      // temporary flag for conjugate operation
 mutable bool transpose_;      // temporary flag for transpose operation
 //to manage data requirements
 bool requireNx;               // true if function requires normal or x-normal vector
 bool requireNy;               // true if function (kernel) requires y-normal vector
 bool requireElt;              // true if function requires element
 bool requireDom;              // true if requires domain
 bool requireDof;              // true if requires dof
 //special attributes for kernel
 mutable bool xpar;            // true if x is consider as a parameter
 mutable Point xory;           //  x or y as parameter of the kernel
 public:
 static std::map<String,std::pair<ValueType,StrucType> > returnTypes;
 static std::map<String,std::pair<ValueType,StrucType> > returnArgs;
}
```

which manages the user function storing its pointer in the void pointer *fun_*, its parameters list in the Parameters pointer *params_* and a function name (optional) in the string *name_*. There are also members to store characteristics of the function (type and arguments type) allowing to identify quickly the return type of the function. The member *check_type_* is a flag used in safe evaluation process of the function. The two static maps are used to the management of the types.

We choose to use a non templated class for two reasons: to avoid template paradigm to the end users and to have a simpler way to transmit such object function in different part of the library. The counterpart of this choice is a more complex Function class but the complexity is only located in the class.

For each type of function is defined a useful alias of the pointer function:

```
typedef r(fun_xx_t)(const Point&, Parameters&);
typedef Vector<r>(vfun_xx_t)(const Vector<Point>&, Parameters&);
typedef r(ker_xx_t)(const Point&, const Point&, Parameters&);
typedef Vector<r>(vker_xx_t)(const Vector<Point>&, const Vector<Point>&, Parameters&);
```

where *r* is the return type and *xx* a code of the return type (sr,sc,vr,vc,mr,mc); s for scalar, v for vector, m for matrix, r for real and c for complex.
A `Function`, using the `void*` pointer `table_`, can be related to a `Tabular` object that handles tabulated values. `table_` is a `void*` pointer because the `Tabular` is a template class. In that case the function is evaluated using interpolation of tabulated values. By default, the Tabular dimension has to be consistent with the type of function and the dimension of input point. If it is planned to used a Tabular with a dimension less than the point dimension, the `Function` pointer `pointToTabx_` has to be set by a `Function` that relates a `Point` to a `Vector<real_t>` containing the coordinates in the `Tabular`.
The `Function` proposes:

- two constructors for each type of function (named and unnamed):

```
  Function(fun_sr_t& f, Parameters& pa = def_parameters);  //real scalar type
  Function(fun_sr_t& f, const String& na, Parameters& pa = def_parameters);
  Function(fun_sc_t& f, Parameters& pa = def_parameters);  //complex scalar type
  Function(fun_sc_t& f, const String& na, Parameters& pa = def_parameters);
  ...
```

  which initialize the void pointer and compute the return types using the member function *init()*.

  A function may be constructed from tabulated values, specifying a `Tabular` object:

```
template <typename T>
Function(Tabular<T>& tab, dimen_t dp, const string_t& na,
         FunctType ft =_function, Function* fpx =0)
```

  Note that it is also possible to create some tabulated values from the function itself using `createTabular` member functions:

```
void createTabular(real_t x0, real_t dx, number_t nx, const string_t& nax="x") ;
void createTabular(real_t x0, real_t dx, number_t nx, real_t y0, real_t dy,
         number_t ny, const string_t& nax="x", const string_t& nay="y");
...
```

  Up to now, only scalar function (not kernel) can be tabulated.

- evaluation capabilities (unsafe but fast) for each type of function:

```
real_t fun_sr(const Point &x)
complex_t fun_sc(const Point &x)
...
```

  As these functions only recast the void pointer to the required pointer function:

```
real_t fun_sr(const Point &x)
   {return reinterpret_cast<fun_sr_t*>(fun_)(x,*params_);}
```

  they are unsafe !

- templated overloaded operator (), insensitive to the form of function (safe but not as fast as previous)

```
template <typename T_>
T_& operator()(const Point & x, T_ & res) const;
T_& operator()(const Point & x,const Point& y, T_& res) const;
Vector<T_>& operator()(const Vector<Point>& x, Vector<T_>& res);
Vector<T_>& operator()(const Vector<Point>& x,
                       const Vector<Point>& y,Vector<T_> & res);
```

Note that these functions return a reference, contrary to the direct straight functions which return a value. Besides, by testing the input arguments, they are able to deal with single point or vector of points independently of the scalar or vector form of the user function :

```
template<typename T_>
T_& Function::operator()(const Point & x, T_ & res)
{  if(checkType_)checkFunctionType(res, _function); // check the type of arguments
   if(argType_ == _pointArg)  // case of a function of a point
   {
     if(functionType_==_function)
      {if(table_==0)
         { typedef typename PointerF<T>::fun_t* funT;
           funT f = reinterpret_cast<funT>(fun_);
           res = f(x, *params_);
         }
       else res=funTable(x,res);
    }
...
if(transpose_) res=tran(res);
if(conjugate_) res=conj(res);
return res;
}

}
```

Moreover, using the *checkFunctionType()* they can also perform a control of the type of the function. As the checking function uses expensive RTTI capabilities, this possibility is conditioned by the *check_type* state (true or false) which is automatically reset to false by the *checkFunctionType()*.

- accessors to the function characteristics:

```
ValueType typeReturned() const;
StrucType structReturned() const;
ValueType valueType() const;
StrucType strucType() const;
FunctType typeFunction() const;
ArgType typeArg() const ;
bool conjugate() const;
bool& conjugate();
void conjugate(bool v) const;
bool transpose() const;
bool& transpose();
void transpose(bool v) const;
bool isVoidFunction() const;
const void* fun_p() const;
Parameters& params();
Parameters& params() const;
Parameters*& params_p();
const Parameters* params_p() const;
dimPair dims() const;
string_t name() const;
```

- some functions to manage the function parameters and X/Y parameter in kernel:

```
void addParam(Parameter& pa;
template<typename K>
void setParam(K& v, const string_t& name) const;
Parameter& parameter(const string_t&) const;
Parameter& parameter(const char* s) const;
Parameter& parameter(const size_t) const;
void setX(const Point& P) const; // for kernel
void setY(const Point& P) const;
```

- some functions to manage the function data required during computation:

```
bool normalRequired() const;
void require(UnitaryVector uv, bool tf=true);
void require(const string_t& s, bool tf=true);
```

- a print utility:

```
void printInfo() const
```

To deal with some data that are available during FE computation such as normal vectors, current element, current dof or current domain, there is two things to do : tell to XLIFE++ that the Function will use such data

```
Function F(fun);        //link a C++ function fun to a Function object
F.require(_n);          //tell that function fun will use normal vector
F.require("element");   //tell that function fun will use element
```

and get data in the C++ function related to the Function object:

```
 Real fun(const Point& x, Parameters& pars=theDefaultParameters)
 {...
  Vector<Real>& n = getN();        //get the normal vector
  GeomElement& elt=getElement();  //get element
   ...
 }
```

This machinery is based on the ThreadData class that manages one instance of data by thread.

| | |
|---:|---|
| library : | **utils** |
| header : | **Function.hpp** |
| implementation : | **Function.cpp** |
| unitary tests : | **test_Function.cpp** |
| header dependences : | **config.h, Parameters.hpp, Point.hpp, String.hpp, Vector.hpp** |

## 3.16 The Kernel class

The Kernel class is intended to deal with kernel, say function $G(x,y)$ where $x,y$ are two points. Basically, it manages the function itself using Function object that is able to deal with such function but it manages other functions such as $\nabla_x G$, $\nabla_y G$, $\nabla_{xy} G$, $\frac{\partial G}{\partial n_x}$, $\frac{\partial G}{\partial n_y}$:

```
public:
Function kernel;
Function gradx;
Function grady;
Function gradxy;
Function ndotgradx;
Function ndotgrady;
Parameters userData;
```

All functions defined in Kernel class share the same parameters given by **userData**. Besides, the class provides some additional properties:

```
SingularityType singularType;    // singularity type
real_t singularOrder;            // singularity order
complex_t singularCoefficient;   // singularity coefficient
SymType symmetry;                // kernel symmetry
string_t name;                   // kernel name
dimen_t dimPoint;                // dim of points x,y
//temporary data
mutable bool checkType_;        // to activate checking mode
mutable bool conjugate_;        // flag for conjugate operation
mutable bool transpose_;        // flag for transpose operation
mutable bool xpar;              // true if x is consider as a parameter
mutable Point xory;             // x/y as parameter of the kernel
 //to manage data requirements
bool requireNx;               // true if requires normal or x-normal vector
bool requireNy;               // true if requires y-normal vector
bool requireElt;              // true if requires element
bool requireDom;              // true if requires domain
bool requireDof;              // true if requires dof
```

The following singularity types are currently available:

```
enum SingularityType {_notsingular, _r, _logr,_loglogr};
```

It is also possible to specify the singular and regular part using Kernel pointer (0 by default):

```
Kernel* singPart;
Kernel* regPart;
```

There are simple constructors from Function objects or from explicit C++ functions having a kernel form (see Function class):

```
Kernel();                              // default constructor
Kernel(const Kernel&);                 // copy constructor
Kernel& operator=(const Kernel&);      // assign operator
//from Function object
Kernel(const Function& ker, SingularityType st=_notsingular,
       real_t so=0, SymType sy=_noSymmetry);
Kernel(const Function& ker, const string_t& na, SingularityType st=_notsingular,
       real_t so=0, SymType sy=_noSymmetry);
//from explicit function having a kernel form
template <typename T>
Kernel(T(fun)(const Point&, const Point&, Parameters&),
       SingularityType st=_notsingular, real_t so=0, SymType sy=_noSymmetry);
template <typename T>
Kernel(T(fun)(const Point&, const Point&, Parameters&), const string_t& na,
       SingularityType st=_notsingular, real_t so=0, SymType sy=_noSymmetry);
...
virtual void initParameters();  //to share user parameters
```

Note that these simple constructors do not allow to set other functions (gradx, grady, ...).

This class provides some accessors:

```
bool conjugate() const;
bool& conjugate();
void conjugate(bool v) const;
bool transpose() const;
bool& transpose();
void transpose(bool v) const;
virtual bool isSymbolic() const;
virtual ValueType valueType() const;
virtual StrucType structType() const;
virtual dimPair dims() const;
```

It provides also some tools to manage parameters:

```
void setParameters(const Parameters& par);
void setParameter(Parameter& par);
template<typename T>
 void setParameter(const string_t& name, T value);
template<typename T>
 T getParameter(const string_t& name, T value) const;
void setX(const Point& P) const;
void setY(const Point& P) const;
```

and some functions to manage the kernel data required during computation:

```
bool normalRequired() const;
bool xnormalRequired() const;
bool ynormalRequired() const;
void require(UnitaryVector uv, bool tf=true);
void require(const string_t& s, bool tf=true);
```

In some computations, a `Kernel` object has to be viewed as a `Function` object, x or y being considered as a parameter. the following member functions do the job:

```
//move to y->k(x,y) or  x->k(x,y)
const Function& operator()(const Point& x, variableName vn ) const;
const Function& operator()(variableName vn, const Point& y) const;
const Function& operator()(variableName vn) const;
```

**variableName** is defined by the following enumeration:

```
enum VariableName {_x, _x1=_x, _y, _x2=_y, _z, _x3=_z, _t};
```

The class provides function to evaluate kernel:

```
template<typename T>
 T& operator()(const Point&, const Point&, T&) const;//compute at (x,y)
template<typename T>
 T& operator()(const Point&, T&) const;   //compute at (x,P) or (P,y) with P=xory
template<typename T>
 Vector<T>& operator()(const Vector<Point>&,const Vector<Point>&,
                               Vector<T>&) const; //compute at a list of points
```

As the `Kernel` class is the base class of `TensorKernel` class which deals with particular kernel, there are some virtual functions:

```
virtual KernelType type() const;                //_generalKernel, _tensorKernel
virtual const TensorKernel* tensorKernel() const;//downcast to tensorkernel
virtual TensorKernel* tensorKernel();           //downcast to tensorkernel*
```

To deal with some data that are available during FE computation such as normal vectors, current element, current dof or current domain, there is two things to do : tell to XLIFE++ that the Kernel will use such data

```
Kernel K(ker);      //link a C++ function(kernel) to a Kernel object
K.require(_nx);     //tell that function ker will use normal vector
```

and get data in the C++ function related to the Kernel object:

```
Real ker(const Point& x, const Point&y, Parameters& pars=theDefaultParameters)
{...
Vector<Real>& n = getN();       //get the normal vector
...
}
```

This machinery is based on the `ThreadData` class that manages one instance of data by thread.

As an example, we give the sketch of the program constructing the Laplace kernel in 3d:

```
Kernel Laplace3dKernel(Parameters& pars)
{
    Kernel K;
    K.name="Laplace 3D kernel";
    K.singularType =_r;
    K.singularOrder = -1;
    K.singularCoefficient = over4pi;
    K.symmetry=_symmetric;
    K.userData.push(pars);
    K.kernel = Function(Laplace3d, K.userData);
    K.gradx = Function(Laplace3dGradx, K.userData);
    K.grady = Function(Laplace3dGrady, K.userData);
    K.ndotgradx = Function(Laplace3dNxdotGradx, K.userData);
    K.ndotgrady = Function(Laplace3dNydotGrady, K.userData);
    return K;
}

real_t Laplace3d(const Point& x, const Point& y, Parameters& pars)
{
  real_t r = x.distance(y);
  return over4pi / r;
}

//derivatives
Vector<real_t> Laplace3dGradx(const Point& x, const Point& y,Parameters& pars)
{
  real_t r2 = x.squareDistance(y);
  real_t r = std::sqrt(r2);
  Vector<real_t> g1(3);
  scaledVectorTpl(over4pi / (r*r2), x.begin(), x.end(), y.begin(), g1.begin());
  return g1;
}

Vector<real_t> Laplace3dGrady(const Point& x, const Point& y,Parameters& pars)
{
  real_t r2 = x.squareDistance(y);
  real_t r = std::sqrt(r2);
  Vector<real_t> g1(3);
  scaledVectorTpl(-over4pi / (r*r2), x.begin(), x.end(), y.begin(), g1.begin());
  return g1;
}

real_t Laplace3dNxdotGradx(const Point& x, const Point& y, Parameters& pars)
{
 Vector<real_t>& nxp = getNx(); //get normal at x point
 std::vector<real_t>::const_iterator itx=x.begin(),ity=y.begin(), itn=nxp.begin();
 real_t d1=(*itx++ - *ity++), d2=(*itx++ - *ity++), d3=(*itx - *ity);
 real_t r = d1* *itn++; r+= d2* *itn++; r+=d3* *itn;
 real_t r3= d1*d1+d2*d2+d3*d3; r3*=std::sqrt(r3);
 return -r*over4pi_/r3;
}
...
```

See in the *mathRessources* directory, the kernels that are avalaible.

| | |
|---|---|
| library : | **utils** |
| header : | **Kernel.hpp** |
| implementation : | **Kernel.cpp** |
| unitary tests : | **test_Function.cpp** |
| header dependences : | **config.h, Parameters.hpp, Point.hpp, String.hpp, Vector.hpp, Function.hpp** |

## 3.17 The `TensorKernel` class

The `TensorKernel` class, inherited from the `Kernel` class, deals with kernels of the form:

$$K(x,y)=\sum_{1\le m\le M}\sum_{1\le n\le N}\psi_m(x)\mathbb{A}_{mn}\phi_n(y)$$

with $\mathbb{A}$ a $M\times N$ matrix. Such kernel is involved, for instance, in Dirichlet to Neumann method using spectral expansion. In many cases, this matrix is a diagonal one:

$$K(x,y)=\sum_{1\le n\le N}\psi_n(x)\lambda_n\phi_n(y).$$

In the meaning of XLiFE++, the families $(\psi_m)_{1\le m\le M}$ and $(\psi_n)_{1\le n\le N}$ may be considered as some basis of spectral space, say `SpectralBasis` object. So, the `TensorKernel` class is defined as follow:

```
protected :
 const SpectralBasis* phi_p;
 const SpectralBasis* psi_p;
 VectorEntry* matrix_p;
public :
 bool isDiag;         // true if matrix is a diagonal one
 Function xmap;       // geometric transformation applied to x
 Function ymap;       // geometric transformation applied to y
 bool isConjugate;    // conjugate phi_p in computation (default=false)
```

The **xmap** and **ymap** functions allow to map the basis functions from a reference space to an other one. For instance, suppose the basis $\cos(n\pi x)$ on the segment $]0,1[$ is given:

```
Real cosn(const Point& P, Parameters& pars)
{ Real x=P(1);
  Int n=pa("basis index")-1;  //get the index of function to compute
  return cos(n*pi*x);
}
```

and has to be used on the boundary $\Sigma=\{(0,y),0<y<h\}$. The basis will be map onto using the function:

```
Point sigmaTo(const Point& P, Parameters& pars)
{
  return Point(P(2)/h);
}
```

The `SpectralBasis` class manages either a basis given by an explicit C++ function (analytic form) or a basis given by a set of **TermVector** objects (numerical form). So the constructors provided by the `TensorKernel` class manages these different cases too:

```
TensorKernel();     //default constructor
template<typename T>
 //from one or two SpectralBasis objects
 TensorKernel(const SpectralBasis&, const vector<T>&, bool conj=false);
 TensorKernel(const SpectralBasis&, const vector<T>&, const SpectralBasis&);
 //from one or two Unknown objects belonging to spectral spaces
 TensorKernel(const Unknown&, const vector<T>&, bool conj=false);
 TensorKernel(const Unknown&, const vector<T>&, const Unknown&);
 //from one or two Function objects
```

```
TensorKernel(Function, const vector<T>&, bool conj=false);
TensorKernel(Function, const vector<T>&, Function);
//from one or two set of TermVector objects
TensorKernel(const vector<TermVector>&, const vector<T>&, bool conj =false);
TensorKernel(const vector<TermVector>&, const vector<T>&,
             const vector<TermVector>&);
```

Note that these constructors does not allow to set maps! They have to be set after construction. When the user defines TensorKernel from an explicit function, it has to get the index from the parameters related to the function. This index is automatically set by the computation functions and its name in parameters is "basis index".

The TensorKernel class provides some accessors ans properties:

```
const VectorEntry& vectorEntry() const;
const SpectralBasis* phip() const;
const SpectralBasis* psip() const;
const SpectralBasis& phi()  const;
const SpectralBasis& psi()  const;
dimen_t dimOfPhi() const;
dimen_t dimOfPsi() const;
number_t nbOfPhi() cons;
number_t nbOfPsi() cons;
bool phiIsAnalytic() const;
bool psiIsAnalytic() const;
virtual KernelType type() const;
virtual bool isSymbolic() const;
virtual ValueType valueType() const;
virtual StrucType structType() const;
bool sameBasis() const;
virtual const TensorKernel* tensorKernel() const;
virtual TensorKernel* tensorKernel();
```

It implements the computation of kernel:

```
template<typename T>
 T kernelProduct(number_t, const T&) const;
template<typename T>
 T kernelProduct(number_t, number_t, const T&) const;
```

| | |
|---:|---|
| library : | **terms** |
| header : | **TensorKernel.hpp** |
| implementation : | **TensorKernel.cpp** |
| unitary tests : | **test_Function.cpp** |
| header dependences : | **config.h, Parameters.hpp, Point.hpp, String.hpp, Vector.hpp, Function.hpp, TermVector.hpp, SpectralBasis.hpp** |

## 3.18 The ThreadData class

The ThreadData class is a utility class that manages some FE computation data (normal vectors, current element, current dof, current domain) that may be get by user function or user kernel. When the computation is done on several threads, these data have multiple instances (one by thread), this a reason why a ThreadData object handles some vectors of data pointers:

```
vector<Vector<real_t>*> theCurrentNxs;      // normal pointers or x-normal pointers
vector<Vector<real_t>*> theCurrentNys;      // y-normal pointers
vector<GeomElement*> theCurrentElements;    // element pointers
```

```
vector<Dof*> theCurrentDofs;              // dof pointers
GeomDomain* currentDomainx;               // domain pointer or domain_x pointer
GeomDomain* currentDomainy;               // domain_y pointer
```

It has only one a basic constructor and a resize function that is called when the number of threads changes:

```
ThreadData(number_t s=1);
void resize(number_t);
```

Besides, it offers various functions to set or get the data:

```
void setNx(Vector<real_t>*);
void setNy(Vector<real_t>*);
void setElement(GeomElement*);
void setDomainx(GeomDomain*);
void setDomainy(GeomDomain*);
void setDof(Dof*);
void setNx(Vector<real_t>*, number_t);
void setNy(Vector<real_t>*, number_t);
void setElement(GeomElement*, number_t);
void setDof(Dof*, number_t);

Vector<real_t>& getNx(number_t) const;
Vector<real_t>& getNx() const;
Vector<real_t>& getNy(number_t ) const;
Vector<real_t>& getNy() const;
GeomElement& getElement(number_t);
GeomElement& getElement() const;
GeomDomain& getDomainx() const;
GeomDomain& getDomainy() const;
Dof& getDof(number_t ) const;
Dof& getDof() const;
FeDof& getFeDof(number_t) const;
FeDof& getFeDof() const;
```

Print utility are also available

```
void print(std::ostream&) const;
void print(PrintStream& os) const {print(os.currentStream());}
```

When starting, XLiFE++ create one instance of `ThreadData` : `theThreadData` (see *globalScopeData.hpp*, *config.hpp*). To avoid the user to deal explicitely with it, some extern functions (wrappers to member functions) are also proposed:

```
inline void setNx(Vector<real_t>* p, number_t t);
inline void setNy(Vector<real_t>* p, number_t t);
inline void setElement(GeomElement* p, number_t t);
inline void setDof(Dof* p,number_t t);
inline void setNx(Vector<real_t>* p);
inline void setNy(Vector<real_t>* p);
inline void setElement(GeomElement* p);
inline void setDomain(GeomDomain* p);
inline void setDomainx(GeomDomain* p);
inline void setDomainy(GeomDomain* p);
inline void setDof(Dof* p);
inline Vector<real_t>& getN(number_t t);
inline Vector<real_t>& getNx(number_t t);
inline Vector<real_t>& getNy(number_t t ;
inline GeomElement& getElement(number_t t);
inline Dof& getDof(number_t t);
inline FeDof& getFeDof(number_t t);
inline Vector<real_t>& getN();
inline Vector<real_t>& getNx();
inline Vector<real_t>& getNy();
inline GeomElement& getElement();
inline GeomDomain& getDomain();
inline GeomDomain& getDomainx();
inline GeomDomain& getDomainy();
inline Dof& getDof();
inline FeDof& getFeDof();
```

This machinery allows the user to simply deal with such computation data:

```
Real fun(cons Point& x, Parameters& pars=theDefaultParameters)
{...
Vector<Real>& n = getN();       //get the normal vector
GeomElement& elt=getElement(); //get element
...}

int main()
{...
 Function F(fun);      //link a C++ function fun to a Function object
 F.require(_n);        //tell that function fun will use normal vector
 F.require("element"); //tell that function fun will use element
...
}
```

| | |
|---|---|
| library : | **utils** |
| header : | **ThreadData.hpp** |
| implementation : | **ThreadData.cpp** |
| unitary tests : | **test_ThreadData.cpp** |
| header dependences : | **config.h, utils.h** |

## 3.19 The SymbolicFunction class

The SymbolicFunction class handles a function described in a symbolic way, that is an expression involving variables, constant and operators. In fact, a SymbolicFunction object is a node of a tree :

```
class SymbolicFunction
{
   public :
   const SymbolicFunction* fn1, *fn2;  //nodes involved 0, 1 or 2 (0 by default)
   VariableName var;                   //variable involved (undef by default)
   SymbolicOperation op;               //operation involved (id by default)
   complex_t coef;                     //coefficient to apply to
   complex_t par;                      //additional parameter
   ...
}
```

A node may be

- a constant value stored in coef with fn1=fn2=0 and var=_varundef
- a variable (_x1, or _x2 or _x3) stored in var, with fn1=fn2=0
- a unary operation stored in op and acting either on the variable or the SymbolicFunction object fn1
- a binary operation stored in op and acting on the SymbolicFunction objects fn1 and fn2

The unary and binary operators are given by the enumeration:

```
enum SymbolicOperation
{_idop=0, _plus, _minus, _multiply, _divide, _power,
 _equal, _different, _less, _lessequal, _greater, _greaterequal, _and, _or,
 _abs, _realPart, _imagPart, _sqrt, _squared, _sin, _cos, _tan,          //unary
 _asin, _acos, _atan, _sinh, _cosh, _tanh, _asinh, _acosh, _atanh,       //unary
 _exp, _log, _log10, _pow, _not                                          //unary
};
```

As an example, the function `f(x_1,x_2)= (x_1+x_2)<1 && exp(x_1)>2` has the following tree representation:

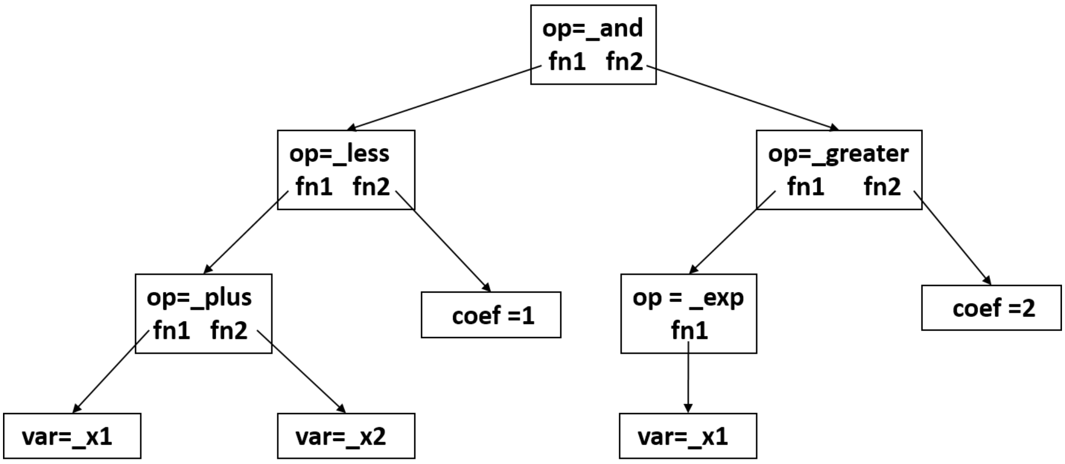


Figure 3.1: exemple of SymbolicFunction tree

> The function asinh, acosh, atanh are only available when compiling with a C++ version greater than 2011.

The `SymbolicFunction` class provides some basic constructors for each kind of node:

```
explicit SymbolicFunction(VariableName v=_varUndef);
explicit SymbolicFunction(const real_t&);
explicit SymbolicFunction(const complex_t&);
SymbolicFunction(const SymbolicFunction&, SymbolicOperation,
                 complex_t c=1.,complex_t p=0.);
SymbolicFunction(const SymbolicFunction&, const SymbolicFunction&,
                 SymbolicOperation, complex_t c=1., complex_t p=0.);
SymbolicFunction(const SymbolicFunction&);
~SymbolicFunction();
SymbolicFunction& operator=(const SymbolicFunction&);
```

The copy constructor and the assign operator do full copy of object referenced by pointers `fn1` and `fn2`. So, the destructor deletes them if they are assigned. Note that the variable `coef` and `par` are complex. Obviously, they may store some real scalars and the code interprets the imaginary part to know if they are real.

In order to make easier the construction of `SymbolicFunction` object, a lot of function or operator are provided, for instance :

```
//binary operation on SymbolicFunction's
SymbolicFunction& operator+ (const SymbolicFunction&, const SymbolicFunction&);
SymbolicFunction& operator- (const SymbolicFunction&, const SymbolicFunction&);
SymbolicFunction& operator* (const SymbolicFunction&, const SymbolicFunction&);
SymbolicFunction& operator/ (const SymbolicFunction&, const SymbolicFunction&);
```

```
SymbolicFunction& operator^ (const SymbolicFunction&, const SymbolicFunction&);
SymbolicFunction& operator==(const SymbolicFunction&, const SymbolicFunction&);
SymbolicFunction& operator!=(const SymbolicFunction&, const SymbolicFunction&);
SymbolicFunction& operator> (const SymbolicFunction&, const SymbolicFunction&);
SymbolicFunction& operator>=(const SymbolicFunction&, const SymbolicFunction&);
SymbolicFunction& operator< (const SymbolicFunction&, const SymbolicFunction&);
SymbolicFunction& operator<=(const SymbolicFunction&, const SymbolicFunction&);
SymbolicFunction& operator&&(const SymbolicFunction&, const SymbolicFunction&);
SymbolicFunction& operator||(const SymbolicFunction&, const SymbolicFunction&);
```

```
//unary operation on SymbolicFunction
SymbolicFunction& operator-(const SymbolicFunction&);
SymbolicFunction& operator+(const SymbolicFunction&);
SymbolicFunction& operator!(const SymbolicFunction&);
SymbolicFunction& abs(const SymbolicFunction&);
SymbolicFunction& real(const SymbolicFunction&);
SymbolicFunction& imag(const SymbolicFunction&);
SymbolicFunction& sqrt(const SymbolicFunction&);
SymbolicFunction& squared(const SymbolicFunction&);
SymbolicFunction& sin(const SymbolicFunction&);
SymbolicFunction& cos(const SymbolicFunction&);
SymbolicFunction& tan(const SymbolicFunction&);
SymbolicFunction& asin(const SymbolicFunction&);
SymbolicFunction& acos(const SymbolicFunction&);
SymbolicFunction& atan(const SymbolicFunction&);
SymbolicFunction& sinh(const SymbolicFunction&);
SymbolicFunction& cosh(const SymbolicFunction&);
SymbolicFunction& tanh(const SymbolicFunction&);
SymbolicFunction& exp(const SymbolicFunction&);
SymbolicFunction& log(const SymbolicFunction&);
SymbolicFunction& log10(const SymbolicFunction&);
SymbolicFunction& pow(const SymbolicFunction&, const double&);
#if __cplusplus > 199711L
SymbolicFunction& asinh(const SymbolicFunction&);
SymbolicFunction& acosh(const SymbolicFunction&);
SymbolicFunction& atanh(const SymbolicFunction&);
#endif
```

The binary operators are also provided for `SymbolicFunction` object and constant (real or complex).

Besides, some basic tools are proposed by the class:

```
bool isSingle() const;  //true if a constant or variable
bool isConst() const;   //true if a constant expression
set<VariableName> listOfVar() const; //list of involved variables
number_t numberOfVar() const; //number of involved variables
void print(ostream& = cout) const;
void printTree(ostream& =cout, int lev=0) const;
```

Finally, by overloading the operator (), the symbolic function can be evaluated for any set of real values or complex values:

```
complex_t operator()(const vector<complex_t>& xs) const;
complex_t operator()(const complex_t& x1) const;
complex_t operator()(const complex_t& x1, const complex_t& x2) const;
complex_t operator()(const complex_t& x1, const complex_t& x2,
                     const complex_t& x3) const;
real_t operator()(const vector<real_t>& xs) const;
real_t operator()(const real_t& x1) const;
real_t operator()(const real_t& x1, const real_t& x2) const;
real_t operator()(const real_t& x1, const real_t& x2, const real_t& x3) const;
```

These member functions use the fundamental functions that performs computations:

```
inline real_t evalOp(SymbolicOperation op,const real_t& x,const real_t& y);
inline real_t evalFun(SymbolicOperation op,const real_t& x,const real_t& p=0.);
inline complex_t evalOp(SymbolicOperation op,const complex_t& x,
                        const complex_t& y);
inline complex_t evalFun(SymbolicOperation op,const complex_t& z,
                         const complex_t& p=0.);
```

Hereafter, some examples of construction of `SymbolicFunction` objects:

```
SymbolicFunction fs;
fs = x_1+x_2-1;
fs = 2*x_1-3*x_2;
fs = 5*(2*x_1-3*x_2);
fs = 4*sqrt(2*x_1-3*x_2)/x_2;
fs = sin(cos(sqrt(abs(log(x_1*x_1+x_2*x_2+x_3*x_3)))));
fs = (1.-sin(x_1))*(cos(1.+x_1)/5 + 2*sin(3*x_1));
fs = pow(squared(x_1), 0.5);
fs = SymbolicFunction(3);
fs = -sin(x_1);
fs = +sin(-x_1);
fs = cos(x_2)-2*sqrt(x_1*x_2);
fs = x_1 < 1;
fs = (x_1+x_2)<=1 && exp(x_1)>2;
fs = (x_1+x_2)^3;
```

| | |
|---|---|
| library : | **utils** |
| header : | **SymbolicFunction.hpp** |
| implementation : | **SymbolicFunction.cpp** |
| unitary tests : | **unit_SymbolicFunction.cpp** |
| header dependences : | **config.h, Messages.hpp** |

## 3.20 The `Graph` class

The `Graph` class is a simple class representing a numbering graph well suited to deal with storage of matrices, in particular to optimize the matrix numbering in order to minimize its bandwith. It is not a general `Graph` class.

Each node, represented by a `vector<Number>`, contains the connection between this node and others. Node $n_i$ and $n_j$ are "connected" if $n_j$ belongs to `vector<Number>` defining $n_i$. The degree of a node is the number of nodes connected to it. It is implemented as a child class of `vector<vector<Number> >`:

```
class Graph : public std::vector<std::vector<Number> >
{
public:
   Graph(Number);   //basic constructor
   Number nodeDegree(Number) const;
   Number maximumDegree() const;
   ...
};
```

It provides some tools to compute matrix bandwidth and length of skyline storage of matrix, and to optimize numbering to reduce the bandwidth:

```
pair<Number, Number> bandWidthAndSkyline() const;
Number bandWidth() const;
Number skylineSize() const;
```

```
vector<Number> renumber(Number);
Number renumEngine(vector<bool>&, vector<Number>&, Number& ,Number,
                  Number&, Number&);
```

and some printing facilities:

```
void print(std::ostream&, const String&) const;
void print(const String& title = "") const;
void printNodes(std::ostream&, const vector<Number>&);
void printNodes(const vector<Number>&);
```

| | |
|---|---|
| library : | **utils** |
| header : | **Graph.hpp** |
| implementation : | **Graph.cpp** |
| unitary tests : | **test_Graph.cpp** |
| header dependences : | |

## 3.21 The `Value` class

The `Value` class is a utility class to encapsulates user's data involved in a differential expression. Such data may be a function (`Function` object) or any real or complex scalar, vector or matrix value. This class is designed as follows:

```
class Value
{
protected :
  ValueType type_;    //type of returned value ( _real, _complex)
  StrucType struct_; //structure of returned value (_scalar, _vector, _matrix,
                            _vectorofvector, _vectorofmatrix, _matrixofmatrix)
  void * value_p;          //void pointeur to the true value
  mutable bool conjugate_; //temporary conjugate state flag
  mutable bool transpose_; //temporary transposition state flag
```

The attributes *conjugate_* and *transpose_* are temporary flags used when chaining Value object in a differential expression. They have no meaning outside a particular context!
In order to recast safely the void pointer *value_p* pointing to the actual data, this class uses the Run Time Information, to store the names of data type supported:

```
typedef std::pair<ValueType,StrucType> structPair;
typedef std::pair<String,structPair> mapPair;
static std::map<String,structPair > theValueTypeRTInames;
static void valueTypeRTINamesInit();
```

The only constructors allowed are the following:

```
Value(const real_t &);
Value(const Vector<real_t> &);
Value(const Matrix<real_t> &);
Value(const Vector<Vector<real_t> > &);
Value(const Vector<Matrix<real_t> >&);
Value(const Matrix<Matrix<real_t> >&);
Value(const complex_t &);
Value(const Vector<complex_t> &);
Value(const Matrix<complex_t> &);
Value(const Vector<Vector<complex_t> > &);
Value(const Vector<Matrix<complex_t> >&);
Value(const Matrix<Matrix<complex_t> >&);
```

They correspond to the data types that are supported by this encapsulation class. These constructors create in memory a copy of the given value.

There are two templated functions to check the data types:

```
template<typename T> static bool checkTypeInList(const T &);
template<typename T> static bool isTypeInList(const T&);
template<typename T> void checkType(const T&) const;
```

The two first ones checks if the type T is in the list of allowed types and the second one compares the type T to the type of the current Value. To get the actual value, you have to use the templated member function:

```
template<class T> T& value() const;
```

Note that you have to explicit the template argument T. This function checks the value type and recasts the void pointer.

Besides, there are accessors/modifiers member functions:

```
ValueType valueType() const{return type_;}
StrucType strucType() const{return struct_;}
bool  conjugate()const {return conjugate_;}
bool& conjugate() {return conjugate_;}
void  conjugate(bool v) const {conjugate_=v;}
bool  transpose()const {return transpose_;}
bool& transpose() {return transpose_;}
void  transpose(bool v) const {transpose_=v;}
```

In order to conjugate or transpose (or both) a value in an expression, this class provides the functions:

```
Value& conj(Value &);
Value& trans(Value &);
Value& adj(Value &);
```

Be care, these functions do not modify the value but just set the *conjugate_/transpose_* flag to its opposite.

Finally, there are some printing functions:

```
static void Value::printValueTypeRTINames(std::ostream&);
void Value::print(std::ostream &) const;
friend std::ostream& operator<<(std::ostream&,const Value &);
```

Here, we give a small example to illustrate how the `Value` class works:

```
Value::printValueTypeRTINames(cout);     //print on stdout the RTI names of value types
real_t s=1.;
Value Vs(s);                             //create Value object
cout<<"real Value Vs(s) :"<<Vs;          //print Value
real_t r =Vs.value<real_t>();            //get as a real
Vector<complex_t> vc(3,complex_t(0,1));  //a vector of complex values
Value Vvc(vc);
cout<<"complex vector Value Vvc(vc) :"<<Vvc;          //print Value
Vector<complex_t> wc=Vvc.value<Vector<complex_t> >(); //get as a complex vector
```

|  |  |
|---|---|
| library : | **operator** |
| header : | **Value.hpp** |
| implementation : | **Value.cpp** |
| unitary tests : | **test_operator.cpp** |
| header dependences : | **config.h, utils.h** |

## 3.22 The `KdTree` class

The `KdTree` class implements the well known kdtree which is a binary tree where objects are separated using component by component separation. Usually objects are points but the following implementation is templated to deal with any class T that have components that can be separated. More precisely, the T class has to provide the following:

```
T::SepValueType;
T::operator()(int);
T::dim();
int Tcompare(const T& t, int c, const T::SepValueType& s);
//return  -1 (t_c<s), 1 (t_c>s) or 0 (t_c=s)
int maxSeparator(const T& t1, const T& tT2, int &c, T::SepValueType& s);
// find the component index c where separation is maximal, update s as the middle value and
    return the comparison of t1 and t2 (1,-1,0)
```

Such tree may find the nearest object of a given object in a fast way ($n\log n$ in the most cases and $n$ in worst cases).

The `KdTree` class is based on the `KdNode` class which is in fact the main class, `KdTree` handling the root node. A `KdNode` is either a separation line (component that separates two points and value of separation) or a terminal leaf containing a separated object.

### `KdNode` class

```
template <class T>
class KdNode
{
private :
   typedef typename T::SepValueType SvType;
   KdNode * parent_;      //!< pointer to parent node
   KdNode * left_;        //!< pointer to left node
   KdNode * right_;       //!< pointer to right node
   const T * obj_;        //!< object pointer linked to node
   int separator_;        //!< separation component
   SvType sv_;            //!< separation value
}
```

It has two basic constructors, a destructor and a node insertion function

```
KdNode();
KdNode(const T *O,int s, KdNode * p);
~KdNode();
void insert(const T *);
```

The `insert` function is the fundamental function used in building of kdtree : it travels in tree up to find a free box containing the object to be inserted; if no free box is found, the last non empty box containing object to be inserted and an other object is split in two boxes. The tree obtained by this method has not an optimal balancing !

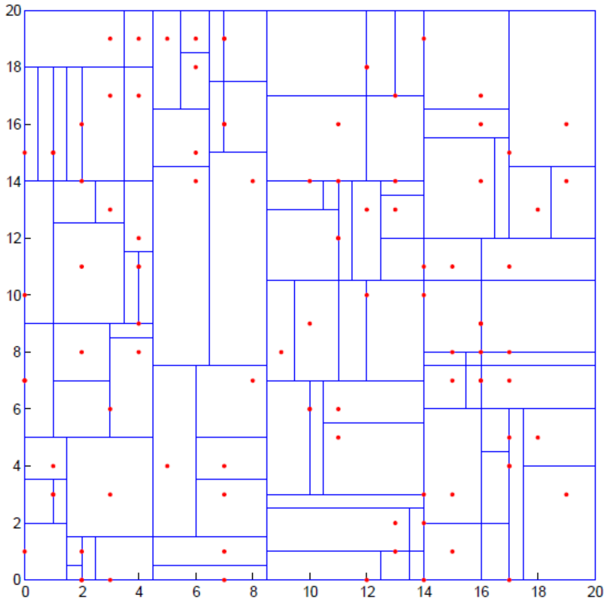


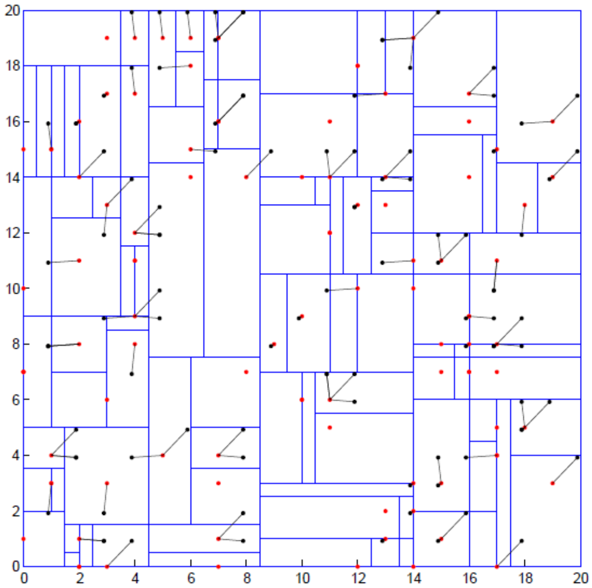
Figure 3.2: exemple of separation of 2d points

The class provides some utitilities

```
Number& depth(Number &) const;        //!< return node depth
void print(std::ostream&, std::string &) const;
void printBoxes(std::ostream &os, Box<SvType> b) const;
template <class S>
friend std::ostream& operator<<(std::ostream& os,const KdNode<S> & node);
```

and the important function to search the nearest object of a given object:

```
void searchNearest(const T *, const T *&, SvType &);
```



### KdTree class

As already mentioned KdTree handles the root node of tree and mainly encapsulated the KdNode functions

```
template <class T>
class KdTree
{
private :
 typedef typename T::SepValueType SvType;    //separator value type
 KdNode<T>* root;                            //rootnode of the tree
 Dimen dimT;                                 //object dimension
 }
```

```
KdTree() {root=new KdNode<T>();dimT=0;}
KdTree(const std::vector<T>&);
~KdTree() {delete root;};
bool isVoid() const;
Dimen dim() const;
void insert(const T&);
void insert(const std::vector<T>&);
Number depth() const;
const T* searchNearest(const T &) const;
void print(std::ostream& out) const;
template <typename R>
 void printBoxes(std::ostream &os, const Box<R>& rb);
template <typename R>
 void printBoxes(const std::string& file , const Box<R>& rb);
template <class S>
   friend std::ostream& operator<<(std::ostream& os,const KdTree<S>& node);
```

| | |
|---:|---|
| library : | **utils** |
| header : | **KdTree.hpp** |
| implementation : | **KdTree.hpp** |
| unitary tests : | **test_KdTree.cpp** |
| header dependences : | **space.h, config.h, utils.h** |

## 3.23 The polynomials classes

In order to deal with general polynomial spaces (using formal polynomials), XLIFE++ provides the following template classes

- MonomialT to deal with monomials of the form $x^i y^j z^k$
- PolynomialT to deal with polynomials as combination of monomials, say

$$p(x,y,z)=\sum_{i,j,k\geq 0}\alpha_{ijk}x^i y^j z^k$$

- PolynomialBasisT to deal with set of polynomials, may be a poynomials basis:

$$P[x,y,z]=\text{span}\{P_\ell,\ \ell=1,L\}$$

- PolynomialsBasisT to deal with set of vector polynomials, may be a poynomial basis:

$$\mathbf{P}[x,y,z]=\text{span}\left\{\mathbf{P}_\ell=\begin{pmatrix}P^x_\ell\\ P^y_\ell\\ P^z_\ell\end{pmatrix},\ \ell=1,L\right\}$$

- PolyNodeT to represent a polynomial as tree, useful to evaluate polynomial in a best way (Horner algorithm)

These classes can manage one, two or three variables and are templated by the type of the variable (K) which is of real_t type by default.

Note that there is no specific class to deal with vector polynomial, they are described as std::vector<PolynomialT>.

For users, some useful aliases are available :

```
typedef MonomialT<real_t>  Monomial;
typedef PolynomialT<real_t> Polynomial;
typedef PolynomialBasisT<real_t> PolynomialBasis;
typedef PolynomialsBasisT<real_t> PolynomialsBasis;
```

Some usual scalar polynomials spaces may be constructed in 1d, 2d or 3d:

$$\begin{array}{lll}
Pn[x,y,z] & : \sum a_{ijk}x^i y^j z^k & i,j,k \geq 0,\ i+j+k \leq n \\
PHn[x,y,z] & : \sum a_{ijk}x^i y^j z^k & i,j,k \geq 0,\ i+j+k = n \\
Qn[x,y,z] & : \sum a_{ijk}x^i y^j z^k & i,j,k \geq 0,\ i,j,k \leq n \\
Qns[x,y,z] & : \sum a_{ijk}x^i y^j z^k & i,j,k \geq 0,\ i \leq nx, j \leq ny, k \leq nz
\end{array}$$

Some particular vector polynomials spaces related to FE space are also provided (see PolynomialsBasisT class). They can be addressed using the enumeration:

```
enum PolynomialSpace {_Pk,_PHk,_Qk,_Qks,_Rk, _SHk,_Dk,_DQk,_DQ2k};
```

Main algebraic operations are supported and some formal derivative operations too. Polynomials may be evaluated at point $(x, y, z)$ using operator ().

Besides, Polynomials may have a tree representation using PolyNodeT class. It may be useful when evaluating large polynomials.

### 3.23.1 The MonomialT class

This class deals with monomials of the form :

$$x_1^{a_1} x_2^{a_2} x_3^{a_3}$$

storing only the three power numbers $a_1$, $a_2$, $a_3$:

```
template <typename K = real_t>
class MonomialT
{
  public:
    dimen_t a1, a2, a3;
    ...
};
```

Thus, it allows only to deal with monomials of 3 variables of type K. Note that no coefficient is attached to a monomial.

MonomialT class provides only one fundamental constructor, overloaded operator () to evaluate monomial at a point or a vector of points, product by a monomial, comparison operators and print facilities:

```
MonomialT(dimen_t p1=0, dimen_t p2=0, dimen_t p3=0)
K operator()(const K& x1, const K& x2 = K(1), const K& x3 = K(1))const
K operator() (const std::vector<K>& x) const
MonomialT<K>& operator*=(const MonomialT<K>& m);
void swapVar(dimen_t v1, dimen_t v2, dimen_t v3);
string_t asString() const;
void print(std::ostream& out) const;
```

```
MonomialT<K> operator*(const MonomialT<K>& m1, const MonomialT<K>& m2);
friend std::ostream& operator<<(std::ostream& out, const MonomialT& m);
bool operator== (const MonomialT<K>& m1, const MonomialT<K>& m2);
bool operator!= (const MonomialT<K>& m1, const MonomialT<K>& m2);
bool operator < (const MonomialT<K>& m1, const MonomialT<K>& m2);
bool operator > (const MonomialT<K>& m1, const MonomialT<K>& m2);
```

### 3.23.2 The PolynomialT class

The PolynomialT class deals with polynomial up to 3 variables of value type K stored as a list of pairs of MonomialT object and a coefficient of type K:

```
template <typename K=real_t>
class PolynomialT
{
  public:
    std::list<std::pair<MonomialT<K>, K > > monomials;
    real_t epsilon;
    mutable PolyNodeT<K> tree;
    ...
}
```

The member data epsilon is used to round to 0 the very small coefficients of the polynomial. By default its value is 100000*theEpsilon (about $10^{-10}$ in double precision). The member data tree may store a tree representation (PolyNode object) of the polynomial, that is useful to evaluate it at a point in a faster and more stable way (generalized Horner algorithm).

The class provides simple constructors from monomials and a copy constructor:

```
PolynomialT();
PolynomialT(const MonomialT<K>&,const K& =K(1));
PolynomialT(const MonomialT<K>& ,const K&, const MonomialT<K>&, const K&);
PolynomialT(const PolynomialT<K>&);
PolynomialT<K>& operator=(const PolynomialT<K>& p);
```

There are some useful tools:

```
void push_back(const K&, const MonomialT<K>&);  //add a monomial part
(const_) iterator begin() (const) ;
(const_)iterator end()(const) ;
dimen_t degree() const;
void clean(real_t asZero);  //remove "zero" part
void clean();
void swapVar(dimen_t v1, dimen_t v2, dimen_t v3);
static PolynomialT<K> zero();
bool isZero() const;
```

To evaluate the polynomial two methods are available. One evaluating the polynomial as a linear combination of monomials, the other one using a generalized Horner algorithm based on a tree representation of the polynomial:

```
void buildTree() const;
K eval (const K& x1, const K& x2 = K(1), const K& x3 = K(1)) const ;
K evalTree(const K& x1, const K& x2 = K(1), const K& x3 = K(1)) const;
K operator() (const K& x1, const K& x2 = K(1), const K& x3 = K(1)) const;
K operator() (const std::vector<K>& x) const;
```

If tree representation is built, the `eval` functions used always tree representation.

Main algebraic operations are avalaible, either as internal or external functions to the class:

```
PolynomialT<K>& operator *=(const MonomialT<K>&);
PolynomialT<K>& operator *=(const K&);
PolynomialT<K>& operator /=(const K& k);
PolynomialT<K>& operator +=(const MonomialT<K>&);
PolynomialT<K>& operator -=(const MonomialT<K>&);
PolynomialT<K>& operator +=(const PolynomialT<K>&);
PolynomialT<K>& operator -=(const PolynomialT<K>&);
PolynomialT<K>& operator *=(const PolynomialT<K>&);

//extern operation
template <typename K>
PolynomialT<K> operator *(const PolynomialT<K>& ,const MonomialT<K>&);
PolynomialT<K> operator *(const MonomialT<K>&, const PolynomialT<K>&);
PolynomialT<K> operator *(const MonomialT<K>&, const K&);
PolynomialT<K> operator *(const K&, const MonomialT<K>&);
PolynomialT<K> operator /(const MonomialT<K>&, const K&);
PolynomialT<K> operator *(const PolynomialT<K>&, const K&);
PolynomialT<K> operator *(const K&, const PolynomialT<K>&);
PolynomialT<K> operator /(const PolynomialT<K>&, const K&);
PolynomialT<K> operator -(const PolynomialT<K>&);
PolynomialT<K> operator +(const PolynomialT<K>&, const PolynomialT<K>&);
PolynomialT<K> operator -(const PolynomialT<K>&, const PolynomialT<K>&);
PolynomialT<K> operator *(const PolynomialT<K>&, const PolynomialT<K>&);
```

Using the operator `(.)`, polynomials may be chained (say $q(p1(x,y,z),p2(x,y,z),p3(x,y,z))$ :

```
template <typename K>
PolynomialT<K> operator()(const PolynomialT<K>& px,
                          const PolynomialT<K>& py=PolynomialT<K>(),
                          const PolynomialT<K>& pz=PolynomialT<K>()) const;
PolynomialT<K>& replace(VariableName, const PolynomialT<K>&);
```

It is also possible to get some derivatives and integrals of polynomials:

```
template <typename K>
PolynomialT<K> dx(const MonomialT<K>&);
PolynomialT<K> dy(const MonomialT<K>&);
PolynomialT<K> dz(const MonomialT<K>&);
vector<PolynomialT<K> > grad(const MonomialT<K>&, dimen_t =3);
vector<PolynomialT<K> > curl(const MonomialT<K>&, dimen_t =3);
PolynomialT<K> derivative(VariableName, const MonomialT<K>&);
PolynomialT<K> integral(VariableName, const MonomialT<K>&);

PolynomialT<K> dx(const PolynomialT<K>&);
PolynomialT<K> dy(const PolynomialT<K>&);
PolynomialT<K> dz(const PolynomialT<K>&);
vector<PolynomialT<K> > grad(const PolynomialT<K>&, dimen_t =3);
```

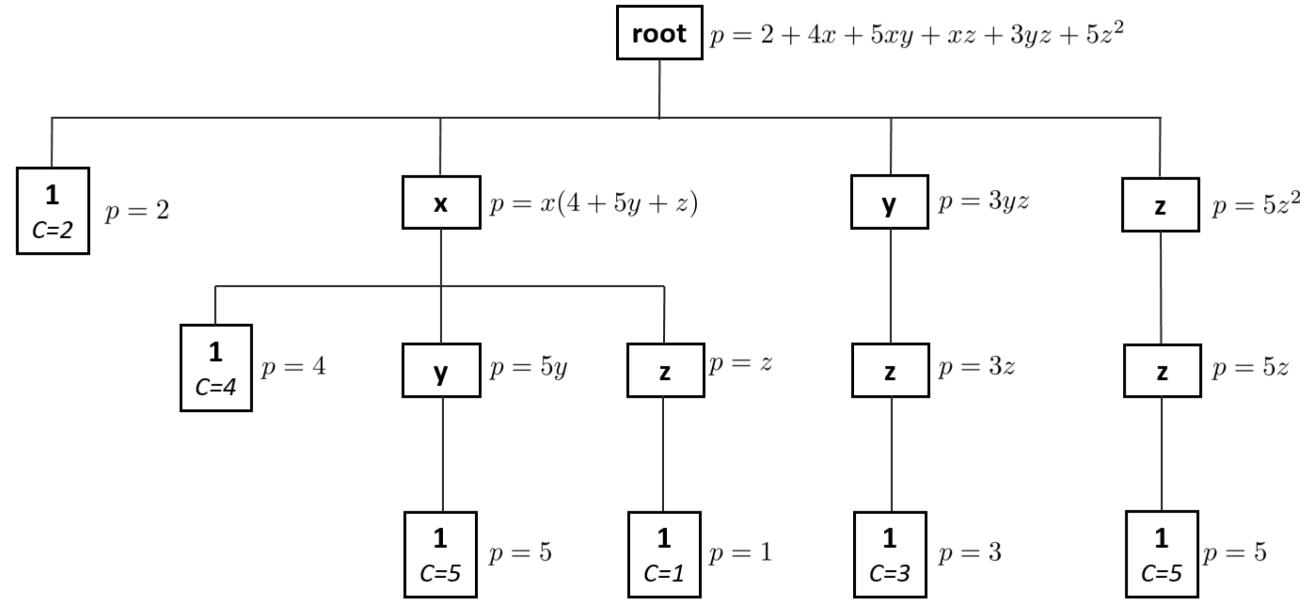
```
vector<PolynomialT<K> > curl(const PolynomialT<K>&, dimen_t =3);
PolynomialT<K> derivative(VariableName, const PolynomialT<K>&);
PolynomialT<K> integral(VariableName, const PolynomialT<K>&);

vector<PolynomialT<K> > dx(const vector<PolynomialT<K> >&);
vector<PolynomialT<K> > dy(const vector<PolynomialT<K> >&);
vector<PolynomialT<K> > dz(const vector<PolynomialT<K> >&);
vector<PolynomialT<K> > curl(const vector<PolynomialT<K> >&);
PolynomialT<K> div(const vector<PolynomialT<K> >&);
PolynomialT<K> dot(const vector<PolynomialT<K> >&, const vector<K>&);
vector<PolynomialT<K> > derivative(VariableName,const vector<PolynomialT<K> >&)
vector<PolynomialT<K> > integral(VariableName,const vector<PolynomialT<K> >);
```

Finally, some print facilities are provided:

```
string_t asString() const;
void print(std::ostream&) const;
friend std::ostream& operator<<(std::ostream&, const PolynomialT&)
```

### 3.23.3 The `PolyNodeT` class

In order to be computed in a faster and a more stable way, a polynomial may be represented as a tree and evaluated by traveling this tree. In this tree representation, each node represents one of the factor $1$, $x_1$, $x_2$ or $x_3$. When it is a leaf, the coefficient of the corresponding monomial is stored. For instance the polynomial $2+4x+5xy+xz+3yz+5z^2$ has the following tree :



Horizontal lines represents addition while vertical lines represent product. Note that the tree representation is not unique.

The `PolyNodeT` class manages for each node a factor type and a coefficient, and some pointers to travel the tree:

```
template <typename K=real_t>
class PolyNodeT
{public:
    dimen_t type;          // 0: 1, 1: x1, 2:x2, 3:x3
    K coef;
    PolyNodeT<K>* parent, *child, *right;
    ...
};
```

It offers only a few member functions to build the polynomial tree:

```
PolyNodeT(dimen_t =0, PolyNodeT<K>* =0, const K& =K(0));
~PolyNodeT();
void clear();
void insert(const MonomialT<K>&, const K&);
bool rootNode() const;
bool isZero() const {return (coef==K(0) && child==0);}
void print(std::ostream&) const;
void printTree(std::ostream&, std::string&) const;
string_t varString() const;
```

The most important function is the operator ():

```
K operator()(const K& x, const K& y=K(1), const K& z=K(1)) const;
```

that evaluates the polynomial at a point $(x, y, z)$.

### 3.23.4 The `PolynomialBasisT` class

A space of polynomials (of finite dimension $p$) may be described by one of its basis, say a set of $p$ polynomials. The `PolynomialBasisT` class manages this basis as a list of `PolynomialT` objects. In fact it inherits from std::list<PolynomialT<K> >:

```
template <typename K=real_t>
class PolynomialBasisT : public std::list<PolynomialT<K> >
{public:
    dimen_t dim;        // number of variables in Polynomials
    string_t name;      // basis name
  ...
};
```

There exists some basic constructors from monomials and a general constructor for rather standard polynomial spaces identified by the enumerator `PolynomialSpace`:

```
enum PolynomialSpace {_Pk,_PHk,_Qk,_Qks,_Rk, _SHk,_Dk,_DQk,_DQ2k};

PolynomialBasisT(dimen_t =0, const string_t& ="");
PolynomialBasisT(dimen_t, const MonomialT<K>&, const string_t& na="");
PolynomialBasisT(dimen_t, const MonomialT<K>&, const MonomialT<K>&,
                 const string_t& ="");
PolynomialBasisT(PolynomialSpace, dimen_t, dimen_t, dimen_t =0, dimen_t =0);
void buildPk(dimen_t);
void buildPHk(dimen_t);
void buildQk(dimen_t);
void buildQks(dimen_t , dimen_t =0, dimen_t=0);
void buildTree();
```

The (scalar) polynomial spaces that can be constructed are ($n$ number of variables, $\alpha$ multi-index):

| polynomial space | dimension | XLIFE++ |
|---|---|---|
| $P_k = \left\{ \sum_{\lvert a \rvert \le k} a_\alpha x^\alpha \right\}$ | $C_k^{n+k} = \frac{(n+k)!}{k!\,n!}$ | _Pk |
| $\tilde{P}_k = \left\{ \sum_{\lvert \alpha \rvert = k} a_\alpha x^\alpha \right\}$ | $n=2\ :\ k+1$<br>$n=3\ :\ \frac{1}{2}(k+2)(k+1)$ | _PHk |
| $Q_k = \left\{ \sum_{\alpha_1 \le k, \alpha_2 \le k, \alpha_3 \le k} a_\alpha x^\alpha \right\}$ | $(k+1)^n$ | _Qk |
| $\tilde{Q}_{lmn} = \left\{ \sum_{\alpha_1 \le l, \alpha_2 \le m, \alpha_3 \le n} a_\alpha x^\alpha \right\}$ | $(l+1)(m+1)(n+1)$ | _Qks |

Several functions are devoted to the managment of the list:

```
void push_back(const PolynomialT<K>&);
void add(const MonomialT<K>&);
void add(const PolynomialT<K>&);
void add(const PolynomialBasisT&);
iterator begin();
iterator end();
const_iterator begin() const;
const_iterator end() const;
size_t size() const;
void resize(size_t n);
void clean();
void clean(real_t asZero);
dimen_t degree() const;
void swapVar(dimen_t v1, dimen_t v2, dimen_t v3);
```

The PolynomialsBasisT class is intended to deal with polynomial basis but there is no tool to check independance of polynomials!

It is also possible to evaluate all the polynomials at a point using different ways:

```
std::vector<K>& eval(std::vector<K>& res, const K& x1, const K& x2 = K(1),
                     const K& x3 = K(1)) const;
std::vector<K> eval(const K& x1, const K& x2 = K(1), const K& x3 = K(1)) const;
std::vector<K>& evalTree(std::vector<K>& res, const K& x1, const K& x2 = K(1),
                         const K& x3 = K(1)) const;
std::vector<K> evalTree(const K& x1, const K& x2 = K(1),
                        const K& x3 = K(1)) const;
std::vector<K> operator()(const K& x1, const K& x2 = K(1),
                          const K& x3 = K(1)) const;
std::vector<K>& operator()(std::vector<K>& res, const K& x1, const K& x2 = K(1),
                           const K& x3 = K(1)) const:
```

As usual, there are some print facilities:

```
void print(std::ostream&) const;
friend std::ostream& operator<<(std::ostream&, const PolynomialBasisT<K>& );
```

### 3.23.5 The PolynomialsBasisT class

In finite element approximation, some vector polynomial spaces are required. This is the role of the PolynomialsBasisT class. There is no class to deal with vector polynomial, they are represented by some vector<PolynomialT>. As a consequence, the PolynomialsBasisT class inherits from list<std::vector<PolynomialT<K> > >:

```
template <typename K=real_t>
class PolynomialsBasisT : public std::list<std::vector<PolynomialT<K> > >
{
public:
dimen_t dimVar;           // dimension of Polynomials (number of variables)
dimen_t dimVec;           // dimension of vectors of Polynomials
string_t name;            // basis name
...
};
```

Several constructors are available. Some construct product spaces from PolynomialBasisT objects. There is a general constructor allowing to get particular vector polynomial spaces enumerated in PolynomialSpace:

```
PolynomialsBasisT(dimen_t =0, dimen_t =0, const string_t& ="");
PolynomialsBasisT(const PolynomialBasisT<K>&, dimen_t, const string_t& na="");
PolynomialsBasisT(const PolynomialBasisT<K>&, const PolynomialBasisT<K>&,
                  const string_t& ="");
PolynomialsBasisT(const PolynomialBasisT<K>&, const PolynomialBasisT<K>&,
                  const PolynomialBasisT<K>&, const string_t& na="");
PolynomialsBasisT(PolynomialSpace, dimen_t, dimen_t);
void buildSHk(dimen_t);
void buildRk(dimen_t);
void buildDk(dimen_t);
void buildDQk(dimen_t);
void buildDQ2k(dimen_t);
void buildTree();
```

The following FE spaces are available:

| polynomial space | dimension | XLiFE++ |
|---|---|---|
| $S_k = \{p \in (\tilde{P}_k)^n;\ x.p = 0\}$ | $n \dim \tilde{P}_k - \dim \tilde{P}_{k+1}$ | _Sk |
| $D_k = (P_{k-1})^n \oplus \tilde{P}_{k-1} x$ | $n \dim P_{k-1} + \dim \tilde{P}_{k-1}$ | _Dk |
| $R_k = (P_{k-1})^n \oplus Sk$ | $n \dim P_{k-1} + \dim S_k$ | _Rk |
| $DQk = Q_{k,k-1,k-1} \times Q_{k-1,k,k-1} \times Q_{k-1,k-1,k}$ | $3k(k-1)^2$ | _DQk |
| $DQ2k_{2d} = (P_k)^2 \oplus \mathrm{span}\{\mathrm{curl}\, x_1^{k+1} x_2, \mathrm{curl}\, x_2^{k+1} x_1\}$ | $2(\dim P_k + 1)$ | _DQ2k |

The operator * allows to build tensor polynomials space, say if $P[x_1, x_2]$ and $Q[x_3]$ are two polynomials sets, $(P * Q)[x_1, x_2, x_3]$ is the set:

$$\{p_i(x_1, x_2) q_j(x_3),\ i = 1, m,\ j = 1, n\},$$

```
PolynomialBasisT<K> operator*(const PolynomialBasisT<K>& P,
                              const PolynomialBasisT<K>& Q)
```

Member functions are similar to member functions of the PolynomialBasisT class:

```
void push_back(const std::vector<PolynomialT<K> >&);
void add(const PolynomialT<K>&);
void add(const PolynomialT<K>&, const PolynomialT<K>&);
void add(const PolynomialT<K>&, const PolynomialT<K>&,
         const PolynomialT<K>&);
void add(const std::vector<PolynomialT<K> >&);
void add(const PolynomialsBasisT&);
iterator begin();
iterator end();
const_iterator begin() const;
const_iterator end() const;
size_t size() const;
void resize(size_t);
dimen_t degree() const;
void swapVar(dimen_t, dimen_t, dimen_t);
void clean();
void clean(real_t asZero);

//evaluation of basis
vector<vector<K> >& eval(vector<vector<K> >&, const K&, const K& = K(1),
                         const K& = K(1)) const;
vector<vector<K> >  eval(const K&, const K& = K(1), const K& = K(1)) const;
vector<vector<K> >& evalTree(vector<vector<K> >&, const K&,
                             const K& = K(1), const K& = K(1)) const;
vector<vector<K> >  evalTree(const K&, const K& = K(1), const K& = K(1)) const;
vector<vector<K> >& operator()(vector<vector<K> >&, const K&,
                               const K& = K(1), const K& = K(1)) const;

//print facilities
void print(std::ostream&) const;
friend std::ostream& operator<<(std::ostream&, const PolynomialsBasisT<K>&)
```

| | |
|---|---|
| library : | **utils** |
| header : | **polynomials.hpp** |
| implementation : | **polynomials.hpp** |
| unitary tests : | **test_polynomials.cpp** |
| header dependences : | **config.h, utils.h** |

# 4 The *geometry* library

The *geometry* library collects all the classes and functionalities related to meshes. The main class is the `Mesh` class which handles all stuff to describe a 1D, 2D or 3D mesh. This class provides also basic meshing tools (for simple geometries such as quadrangle, hexahedron, disk, sphere, ...), and import and export tools. The other important class is the `GeomDomain` class, which means geometrical domain, describing parts of mesh, in particular boundaries or parts of boundary. `GeomDomain` objects are involved in integral linear or bilinear forms as integration domain (see the *form* lib). The atomic object of any mesh or geometric domain is the geometric element (`GeomElement` class) which can handle either a full description of a geometric element (`MeshElement` class) or the description of a side of geometric element (say parent elements and side numbers). Note that a side element may also carry a `MeshElement` structure if required; by default it does not.

So the *geometry* library is organized as follows:

`Mesh` class to deal with 1D, 2D or 3D mesh,

`Geometry` class to h andles global geometric data such as bounding box, parametrization,

`GeomDomain` class to deal with geometrical domains (whole computational domain, sub-domains, ...),

`GeomElement` class to deal with elements of a mesh or geometrical domains,

`MeshElement` class handling full description of an element of mesh (nodes, numbering, ...),

`GeomMapData` class storing geometric data (Jacobian matrix of the map to reference element, differential element, normal vector, ...).

The scheme on figure 4.1 shows the organization of the *geometry* library and its interactions with the *space* and *finiteElements* libraries.

## 4.1 Defining geometries

Whatever the geometry is, the common characteristics are a dimension, a shape, a name, a bounding box and a more convenient box for geometry inclusion than the previous one, and easier to define than the convex hull, the so-called "minimal box". This is the reason why we define 3 classes: `BoundingBox`, `MinimalBox` and `Geometry`.

### 4.1.1 `BoundingBox` and `MinimalBox` classes

The bounding box is the smallest box whose faces are parallel to axis containing the geometry. As a segment in 1D, a rectangle in 2D or a parallelepiped in 3D, it can be defined from 2, 3 or 4 points, as illustrated in the following figure:

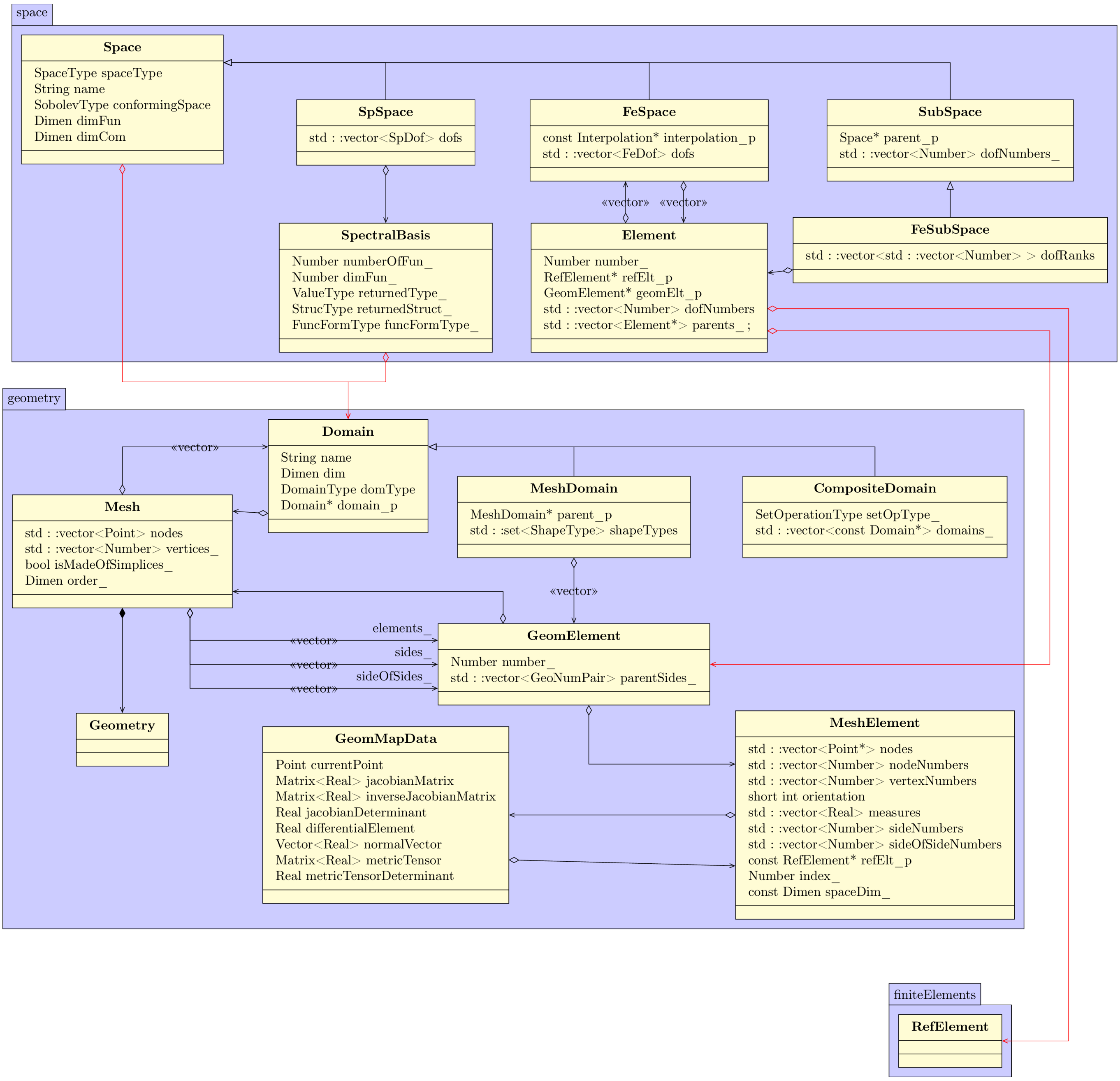

space
Space
SpaceType spaceType
String name
SobolevType conformingSpace
Dimen dimFun
Dimen dimCom
SpSpace
std : :vector<SpDof> dofs
FeSpace
const Interpolation* interpolation_p
std : :vector<FeDof> dofs
SubSpace
Space* parent_p
std : :vector<Number> dofNumbers_
«vector»
«vector»
SpectralBasis
Number numberOfFun_
Number dimFun_
ValueType returnedType_
StrucType returnedStruct_
FuncFormType funcFormType_
Element
Number number_
RefElement* refElt_p
GeomElement* geomElt_p
std : :vector<Number> dofNumbers
std : :vector<Element*> parents_;
FeSubSpace
std : :vector<std : :vector<Number> > dofRanks
geometry
Domain
String name
Dimen dim
DomainType domType
Domain* domain_p
«vector»
Mesh
std : :vector<Point> nodes
std : :vector<Number> vertices_
bool isMadeOfSimplices_
Dimen order_
MeshDomain
MeshDomain* parent_p
std : :set<ShapeType> shapeTypes
CompositeDomain
SetOperationType setOpType_
std : :vector<const Domain*> domains_
«vector»
elements_
«vector»
sides_
«vector»
sideOfSides_
«vector»
GeomElement
Number number_
std : :vector<GeoNumPair> parentSides_
Geometry
GeomMapData
Point currentPoint
Matrix<Real> jacobianMatrix
Matrix<Real> inverseJacobianMatrix
Real jacobianDeterminant
Real differentialElement
Vector<Real> normalVector
Matrix<Real> metricTensor
Real metricTensorDeterminant
MeshElement
std : :vector<Point*> nodes
std : :vector<Number> nodeNumbers
std : :vector<Number> vertexNumbers
short int orientation
std : :vector<Real> measures
std : :vector<Number> sideNumbers
std : :vector<Number> sideOfSideNumbers
const RefElement* refElt_p
Number index_
const Dimen spaceDim_
finiteElements
RefElement

Figure 4.1: *geometry* library organization

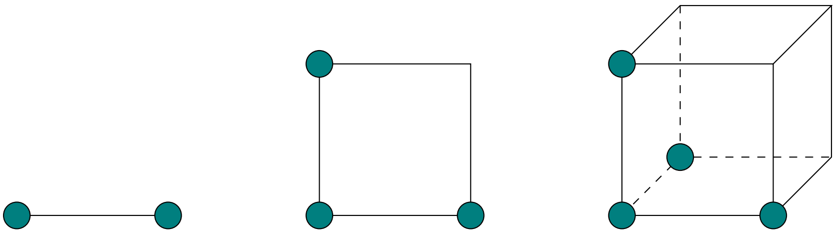


Figure 4.2: Definition of a box from points

For example, if we define a segment whose boundaries are the points $A(0,0,-1)$ and $B(1,2,3)$, the bounding box is $[0;1]\times[0;2]\times[-1;3]$. The `BoundingBox` class is then defined as a vector of pairs of real numbers:

```
typedef std::pair<Real, Real> RealPair;
class BoundingBox
{
  private:
    std::vector<RealPair> bounds_; //!< Bounding values of the box
        [xmin,xmax]x[ymin,ymax]x[zmin,zmax]
```

It offers a various list of constructors, from set of real pairs or set of `Point`:

```
BoundingBox() {}
BoundingBox(const std::vector<RealPair>&);
BoundingBox(Real, Real, Real, Real, Real, Real);
BoundingBox(Real, Real, Real, Real);
BoundingBox(Real, Real);
BoundingBox(const Point&, const Point&, const Point&, const Point&);
BoundingBox(const Point&, const Point&, const Point&);
BoundingBox(const Point&, const Point&);
BoundingBox(const std::vector<Point>& vp);
```

There is also:

- a various list of accessors:

```
std::vector<RealPair> bounds() const; // return bounds in all direction
RealPair bounds(Dimen i) const;    // return bounds in direction i (1 to dim)
RealPair xbounds() const;          // return bounds in first direction
RealPair ybounds() const;          // return bounds in second direction
RealPair zbounds() const;          // return bounds in third direction
Point minPoint() const;            // return the min point (left,bottom,front)
Point maxPoint() const;            // return the max point (right,top,back)
```

- print facilities:

```
void print(std::ostream&) const; // print BoundingBox
String asString() const;         // format as string: [a,b]x[c,d]x[e,f]

std::ostream& operator<<(std::ostream&, const BoundingBox&); //output box
std::ostream& operator<<(std::ostream&, const RealPair&); //output pair of reals
```

- some utility functions, such as merging 2 bounding boxes or giving its dimension:

```
Dimen dim() const; // dimension of the bounding box
BoundingBox& operator +=(const BoundingBox&); // merge a bounding box
```

As the segment example shows, the dimension of the geometry and the dimension of the bounding box are independent. So if we want to check if a geometry is inside another geometry, this is not the right box to use, if we want to be independent of the true shape of the geometry. That is why the `MinimalBox` class is defined:

```
class MinimalBox
{
  protected:
    std::vector<Point> bounds_;
```

You can notice that it is `Point` that are stored, and only the 2, 3 or 4 points necessary to define the box, as shown in Figure 4.2
The `MinimalBox` class offers quite the same constructors as the `BoundingBox` class:

```
MinimalBox() {}
MinimalBox(const std::vector<Point>&);
MinimalBox(const std::vector<RealPair>&);
MinimalBox(Real, Real, Real, Real, Real, Real);
MinimalBox(Real, Real, Real, Real);
MinimalBox(Real, Real);
MinimalBox(const Point&, const Point&, const Point&, const Point&);
MinimalBox(const Point&, const Point&, const Point&);
MinimalBox(const Point&, const Point&);
```

It also offers:

- some accessors:

```
std::vector<Point> bounds() const;
Point boundPt(Dimen i) const; // return bounds in direction i (1 to dim)
Point minPoint() const;
Point maxPoint() const;
```

- print facilities:

```
void print(std::ostream&) const;
String asString() const;


std::ostream& operator<<(std::ostream&, const MinimalBox&); // output MinimalBox
```

- some utility functions, the same as in `BoundingBox`, plus a function to return all vertices of the box, not only the points stored in `bounds_`.

```
Dimen dim() const;
MinimalBox& operator +=(const MinimalBox&);
std::vector<Point> vertices() const;
```

A minimal box of a segment will always be a segment. A minimal box of a 2D plane geometry will always be a rectangle.

Now that both boxes classes are clarified, we can now look at the main class: `Geometry`.

### 4.1.2 The `Geometry` class

A geometry can be of 3 natures: canonical geometries, such as `Rectangle` or `Ball`, so-called "loop" geometries defined by its set of geometrical boundaries, and so-called "composite" geometries defined by union of elementary geometries and holes. The definition of the `Geometry` class takes into account these different natures using inherited classes:

```
enum ShapeType
{
  _noshape=0,
  _point  ,
  _segment, segment=_segment,
  _triangle, triangle=_triangle,
  _quadrangle, quadrangle=_quadrangle,
  _tetrahedron, tetrahedron=_tetrahedron,
  _hexahedron, hexahedron=_hexahedron,
  _prism, prism=_prism,
  _pyramid, pyramid=_pyramid,
  _ellArc, _circArc,_splineArc,_parametrizedArc, _parametrizedSurface,
  _polygon, _parallelogram, _rectangle, _square, _ellipse, _disk, _ellipsoidPart,
  _spherePart,
  _setofelems, _trunkPart, _cylinderPart, _conePart,
  _polyhedron, _parallelepiped, _cuboid, _cube, _ellipsoid, _ball, _trunk,
  _revTrunk, _cylinder, _revCylinder, _cone, _revCone,
  _composite, _loop, _extrusion
};

class Geometry
{
  public:
    BoundingBox boundingBox;
    MinimalBox minimalBox;
    mutable bool force; // tag to force inclusion when geometry engines fails
    mutable bool crackable; // tag to define if the geometry should be cracked or not
  protected:
    string_t domName_;     //geometry name
    Dimen dim_;            //physical space dimension
    ShapeType shape_;      //geometrical shape
    vector<string_t> sideNames_; //names of sides (boundaries)
    vector<string_t> theNamesOfVariables_; // variable names (x,y,z),...
    string_t teXFilename_;  // name of the file containing the tex code
  private:
    mutable map<number_t, Geometry*> components_;// for composite/loop
    map<number_t,vector<number_t> > geometries_; // for composite
    map<number_t,vector<number_t> > loops_;      // for loop geometry
    vector<vector<int_t> > connectedParts_;      // connected parts
    mutable Transformation* extrusion_; // for extrusion geometry
    number_t layers_;                   // for extrusion geometry
  protected:
    Parametrization* parametrization_;    //pointer to parametrization
    Parametrization* boundaryParametrization_; //!pointer to boundary parametrization
```

name and sideNames_ are devoted to store domain names or side domain names. parametrization_ and boundaryParametrization_ are pointers to Parametrization objects that are allocated when building geometries (see particular geometries).

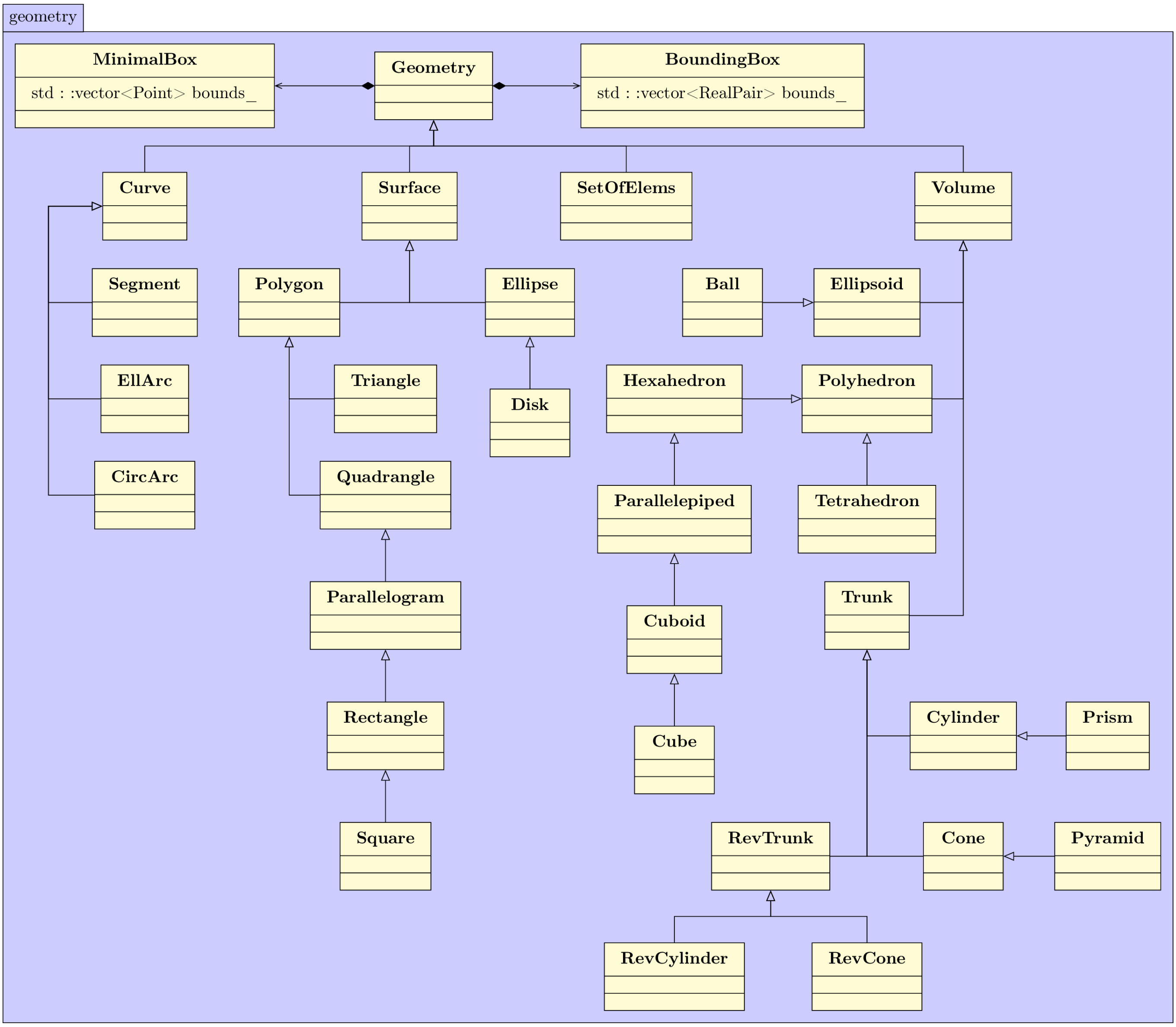


Figure 4.3: Geometry child classes

The Geometry is the base class for a large set of canonical geometries, so the management of "composite" and "loop" geometries implies 2 main vectors of Geometry pointers and a set of virtual functions to cast a Geometry into one of its child:

```
//! access to child Xxxxxxx object (const)
virtual const Xxxxxxx* xxxxxxx() const { error("bad_geometry", name, words("shape",shape_),
    words("shape",_yyyyyyy)); return 0; }
//! access to child Xxxxxxx object
virtual Xxxxxxx* xxxxxxx() { error("bad_geometry", name, words("shape",shape_),
    words("shape",_yyyyyyy)); return 0; }
```

xxxxxxx must be one of the following keyword: segment, ellArc, circArc, splineArc, parametrizedArc, polygon, triangle, quadrangle, parallelogram, rectangle, square, ellipse, disk, polyhedron, tetrahedron, hexahedron, parallelepiped, cuboid, cube, ellipsoid, ball, revTrunk, trunk, cylinder, revCylinder, prism, cone, revCone, pyramid, setOfElems
yyyyyyy must be the corresponding ShapeType item.

Geometry manages also some additional data if useful : cracking and extrusion data, parametrization data (pointers to Parametrization objects). Parametrizations are automatically set for canonical geometries and are not defined for composite geometries. The Geometry class offers constructors from BoundingBox, dimension or both:

```
Geometry(): force(false), crackable(false), domName_(""), dim_(0), shape_(_noshape),
    extrusion_(0), layers_(0) { sideNames_.resize(0); }  // void constructor
Geometry(const Geometry& g);                             // copy constructor
// basic constructor from bounding box
Geometry(const BoundingBox&, const string_t& na = "?", ShapeType sht=_noshape,
     const string_t& nx = "x", const string_t& ny = "y", const string_t& nz = "z");
Geometry(const BoundingBox&, dimen_t, const string_t& na = "?",
     ShapeType sht=_noshape, const string_t& nx = "x", const string_t& ny = "y",
     const string_t& nz = "z");
Geometry(dimen_t, const string_t& na = "?", ShapeType sht=_noshape,
     const string_t& nx = "x", const string_t& ny = "y", const string_t& nz = "z");
virtual ~Geometry()  {}
```

It also offers:

- some accessors:

```
dimen_t dim() const;
ShapeType shape() const;
void shape(ShapeType sh);
string_t domName() const;
void domName(const string_t& nm);
string_t teXFilename() const;
void teXFilename(const string_t& fn);
const std::vector<string_t> sideNames() const;
std::vector<string_t> sideNames();
std::map<number_t, Geometry*> components();
const std::map<number_t, Geometry*> components() const;
const std::map<number_t, std::vector<number_t> > geometries() const;
std::map<number_t, std::vector<number_t> > loops() const;
number_t layers() const;
Transformation* extrusion();
const Transformation* extrusion() const;
```

- some print facilities:

```
void print(std::ostream&) const;             //!< print Geometry
friend std::ostream& operator<<(std::ostream&, const Geometry&); //!< output Geometry
```

- some functions to compute or update boxes:

```
virtual void computeMB(); //! compute the minimal box
void updateBB(const std::vector<RealPair>& bb) {boundingBox = BoundingBox(bb);}
```

  As the minimal box depends on the true shape of the geometry, it is a virtual function reimplemented in child classes.

- some virtual functions to get data from canonical geometries, such as the vector of points defining the geometry, or the parameters for the subdivision mesh algorithm:

```
virtual std::vector<const Point*> boundNodes() const;
virtual std::vector<Point*> nodes();
virtual std::vector<const Point*> nodes() const;
virtual std::vector<std::pair<ShapeType,std::vector<const Point*> > > curves() const;
virtual std::vector<std::pair<ShapeType,std::vector<const Point*> > > surfs() const;
```

- member functions to determine if a geometry is coplanar to another geometry or inside another geometry, and external functions or operators to define "composite", "loop" or "extrusions" geometries.

```
bool isCoplanar(const Geometry& g) const;
bool isInside(const Geometry&) const; //check if geometry is inside an other one

friend Geometry operator+(const Geometry&, const Geometry&); //union
Geometry& operator+=(const Geometry&);
friend Geometry operator-(const Geometry&, const Geometry&); //difference (hole)
Geometry& operator-=(const Geometry&);

// definition of a geometry 2D/3D from its boundary 1D/2D
friend Geometry surfaceFrom(const Geometry&, String name = "");
friend Geometry volumeFrom(const Geometry&, String name = "");
friend Geometry extrude(const Geometry& g, const Transformation& t, number_t layers, string_t
    domName, std::vector<string_t> sidenames);
friend Geometry extrude(const Geometry& g, const Transformation& t, number_t layers,
    std::vector<string_t> sidenames);
```

Operators + and - work as follows:

- if both arguments are canonical geometries (neither "composite" nor "loop"), it puts pointers to them in the components_ attribute and if one geometry is inside the other, it puts it in the geometries attribute.
- If at least one of the argument is "composite" or "loop", it inserts the canonical geometry correctly, or merge the 4 maps.

surfaceFrom and volumeFrom allow to define surfaces and respectively volumes from their boundaries, so-called "loop" geometries. The mechanism is the same: taking a "composite" geometry as argument, it puts every component in the borders_ attribute and defines the loop in the loops_ attribute, so that we can define "composite" geometries of "loop" geometries, but it is for the moment forbidden.

### 4.1.3 Curve, Surface and Volume classes

The Curve class is the base class for every canonical 1D geometry. It has no attributes and only general constructors:

```
class Curve: public Geometry
{
  public:
    Curve();
  protected:
    void buildParam(const Parameter& p);
    void buildDefaultParam(ParameterKey key);
    std::set<ParameterKey> getParamsKeys();
  public:
    Curve(const Curve& c): Geometry(c) {} //!< copy constructor
    virtual Geometry* clone() const { return new Curve(*this); } //!< virtual copy constructor
        for Geometry
    virtual ~Curve() {} //!< virtual destructor
};
```

The Surface class is the base class for every canonical 2D geometry. Actually, it has no attributes and only constructors:

```
class Surface: public Geometry
{
  public:
    //! default constructor for 2D geometries
    Surface();

  protected:
    void buildParam(const Parameter& p);
    void buildDefaultParam(ParameterKey key);
    std::set<ParameterKey> getParamsKeys();

  public:
    Surface(const Surface& s): Geometry(s) {} //!< copy constructor
    virtual Geometry* clone() const { return new Surface(*this); } //!< virtual copy constructor
        for Geometry
    virtual Surface* cloneS() const { return new Surface(*this); } //!< virtual copy constructor
        for Surface
    virtual ~Surface() {} //!< virtual destructor

    virtual std::vector<Point> p() const
    { error("not_yet_implemented","std::vector<Point> Surface::p() const"); return
        std::vector<Point>(); }
    virtual std::vector<number_t> n() const
    { error("not_yet_implemented","std::vector<Point> Surface::n() const"); return
        std::vector<number_t>(); }
    virtual Point p(number_t i) const
    { error("not_yet_implemented","Point Surface::p(Number i) const"); return Point(); }
    virtual number_t n(number_t i) const
    { error("not_yet_implemented","Number Surface::n(Number i) const"); return 0; }
    virtual number_t& n(number_t i)
    { error("not_yet_implemented","Number& Surface::n(Number i)"); return *new number_t(0); }
    virtual std::vector<real_t> h() const
    { error("not_yet_implemented","std::vector<Real> Surface::h() const"); return
        std::vector<real_t>(); }
    virtual real_t h(number_t i) const
    { error("not_yet_implemented","Number Surface::h(Number i) const"); return 0.; }
    virtual real_t& h(number_t i)
    { error("not_yet_implemented","Number& Surface::h(Number i)"); return *new real_t(0); }

    bool isPolygon()
    {
      if (shape_ == _polygon || shape_ == _triangle || shape_ == _quadrangle || shape_ ==
          _parallelogram || shape_ == _rectangle ||
          shape_ == _square) { return true; }
      return false;
    }

    //! format as string
    virtual string_t asString() const { error("shape_not_handled", words("shape",shape_)); return
        string_t(); }
};
```

The `Volume` class is the base class for every canonical 3D geometry. Actually, it has no attributes and only constructors:

```
class Volume: public Geometry
{
  public:
    //! default constructor for 3D geometries
    Volume();

  protected:
    void buildParam(const Parameter& p);
    void buildDefaultParam(ParameterKey key);
    std::set<ParameterKey> getParamsKeys();

  public:
    Volume(const Volume& v): Geometry(v) {} //!< copy constructor
    virtual Geometry* clone() const { return new Volume(*this); } //!< virtual copy constructor
        for Geometry
    virtual ~Volume() {} //!< virtual destructor
    //! format as string
    virtual string_t asString() const { error("shape_not_handled", words("shape",shape_)); return
        string_t(); }
};
```

### 4.1.4 The key-value system

All constructors for classes defining canonical geometries are written in the same way: with `Parameter` arguments, so that the user can use a key-value system. Some keys are easy to determine: the center for rectangles, squares, ellipses, disks, cuboids, cubes, ellipsoids and balls, the radius for disks, balls, and cylinders, .... To do so, global keys are defined (type `Parameter`). Here is the list of available keys with authorized data types and classes using them:

| *key* | *authorized types* | *involved classes* |
|---|---|---|
| **_angle1** | single integer or real value | class `Ellipse`, `Disk` |
| **_angle2** | single integer or real value | class `Ellipse`, `Disk` |
| **_apex** | single integer or real value, or `Point` | classes `Cone`, `Pyramid`, `RevCone` |
| **_apogee** | single integer or real value, or `Point` | class `EllArc` |
| **_basis** | classes `Polygon`, `Triangle`, `Quadrangle`, `Parallelogram`, `Rectangle`, `Square`, `Ellipse`, `Disk` | classes `Trunk`, `Cylinder`, `Prism`, `Cone`, `Pyramid` |
| **_center** | single integer or real value, or `Point` | classes `EllArc`, `CircArc`, `Rectangle`, `Square`, `Ellipse`, `Disk`, `Cuboid`, `Cube`, `Ellipsoid`, `Ball`, `RevCone` |
| **_center1** | single integer or real value, or `Point` | classes `Trunk`, `Cylinder`, `Cone`, `RevTrunk`, `RevCylinder` |
| **_center2** | single integer or real value, or `Point` | classes `Trunk`, `Cylinder`, `RevTrunk`, `RevCylinder` |
| **_degree** | single unsigned integer | class `SplineArc` |
| **_direction** | std::vector of real values or `Point` | classes `Cylinder`, `Prism` |
| **_domain_name** | single string | every class |
| **_end_shape** | enum `GeometricEndShape` | class `RevCone` |
| **_end1_shape** | enum `GeometricEndShape` | classes `RevTrunk`, `RecCylinder` |
| **_end2_shape** | enum `GeometricEndShape` | classes `RevTrunk`, `RecCylinder` |
| **_end_distance** | single unsigned integer or real positive value | class `RevCone` |
| **_end1_distance** | single unsigned integer or real positive value | classes `RevTrunk`, `RecCylinder` |
| **_end2_distance** | single unsigned integer or real positive value | classes `RevTrunk`, `RecCylinder` |
| **_faces** | vector of `Polygon` | class `Polyhedron` |
| **_hsteps** | single real value, std::vector of real values or `Reals` | every class but `Polyhedron` |
| **_length** | single unsigned integer or real positive value | classes `Square`, `Cube` |
| **_nboctants** | single unsigned integer value | classes `Parallelepiped`, `Cuboid`, `Cube`, `Ellipsoid`, `Ball` |
| **_nbParts**<br>**_nbsubdomains** | single unsigned integer value<br>single unsigned integer value | classes `ParametrizedArc`<br>classes `RevTrunk`, `RevCylinder`, `RevCone` |
| **_nnodes** | single unsigned integer value, std::vector of integer values or `Numbers` | every class but `Polyhedron` |
| **_origin** | single integer or real value, or `Point` | classes `Rectangle`, `Square`, `Cuboid`, `Cube`, `Trunk`, `Cylinder`, `Prism` |

| | | |
|---|---|---|
| **_parametrization** | Parametrization | ParametrizedArc |
| **_partitioning** | enum Partitioning | ParametrizedArc |
| **_radius** | single unsigned integer or real positive value | classes Disk, Ball, RevCylinder, RevCone |
| **_radius1** | single unsigned integer or real positive value | class RevTrunk |
| **_radius2** | single unsigned integer or real positive value | class RevTrunk |
| **_scale** | single unsigned integer or real positive value | class Trunk |
| **_side_names** | single string or std::vector of strings | every class but Polyhedron |
| **_spline** | Spline | class SplineArc |
| **_splineBC** | enum SplineBC | class SplineArc |
| **_spline_parametrization** | enum SplineParametrization | class SplineArc |
| **_spline_type** | enum SplineType | class SplineArc |
| **_tangent_0** | vector of reals | classes SplineArc |
| **_tangent_1** | vector of reals | classes SplineArc |
| **_tmin** | single integer or real value | classes SplineArc, ParametrizedArc |
| **_tmax** | single integer or real value | classes SplineArc, ParametrizedArc |
| **_type** | single unsigned integer value | classes Ellipse, Disk, Ellipsoid, Ball, RevTrunk, RevCylinder, RevCone |
| **_varnames** | single string or std::vector of strings | every class |
| **_vertices** | vector of Point | classes Polygon, SplineArc |
| **_v1** | single integer or real value, or Point | every class, but Polygon, Polyhedron, RevTrunk, RevCylinder, RevCone |
| **_v2** | single integer or real value, or Point | every class, but Polygon, Polyhedron, RevTrunk, RevCylinder, RevCone |
| **_v3** | single integer or real value, or Point | classes Triangle, Quadrangle, Tetrahedron, Hexahedron, Prism, Pyramid |
| **_v4** | single integer or real value, or Point | classes Quadrangle, Parallelogram, Rectangle, Square, Tetrahedron, Hexahedron, Parallelepiped, Cuboid, Cube, Pyramid |
| **_v5** | single integer or real value, or Point | classes Hexahedron, Parallelepiped, Cuboid, Cube |
| **_v6** | single integer or real value, or Point | class Hexahedron |
| **_v7** | single integer or real value, or Point | class Hexahedron |
| **_v8** | single integer or real value, or Point | class Hexahedron |
| **_weights** | real or a vector of reals | classes SplineArc |
| **_xlength** | single unsigned integer or real positive value | classes Rectangle, Ellipse, Cuboid, Ellipsoid |
| **_xmin** | single integer or real value | classes Rectangle, Cuboid |
| **_xmax** | single integer or real value | classes Rectangle, Cuboid |
| **_ylength** | single unsigned integer or real positive value | classes Rectangle, Ellipse, Cuboid, Ellipsoid |
| **_ymin** | single integer or real value | classes Rectangle, Cuboid |
| **_ymax** | single integer or real value | classes Rectangle, Cuboid |
| **_zlength** | single unsigned integer or real positive value | class Cuboid |
| **_zmin** | single integer or real value | class Cuboid |
| **_zmax** | single integer or real value | class Cuboid |

A constructor of a geometry will take several Parameter object and transfer the building work to the 3 main following routines:

```
// main function to build a geometry
void build(const std::vector<Parameter>& ps);
// build the list of available keys
std::set<ParameterKey> getParamsKeys();
// deal with one key and do the appropriate work
void buildParam(const Parameter& gp);
// deal with unused keys having default values and do the appropriate work
void buildDefaultParam(ParameterKey key);
```

For some geometries, there are some additional routines called by `build`.

### 4.1.5 Parametrization management

A `Parametrization` object (`parametrization_` pointer ) is attached to every canonical geometry (say CG) in the following way. For each canonical geometry, two member functions computing the parametrization and its inverse are defined

```
Vector<real_t> funParametrization(const Point& pt, Parameters& pars, DiffOpType d=_id) const;
Vector<real_t> invParametrization(const Point& pt, Parameters& pars, DiffOpType d=_id) const;
```

and two extern functions (inline) calling these member functions are also defined :

```
Vector<real_t> parametrization_CG(const Point& pt,Parameters& pars,DiffOpType d=_id)
{return reinterpret_cast<const CG*>
       (pars("geometry").get_p())->funParametrization(pt,pars,d);}
Vector<real_t> invParametrization_CG(const Point& pt,Parameters& pars,DiffOpType d=_id)
{return reinterpret_cast<const CG*>
        (pars("geometry").get_p())->invParametrization(pt,pars,d);}
```

Then, constructors of canonical geometry build the `Parametrization` object relating the above functions:

```
Parameters pars(reinterpret_cast<const void *>(this),"geometry");
parametrization_ = new Parametrization(tmin, tmax, parametrization_CG,
                                       pars,"CG parametrization");
parametrization_->setinvParametrization(invParametrization_CG);
```

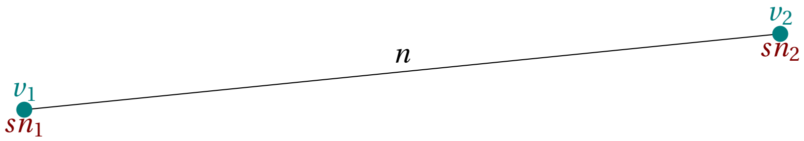
There is a wrapper from member functions to extern functions because `Parametrization` class deals with extern functions but for same arguments, the signature of a member function differs from of an extern function !

By construction, parameter intervals of geometry parametrizations are always $[0,1]$ even if the true parametrizations have other bounds.

### 4.1.6 The `Segment` class

A segment is just a straight line between 2 points, with a number of nodes.

```
class Segment: public Curve
{
  private:
    Point p1_, p2_;
    Number n_;
    std::vector<real_t> h_;
```



It offers constructors, taking from 2 to 5 `Parameter`. Authorized keys and what they do are:

| attribute | key to use to define it | optional | default value |
|---|---|---|---|
| p1_, p2_ | (**_v1**, **_v2**) | no | no |
| n_ | **_nnodes** | yes | 2 |
| | or (**_xmin**, **_xmax**) | | |
| n_ | **_nnodes** | yes | 2 |
| h_ | **_hsteps** | yes | no |
| domName_ | **_domain_name** | yes | "" |
| sideNames_ | **_side_names** | yes | "" |

It also offers:

- some accessors
- implementation of inherited virtual functions concerning segments:

```
virtual void computeMB();
virtual std::vector<Point*> nodes();
virtual std::vector<const Point*> nodes() const;
virtual std::vector<std::pair<ShapeType,std::vector<const Point*> > > curves() const;
```

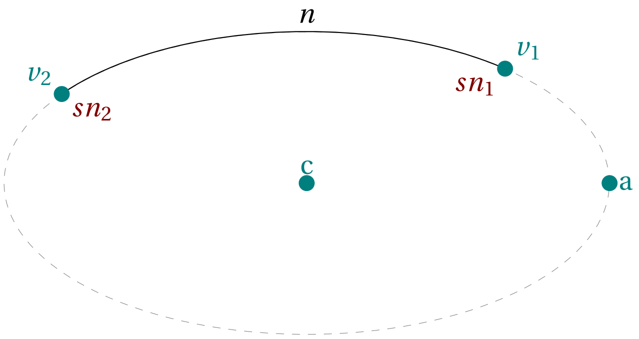
The parametrization is the following :

$$t \in [0,1] \to (1-t)p_1 + tp_2.$$

### 4.1.7 The `EllArc` class

To define an elliptic arc, you need 4 points: the center of the ellipse, a point on the main axis (apogee) and the bounds of the arc. When omitted, the apogee point is defined as the first bound of the arc. An elliptic arc must be smalller than a half-ellipse, to be defined correctly. This is a GMSH restriction. We also store the second apogee deduced from the four previour points and the angles corresponding to the bounds of the arc.

```
class EllArc : public Curve
{
  protected:
    Point c_, a_, b_, p1_, p2_;
    real_t thetamin_, thetamax_;
    number_t n_;
    std::vector<real_t> h_;
```



It offers constructors, taking from 3 to 7 `Parameter`. Authorized keys and what they do are:

| attribute | key to use to define it | optional | default value |
|---|---|---|---|
| c_, a_, p1_, p2_ | (**_center**, **_apogee**, **_v1**, **_v2**)<br>or (**_center**, **_v1**, **_v2**) | no | no |
| n_ | **_nnodes** | yes | 2 |
| h_ | **_hsteps** | yes | no |
| domName_ | **_domain_name** | yes | "" |
| sideNames_ | **_side_names** | yes | "" |

It also offers:

- some accessors
- implementation of inherited virtual functions concerning elliptic arcs:

```
virtual void computeMB();
virtual std::vector<Point*> nodes();
virtual std::vector<const Point*> nodes() const;
virtual std::vector<std::pair<ShapeType,std::vector<const Point*> > > curves() const;
```

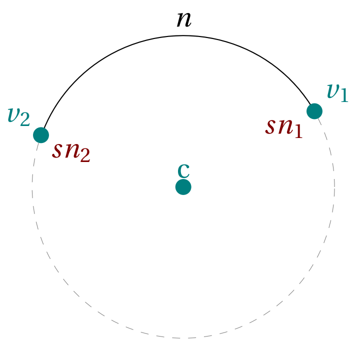
The parametrization is the following :

$$t \in [0,1] \to c + (a-c)\cos\theta + (b-c)\sin\theta \text{ with } \theta = (1-t)\theta_{min} + t\theta_{max}.$$

### 4.1.8 The `CircArc` class

To define a circular arc, you need 3 points: the center of the circle and the bounds of the arc. A circular arc must be smalller than a half-circle, to be defined correctly. This is a GMSH restriction. We consider the first bound as the first apogee of the arc and we also store the second apogee deduced from the four previour points and the angles corresponding to the bounds of the arc (the first one will always be 0):

```
class CircArc : public Curve
{
  protected:
    Point c_, a_, b_, p1_, p2_;
    real_t thetamin_, thetamax_;
    number_t n_;
    std::vector<real_t> h_;
```



It offers constructors, taking from 3 to 6 `Parameter`. Authorized keys and what they do are:

| attribute | key to use to define it | optional | default value |
|---|---|---|---|
| c_, p1_, p2_ | **_center**, **_v1** and **_v2** | no | no |
| n_ | **_nnodes** | yes | 2 |
| h_ | **_hsteps** | yes | no |
| domName_ | **_domain_name** | yes | "" |
| sideNames_ | **_side_names** | yes | "" |

It also offers:

- some accessors
- implementation of inherited virtual functions concerning circular arcs:

```
virtual void computeMB();
virtual std::vector<Point*> nodes();
virtual std::vector<const Point*> nodes() const;
virtual std::vector<std::pair<ShapeType,std::vector<const Point*> > > curves() const;
```

The parametrization is the following ($a$, $b$ the first and second apogee built from $p_1$ and $c$):

$$t \in [0,1] \to c + (a-c)\cos\theta + (b-c)\sin\theta \text{ with } \theta = (1-t)\theta_{min} + t\theta_{max}.$$

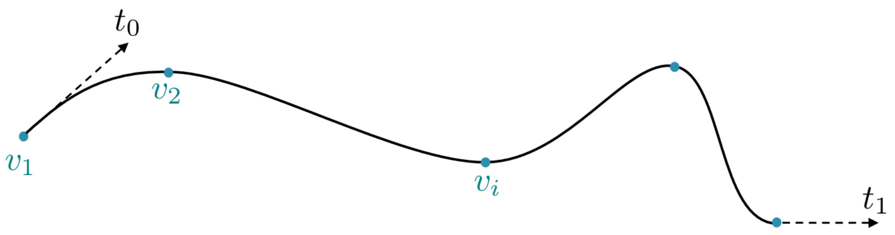
### 4.1.9 The SplineArc class

A spline arc is an arc build from a spline, either a C2-spline, a Catmull-Rom spline, a Bezier curve or a B-spline (see Spline class)

```
class SplineArc: public Curve
{
private:
  Spline* spline_;          //spline pointer
  number_t n_;              //number of nodes
  std::vector<real_t> h_;   //local steps
```

A spline arc may be constructed straightforward from a Spline object or giving spline characteristics. Authorized keys and what they do are:

| attribute | key to use to define it | optional | default value |
|---|---|---|---|
| spline_ | **_spline** | exclusive | no |
| spline_→controlPoints_ | **_vertices** | no | no |
| spline_→type_ | _spline_type | no | no |
| spline_→degree_ | _degree | yes | 3 |
| spline_→bcs_ (bce_) | _splineBC | yes | context |
| spline_→tau_ | _tension | yes (Catmull-Rom spline) | 0.5 |
| spline_→weights_ | _weights | yes (B-spline) | $(1,\dots,1)$ |
| spline_→splinePar_ | _spline_parametrization | yes | uniform |
| spline_→yp0_ | _tangent_0 | yes | $(0,0,0)$ |
| spline_→yp1_ | _tangent_1 | yes | $(0,0,0)$ |
| n_ | **_nnodes** | yes | 2 |
| h_ | **_hsteps** | yes | no |
| domName_ | **_domain_name** | yes | "" |
| sideNames_ | **_side_names** | yes | "" |



Interpolating spline

The parametrization of a spline arc is given by the spline parametrization (see section Spline).

- The standard factory of Gmsh does not support the C2-spline. It is available in OpenCascad machinery of Gmsh which is not yet addressed by XLiFE++.
- By definition, the degree of a Bezier spline is equal to the number of control points minus one. XLiFE++ is compliant with this definition but Gmsh is not. A Bezier curve in Gmsh is a union of Bezier curves of degree 3 with several drawbacks : the curve is C0 but not necessary C1 and the number of points must be of the form $3k+1$. So, if you intend to generate a mesh with Gmsh, only Bezier spline of degree 3 with 4 control points are authorized. However, if you want to use multiple Bezier curves of degree 3, it is possible by concatenating several `SplineArc` built from Bezier spline of degree 3.

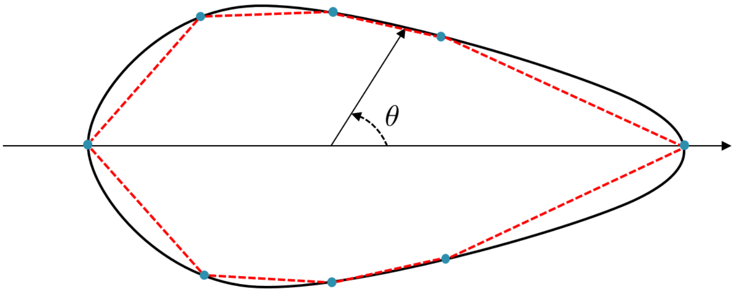
### 4.1.10 The `ParametrizedArc` class

Parametrized arc are defined from a function

$$q(t):\ t \in [t_{min}, t_{max}] \to \mathbb{R}^d \quad (d = 2 \text{ or } d = 3)$$

given either as a C++ function or a symbolic function (see `Parametrization` class). A `Parametrized` object will be mandatory constructed from a `Parametrization` object.
Because Gmsh does not support parametrized arc, additional data related to the way the parametrized arc is split into entities supported by Gmsh (segment and spline), are managed.
When applying linear transformation to a geometry (see `Transformation` class), for most of geometries, it induces only the change of points defining the geometry. But for a parametrized arc, as there is no point of construction (only a function to build points), the linear transformation has to be memorized and applied after each calling of the parametrization function.

```
Parametrization* arc_parametrization_; //Parametrization pointer (must be allocated)
real_t tmin_, tmax_;                   //bounds of parameter t
Point p1_, p2_;                        //vertices of the arc
Partitioning partitioning_;            //partitioning type (_linearPartition or _part_spline)
number_t nbParts_;                     //number of partitions (>0)
vector<Point> p_;                      //vertices of the arc
number_t n_;                           //number of nodes on the ParametrizedArc
vector<real_t> h_;                     //local steps on vertices
Transformation* transformation_;       //pointer to an additional transformation
```



Linear partition of the parametrized arc (nbParts_=8)

A parametrized arc is mandatory constructed from a `Parametrization` object. Authorized keys and what they do are:

| attribute | key to use to define it | optional | default value |
|---|---|---|---|
| spline_ | **_spline** | exclusive | no |
| arc_parametrization_ | **_parametrization** | yes | no |
| tmin_ | _tmin_type | no | no |
| tmax_ | _tmax | yes | 3 |
| partitioning_ | _partitioning | yes | _part_linear |
| nbParts_ | _nbParts | yes | 2 |

| attribute | key to use to define it | optional | default value |
|---|---|---|---|
| n_ | **_nnodes** | yes | 2 |
| h_ | **_hsteps** | yes | no |
| domName_ | **_domain_name** | yes | "" |
| sideNames_ | **_side_names** | yes | "" |

The `Parametrization` object managed by the `Geometry` is an interface to the true `Parametrization` object. Be cautious, its parameter interval is $[0,1]$ and not $[t_{min}, t_{max}]$!

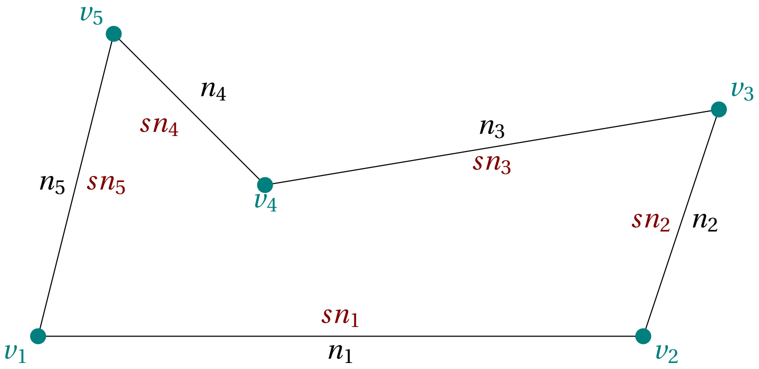
To be consistant with all parametrizations, the parametrization of a Parametrized arc is defined as

$$t \in [0,1] \to q((1-t)\, t_{min} + t\, t_{max}).$$

### 4.1.11 The `Polygon` class

To define a polygon, you give the ordered list of vertices.

```
class Polygon : public Surface
{
  protected:
    std::vector<Point> p_;
    std::vector<real_t> h_;
    std::vector<number_t> n_;
```



It offers constructors, taking from 1 to 4 `Parameter`. Authorized keys and what they do are:

| attribute | key to use to define it | optional | default value |
|---|---|---|---|
| p_ | **_vertices** | no | no |
| n_ | **_nnodes** | yes | 2 |
| h_ | **_hsteps** | yes | no |
| domName_ | **_domain_name** | yes | "" |
| sideNames_ | **_side_names** | yes | "" |

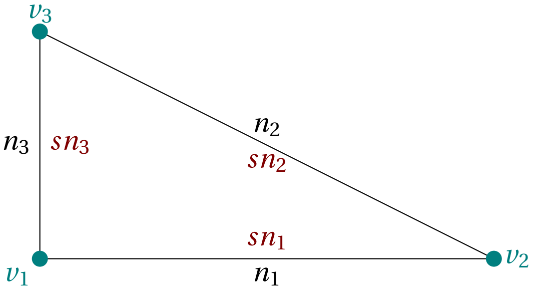
It also offers:

- some accessors
- implementation of inherited virtual functions concerning polygon:

```
virtual void computeMB();
virtual std::vector<const Point*> boundNodes() const;
virtual std::vector<Point*> nodes();
virtual std::vector<const Point*> nodes() const;
virtual std::vector<std::pair<ShapeType,std::vector<const Point*> > > curves() const;
virtual std::vector<std::pair<ShapeType,std::vector<const Point*> > > surfs() const;
```

### 4.1.12 The `Triangle` class

To define a triangle, you give the 3 vertices.



It offers constructors, taking from 3 to 6 `Parameter`. Authorized keys and what they do are:

| attribute | key to use to define it | optional | default value |
|---|---|---|---|
| p_ | **_v1**, **_v2** and **_v3** | no | no |
| n_ | **_nnodes** | yes | 2 |
| h_ | **_hsteps** | yes | no |
| domName_ | **_domain_name** | yes | "" |
| sideNames_ | **_side_names** | yes | "" |

It also offers:

- some accessors
- implementation of inherited virtual functions concerning triangles:

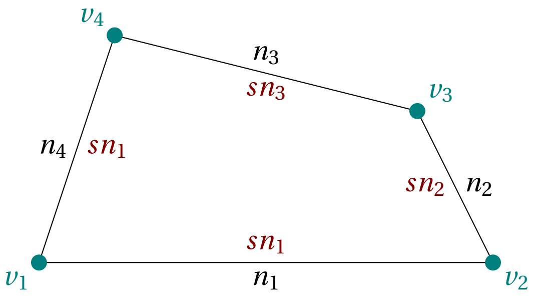
```
virtual void computeMB();
virtual std::vector<const Point*> boundNodes() const;
virtual std::vector<Point*> nodes();
virtual std::vector<const Point*> nodes() const;
virtual std::vector<std::pair<ShapeType,std::vector<const Point*> > > curves() const;
virtual std::vector<std::pair<ShapeType,std::vector<const Point*> > > surfs() const;
```

The parametrization is the following :

$$u \in [0,1],\ v \in [0,1-u] \to (1-u-v)\,p_1 + u\,p_2 + v\,p_3.$$

### 4.1.13 The `Quadrangle` class

To define a quadrangle, you give the 4 vertices.



It offers constructors, taking from 4 to 7 `Parameter`. Authorized keys and what they do are:

| attribute | key to use to define it | optional | default value |
|---|---|---|---|
| p_ | **_v1**, **_v2**, **_v3** and **_v4** | no | no |
| n_ | **_nnodes** | yes | 2 |
| h_ | **_hsteps** | yes | no |
| domName_ | **_domain_name** | yes | "" |
| sideNames_ | **_side_names** | yes | "" |

It also offers:

- some accessors
- implementation of inherited virtual functions concerning quadrangles:

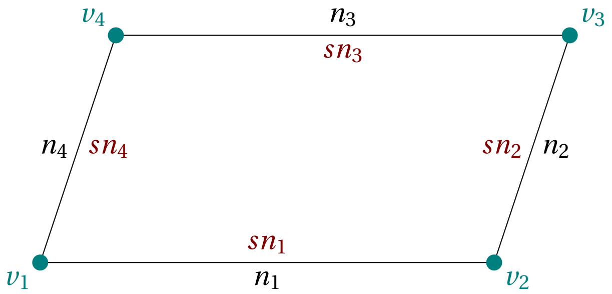
```
virtual void computeMB();
virtual std::vector<const Point*> boundNodes() const;
virtual std::vector<Point*> nodes();
virtual std::vector<const Point*> nodes() const;
virtual std::vector<std::pair<ShapeType,std::vector<const Point*> > > curves() const;
virtual std::vector<std::pair<ShapeType,std::vector<const Point*> > > surfs() const;
```

The parametrization is the following :

$$(u,v) \in [0,1]\times[0,1] \to (1-u-v)\,p_1 + u\,p_2 + v\,p_3 - u\,v\,(p_2 - p_1 + p_4 - p_3).$$

### 4.1.14 The Parallelogram class

To define a parallelogram, you give 3 vertices. $p_3$ is indeed unnecessary. It can be calculated from the 3 other vertices.



It offers constructors, taking from 3 to 6 Parameter. Authorized keys and what they do are:

| attribute | key to use to define it | optional | default value |
|---|---|---|---|
| p_ | **_v1, _v2** and **_v4** | no | no |
| n_ | **_nnodes** | yes | 2 |
| h_ | **_hsteps** | yes | no |
| domName_ | **_domain_name** | yes | "" |
| sideNames_ | **_side_names** | yes | "" |

It also offers:

- some accessors
- implementation of inherited virtual functions concerning parallelograms:

```
virtual void computeMB();
virtual std::vector<const Point*> boundNodes() const;
virtual std::vector<Point*> nodes();
virtual std::vector<const Point*> nodes() const;
virtual std::vector<std::pair<ShapeType,std::vector<const Point*> > > curves() const;
virtual std::vector<std::pair<ShapeType,std::vector<const Point*> > > surfs() const;
```

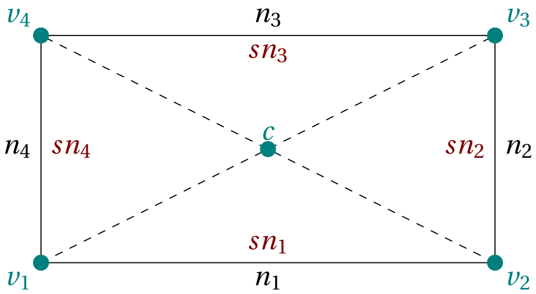
The parametrization is the following :

$$(u,v) \in [0,1]\times[0,1] \to (1-u-v)\,p_1 + u\,p_2 + v\,p_4.$$

### 4.1.15 The Rectangle class

To define a rectangle, you give 3 vertices, as for Parallelogram. You can also give the center (or the origin) and the lengths, or you can gives bounds. To store temporarily these values, the Rectangle class has internal attributes.

```
class Rectangle: public Parallelogram
{
  protected:
    Point center_, origin_;
    bool isCenter_, isOrigin_;
    real_t xlength_, ylength_;
  private:
    real_t xmin_, xmax_, ymin_, ymax_;
    bool isBounds_;
```



It offers constructors, taking from 3 to 7 Parameter. Authorized keys and what they do are:

| attribute | key to use to define it | optional | default value |
|---|---|---|---|
| p_ | (**_v1**, **_v2**, **_v4**)<br>or (**_center**, **_xlength**, **_ylength**)<br>or (**_origin**, **_xlength**, **_ylength**)<br>or (**_xmin**, **_xmax**, **_ymin**, **_ymax**) | no | no |
| n_ | **_nnodes** | yes | 2 |
| h_ | **_hsteps** | yes | no |
| domName_ | **_domain_name** | yes | "" |
| sideNames_ | **_side_names** | yes | "" |

It also offers:

- some accessors
- implementation of inherited virtual functions concerning rectangles:

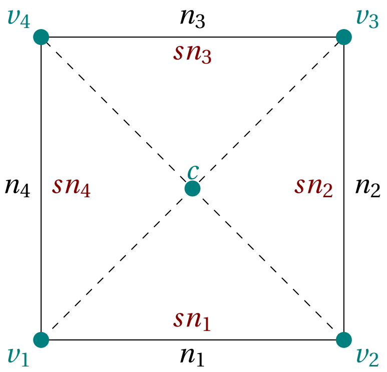
```
virtual void computeMB();
virtual std::vector<const Point*> boundNodes() const;
virtual std::vector<Point*> nodes();
virtual std::vector<const Point*> nodes() const;
virtual std::vector<std::pair<ShapeType,std::vector<const Point*> > > curves() const;
virtual std::vector<std::pair<ShapeType,std::vector<const Point*> > > surfs() const;
```

The parametrization (inherited from Parallelogram) is the following :

$$(u,v) \in [0,1]\times[0,1] \to (1-u-v)\,p_1 + u\,p_2 + v\,p_4.$$

### 4.1.16 The Square class

To define a square, you give 3 vertices. You can also give the center (or the origin) and the length.



It offers constructors, taking from 2 to 6 Parameter. Authorized keys and what they do are:

| attribute | key to use to define it | optional | default value |
|---|---|---|---|
| p_ | (**_v1**, **_v2**, **_v4**)<br>or (**_center**, **_xlength**, **_ylength**)<br>or (**_origin**, **_xlength**, **_ylength**) | no | no |
| n_ | **_nnodes** | yes | 2 |
| h_ | **_hsteps** | yes | no |
| domName_ | **_domain_name** | yes | "" |
| sideNames_ | **_side_names** | yes | "" |

It also offers:

- some accessors
- implementation of inherited virtual functions concerning squares:

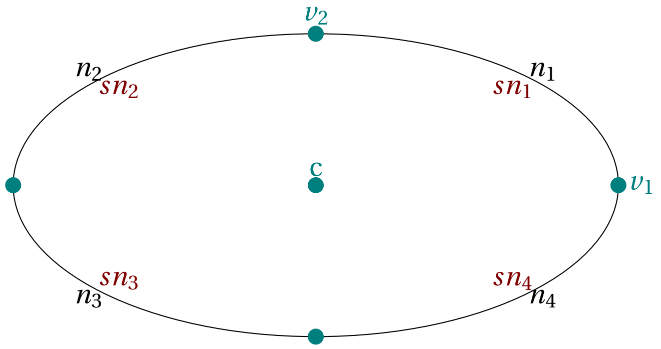
```
virtual void computeMB();
virtual std::vector<const Point*> boundNodes() const;
virtual std::vector<Point*> nodes();
virtual std::vector<const Point*> nodes() const;
virtual std::vector<std::pair<ShapeType,std::vector<const Point*> > > curves() const;
virtual std::vector<std::pair<ShapeType,std::vector<const Point*> > > surfs() const;
```

The parametrization (inherited from Parallelogram) is the following :

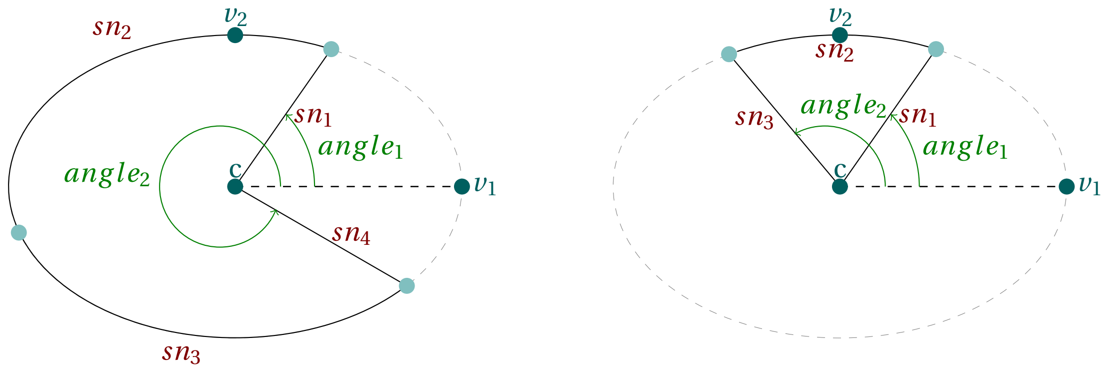
$$(u, v) \in [0,1] \times [0,1] \to (1-u-v)\,p_1 + u\,p_2 + v\,p_4.$$

### 4.1.17 The Ellipse class

To define an elliptic surface, you have to define a center and 2 apogees ($c$, $p1$ and $p2$ in the following figure):



You can also define an ellipse from its center and either the axis or the semi-axis lengths, when axes are x-axis and y-axis. The main attributes are p_, containing the center and the fourth "apogees" of the ellipse, v_, containing the true list of vertices used for meshing, thetamin_ and thetamax_ whose values determines if you are defining a whole ellipse or an elliptical sector.



```
class Ellipse : public Surface
{
  protected :
    std::vector<Point> p_, v_;
    std::vector<number_t> n_;
    std::vector<real_t> h_;
    real_t xradius_, yradius_;
    bool isAxis_;
    real_t thetamin_;
    real_t thetamax_;
    bool isSector_;
    dimen_t type_;
```

It offers constructors, taking from 3 to 9 `Parameter`. Authorized keys and what they do are:

| attribute | key to use to define it | optional | default value |
|---|---|---|---|
| p_, v_ | (**_center**, **_v1** and **_v2**)<br>or (**_center**, **_xlength**, **_ylength**)<br>or (**_center**, **_xradius**, **_yradius**) | no | no |
| n_ | **_nnodes** | yes | 2 |
| h_ | **_hsteps** | yes | no |
| domName_ | **_domain_name** | yes | "" |
| sideNames_ | **_side_names** | yes | "" |
| thetamin_ | **_angle1** | yes | 0 |
| thetamax_ | **_angle2** | yes | 360 |
| type_ | **_type** | yes | 1 |

It also offers:

- some accessors
- implementation of inherited virtual functions concerning elliptic surfaces and disks:

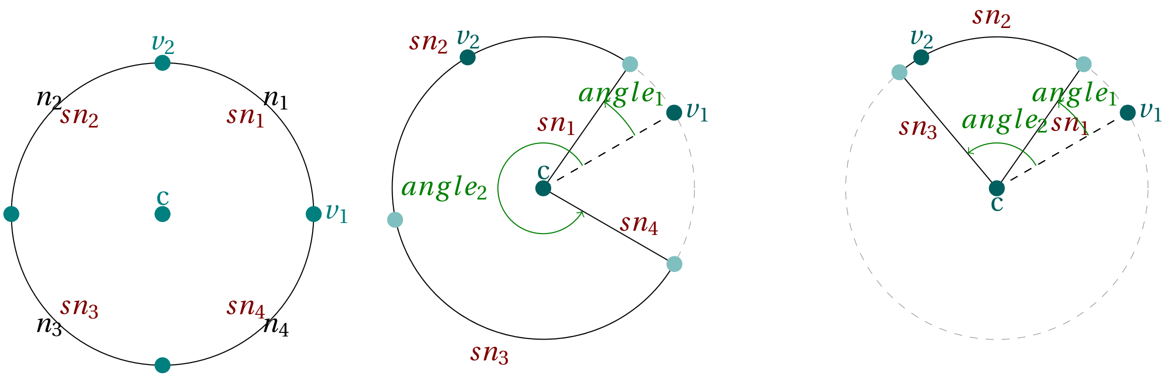
```
virtual void computeMB();
virtual std::vector<const Point*> boundNodes() const;
virtual std::vector<Point*> nodes();
virtual std::vector<const Point*> nodes() const;
virtual std::vector<std::pair<ShapeType,std::vector<const Point*> > > curves() const;
virtual std::vector<std::pair<ShapeType,std::vector<const Point*> > > surfs() const;
```

The parametrization is the following (polar parametrization, $c$ center, $p_1$, $p_2$ first and second apogee):

$$(u,v)\in[0,1]\times[0,1]\to c+(p_1-c)\,u\cos(\theta)+(p_2-c)\,u\sin(\theta)\quad\text{with }\theta=(1-v)\,\theta_{min}+v\,\theta_{max}.$$

### 4.1.18 The `Disk` class

To define a disk, you have to do the same way as `Ellipse`.



It offers constructors, taking from 2 to 9 `Parameter`. Authorized keys and what they do are:

| attribute | key to use to define it | optional | default value |
|---|---|---|---|
| p_, v_ | (**_center**, **_v1** and **_v2**)<br>or (**_center**, **_radius**) | no | no |
| n_ | **_nnodes** | yes | 2 |
| h_ | **_hsteps** | yes | no |
| domName_ | **_domain_name** | yes | "" |
| sideNames_ | **_side_names** | yes | "" |
| thetamin_ | **_angle1** | yes | 0 |
| thetamax_ | **_angle2** | yes | 360 |
| type_ | **_type** | yes | 1 |

It also offers:

- some accessors
- implementation of inherited virtual functions concerning elliptic surfaces and disks:

```
virtual void computeMB();
virtual std::vector<const Point*> boundNodes() const;
virtual std::vector<Point*> nodes();
virtual std::vector<const Point*> nodes() const;
virtual std::vector<std::pair<ShapeType,std::vector<const Point*> > > curves() const;
virtual std::vector<std::pair<ShapeType,std::vector<const Point*> > > surfs() const;
```

The parametrization inherits from Ellispe parametrization ($c$ center, $p_1$, $p_2$ first and second apogee) :

$$(u,v) \in [0,1] \times [0,1] \rightarrow c + (p_1 - c)\, u \cos(\theta) + (p_2 - c)\, u \sin(\theta) \quad \text{with } \theta = (1-v)\,\theta_{min} + v\,\theta_{max}.$$

### 4.1.19 The ParametrizedSurface class

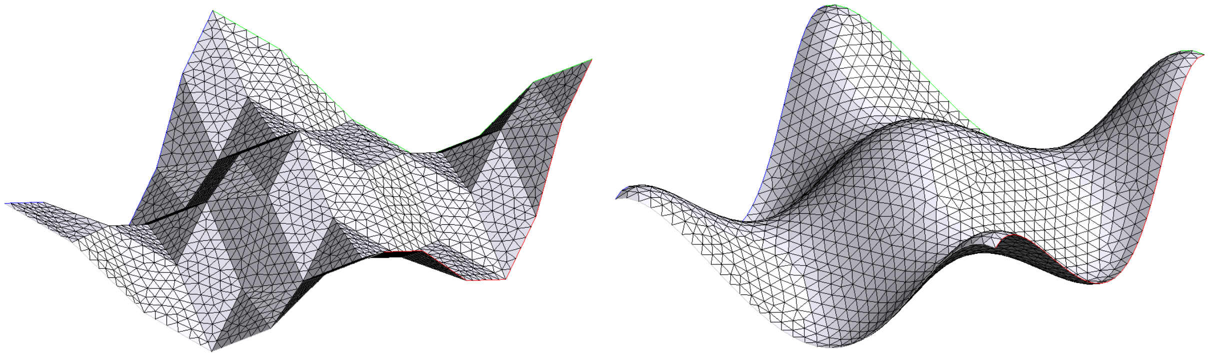
A parametrized surface is defined by a 2D parametrization :

$$(u,v) \in \hat{\Omega} \rightarrow q(u,v) \in \mathbb{R}^d \quad (d = 2,3)$$

handled by an object of the Parametrization class. In most of cases, $\hat{\Omega} = [x_1, x_2] \times [y_1, y_2]$. Since mesh tools, generally, does not support this type of geometry representation, additional data must be provided, to describe how to partition the surface into small plane or spline surfaces :

```
class ParametrizedSurface : public Surface
{
 protected:
  Partitioning partitioning_; //one of _nonePartition*, _linearPartition _splinePartition
  number_t nbParts_;          //number of partitions (>0)
  Transformation* transformation_;  //pointer to an additional linear transformation
```

Be cautious, a partition leads to an approximated surface of the parametrized one. Obviously, the spline (nurbs) partition is better than the linear partition :



In constructors, authorized keys and what they do are:

| attribute | key to use to define it | optional | default value |
|---|---|---|---|
| parametrization_ | **_parametrization** | no | no |
| partitioning_ | **_partitioning** | yes | _part_linear |
| nbParts_ | **_nbParts** | yes | 2 |
| n_ | **_nnodes** | yes | 2 |
| h_ | **_hsteps** | yes | no |
| domName_ | **_domain_name** | yes | "" |
| sideNames_ | **_side_names** | yes | "" |

It also offers:

- some accessors
- implementation of inherited virtual functions concerning :

```
virtual number_t nbSides() const;
virtual std::vector<const Point*> boundNodes() const;
virtual std::vector<Point*> nodes();
virtual std::vector<const Point*> nodes() const;
std::vector<const Point*> nodesOnSide(number_t s=0) const;
virtual std::vector<std::pair<ShapeType,std::vector<const Point*> > > curves() const;
virtual std::vector<std::pair<ShapeType,std::vector<const Point*> > > surfs() const;
```

The parametrization is the original one. Contrary to the parametrized arc, there is no wrapper to map the parameters $(u, v)$ in $[0,1] \times [0,1]$.

Up to now, the ParametrizedSurface geometry can be meshed only with the OpenCascade engine!

### 4.1.20 The SplineSurface class

Spline surface are surface defined by a 2D spline,:

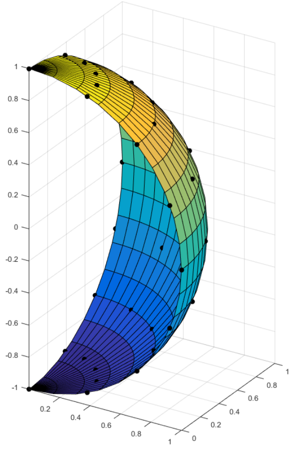
```
class SplineSurface : public Surface
{
        protected:
        Spline* spline_;      //spline pointer (nurbs)
```

Up to now, only NURBS (either appoximation or interpolation nurbs) are available. A NURBS is implicitly parametrized by two scalars $(u, v) \in [0,1] \times [0,1]$. It has at most 4 sides (some may be degenerated).

Constructors of a SplineSurface deal with the following parameters

| attribute | key to use to define it | optional | default value |
|---|---|---|---|
| spline_ | **_spline** | exclusive | no |
| spline subtype_ | **_splineSubtype** | exclusive | _splineInterpolation |
| spline vertices_ | **_vertices** | exclusive | no |
| spline weights_ | **_weights** | exclusive | 1 |
| nb of vertices along u_ | **_nbu** | exclusive | no |
| n_ | **_nnodes** | yes | 2 |
| h_ | **_hsteps** | yes | no |
| domName_ | **_domain_name** | yes | "" |
| sideNames_ | **_side_names** | yes | "" |

The spline surface may be constructed, either by given a Nurbs object or by given a list of vertices (**_vertices**) and some additional spline parameters : **_splineSubtype**, **_weights** and mandatory **_nbu**. Both constructions are exclusive.



All usual stuff is provided and the parametrization is wrapped to the spline (nurbs) parametrization.

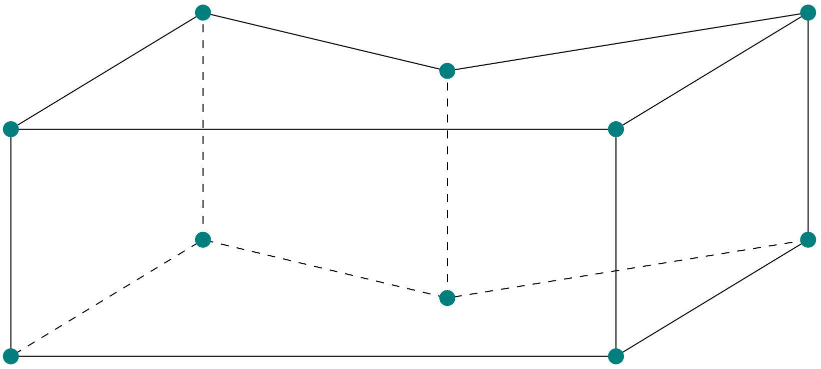
Up to now, the ParametrizedSurface geometry can be meshed only with the OpenCascade engine!

### 4.1.21 The Polyhedron class

A polyhedron is defined bi its polygonal faces.

```
class Polyhedron: public Volume
{
  private:
    std::vector<Polygon*> faces_;
  protected:
    std::vector<Point> p_;
    std::vector<number_t> n_;
    std::vector<real_t> h_;
```

p_, n_ and h_ are defined here but used in child classes.



It offers constructors, taking from 1 to 2 Parameter. Authorized keys and what they do are:

| attribute | key to use to define it | optional | default value |
|---|---|---|---|
| faces_ | **_faces** | no | no |
| domName_ | **_domain_name** | yes | "" |

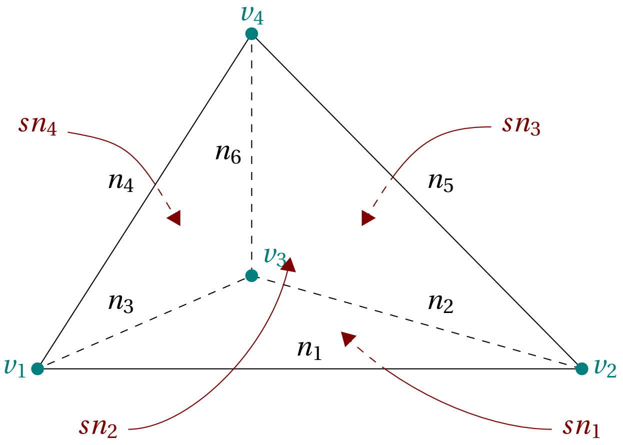
It also offers:

- some accessors
- implementation of inherited virtual functions concerning hexahedron, parallelepipeds and cubes:

```
virtual void computeMB();
virtual std::vector<const Point*> boundNodes() const;
virtual std::vector<Point*> nodes();
virtual std::vector<const Point*> nodes() const;
virtual std::vector<std::pair<ShapeType,std::vector<const Point*> > > curves() const;
virtual std::vector<std::pair<ShapeType,std::vector<const Point*> > > surfs() const;
```

### 4.1.22 The Tetrahedron class

To define a tetrahedron, you just have to give the 4 vertices.



It offers constructors, taking from 4 to 7 `Parameter`. Authorized keys and what they do are:

| attribute | key to use to define it | optional | default value |
|---|---|---|---|
| p_ | **_v1**, **_v2**, **_v3** and **_v4** | no | no |
| n_ | **_nnodes** | yes | 2 |
| h_ | **_hsteps** | yes | no |
| domName_ | **_domain_name** | yes | "" |
| sideNames_ | **_side_names** | yes | "" |

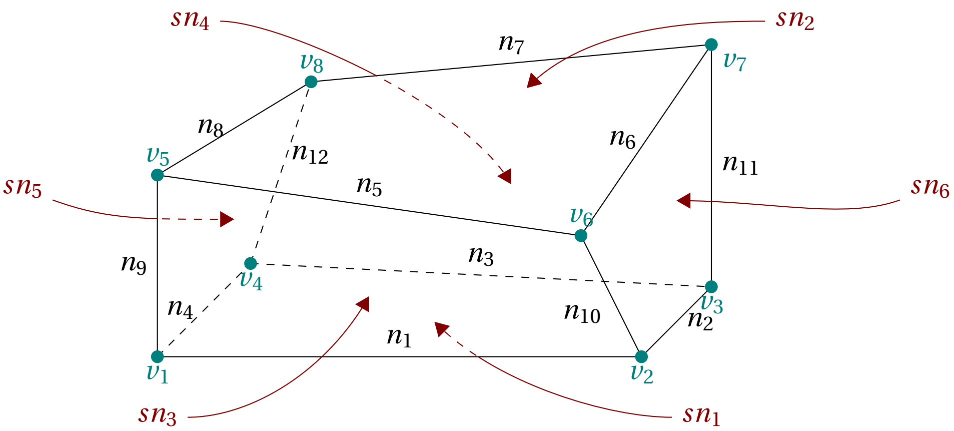
It also offers:

- some accessors
- implementation of inherited virtual functions concerning tetrahedron:

```
virtual void computeMB();
virtual std::vector<const Point*> boundNodes() const;
virtual std::vector<Point*> nodes();
virtual std::vector<const Point*> nodes() const;
virtual std::vector<std::pair<ShapeType,std::vector<const Point*> > > curves() const;
virtual std::vector<std::pair<ShapeType,std::vector<const Point*> > > surfs() const;
```

### 4.1.23 The `Hexahedron` class

To define a hexahedron, you just have to give the 8 vertices.



It offers constructors, taking from 8 to 11 `Parameter`. Authorized keys and what they do are:

| attribute | key to use to define it | optional | default value |
|---|---|---|---|
| p_ | **_v1**, **_v2**, **_v3**, **_v4**, **_v5**, **_v6**, **_v7** and **_v8** | no | no |
| n_ | **_nnodes** | yes | 2 |
| h_ | **_hsteps** | yes | no |
| domName_ | **_domain_name** | yes | "" |
| sideNames_ | **_side_names** | yes | "" |

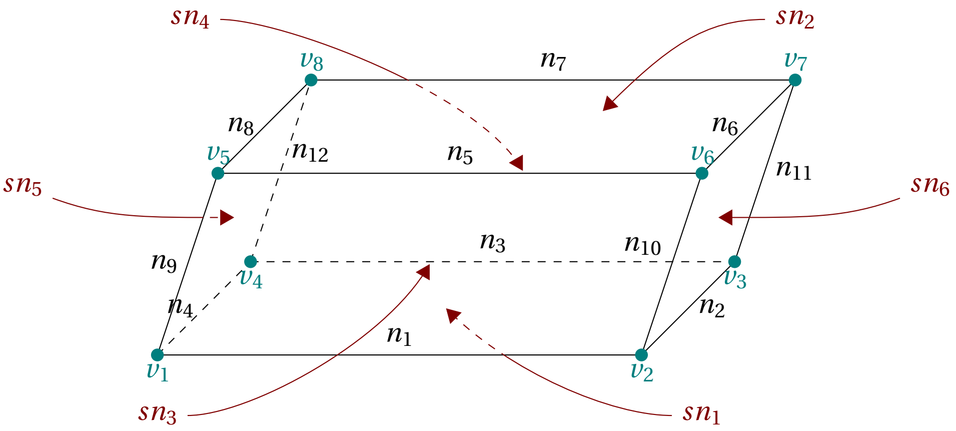
It also offers:

- some accessors
- implementation of inherited virtual functions concerning hexahedra :

```
virtual void computeMB();
virtual std::vector<const Point*> boundNodes() const;
virtual std::vector<Point*> nodes();
virtual std::vector<const Point*> nodes() const;
virtual std::vector<std::pair<ShapeType,std::vector<const Point*> > > curves() const;
virtual std::vector<std::pair<ShapeType,std::vector<const Point*> > > surfs() const;
```

### 4.1.24 The `Parallelepiped` class

To define a parallelepiped, you just have to give 4 vertices ($p_1$, $p_2$, $p_4$ and $p_5$ in the following figure):



In a similar way to angular sectors for `Ellipse` and `Disk` classes, there is an additionnal parameter defining the number of octants to consider. This is the reason why, there is an attribute v_ again, storing the true list of vertices used for meshing:

```
class Parallelepiped : public Hexahedron
{
  protected:
    dimen_t nboctants_;
    std::vector<Point> v_;
```

It offers constructors, taking from 4 to 8 `Parameter`. Authorized keys and what they do are:

| attribute | key to use to define it | optional | default value |
|---|---|---|---|
| p_, v_ | **_v1**, **_v2**, **_v4** and **_v5** | no | no |
| n_ | **_nnodes** | yes | 2 |
| h_ | **_hsteps** | yes | no |
| domName_ | **_domain_name** | yes | "" |
| sideNames_ | **_side_names** | yes | "" |
| nboctants_ | **_nboctants** | yes | 8 |

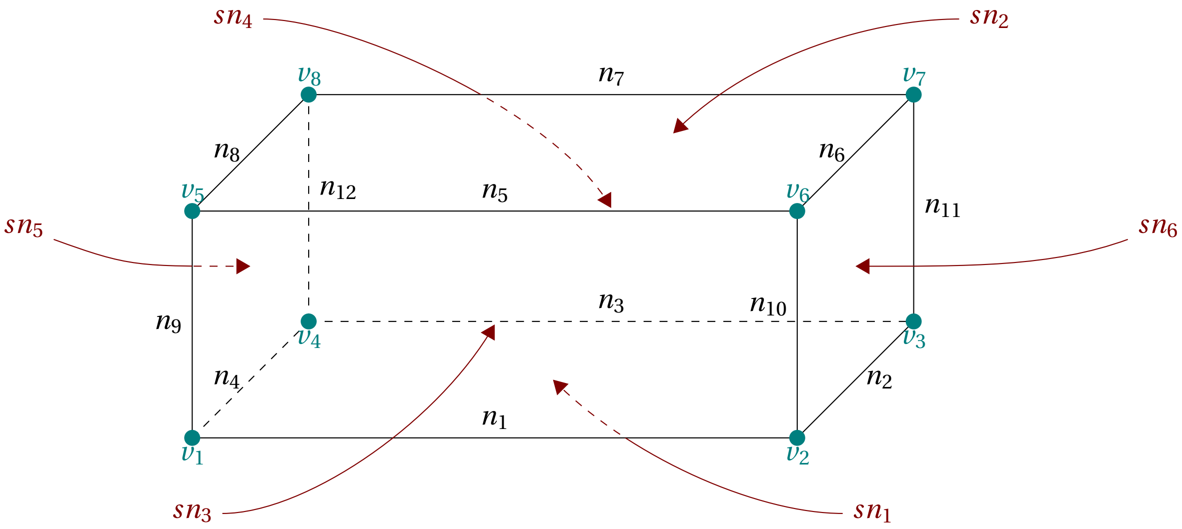
It also offers:

- some accessors
- implementation of inherited virtual functions concerning parallelepipeds:

```
virtual void computeMB();
virtual std::vector<const Point*> boundNodes() const;
virtual std::vector<Point*> nodes();
virtual std::vector<const Point*> nodes() const;
virtual std::vector<std::pair<ShapeType,std::vector<const Point*> > > curves() const;
virtual std::vector<std::pair<ShapeType,std::vector<const Point*> > > surfs() const;
```

### 4.1.25 The Cuboid class

To define a cuboid, you just have to give 4 vertices, as for `Parallelepiped`. And as for `Rectangle`, you can define it by its center or its origin and its lengths, or define it by its bounds



It offers constructors, taking from 4 to 10 `Parameter`. Authorized keys and what they do are:

| attribute | key to use to define it | optional | default value |
|---|---|---|---|
| p_ | (**_v1**, **_v2**, **_v4**, **_v5**)<br>or (**_center**, **_xlength**, **_ylength**, **_zlength**)<br>or (**_origin**, **_xlength**, **_ylength**, **_zlength**)<br>or (**_xmin**, **_xmax**, **_ymin**, **_ymax**, **_zmin**, **_zmax**) | no | no |
| n_ | **_nnodes** | yes | 2 |
| h_ | **_hsteps** | yes | no |
| domName_ | **_domain_name** | yes | "" |
| sideNames_ | **_side_names** | yes | "" |
| nboctants_ | **_nboctants** | yes | 8 |

It also offers:

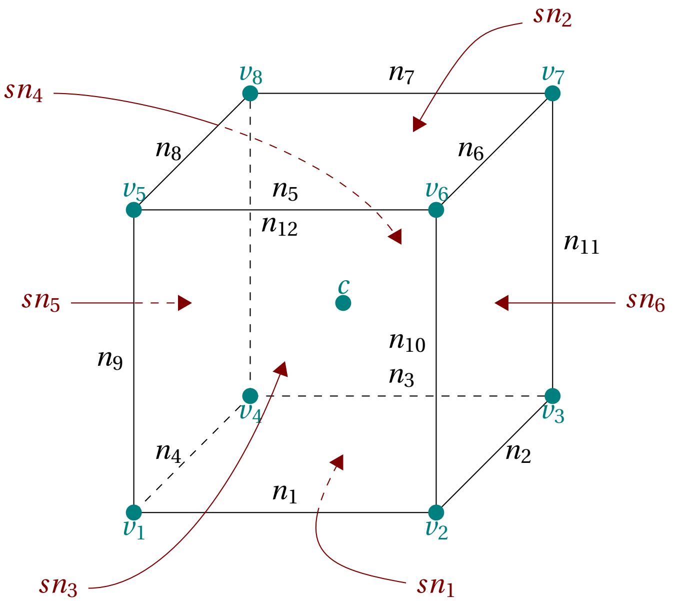
- some accessors
- implementation of inherited virtual functions concerning cuboids:

```
virtual void computeMB();
virtual std::vector<const Point*> boundNodes() const;
virtual std::vector<Point*> nodes();
virtual std::vector<const Point*> nodes() const;
virtual std::vector<std::pair<ShapeType,std::vector<const Point*> > > curves() const;
virtual std::vector<std::pair<ShapeType,std::vector<const Point*> > > surfs() const;
```

### 4.1.26 The Cube class

To define a cube, you just have to give 4 vertices. You can also give the center or the origin and the length.

```
class Cube: public Cuboid
{
  private:
    dimen_t nboctants_;
```



It offers constructors, taking from 2 to 8 `Parameter`. Authorized keys and what they do are:

| attribute | key to use to define it | optional | default value |
|---|---|---|---|
| p_ | (**_v1**, **_v2**, **_v4**, **_v5**)<br>or (**_center**, **_length**)<br>or (**_origin**, **_length**) | no | no |
| n_ | **_nnodes** | yes | 2 |
| h_ | **_hsteps** | yes | no |
| domName_ | **_domain_name** | yes | "" |
| sideNames_ | **_side_names** | yes | "" |
| nboctants_ | **_nboctants** | yes | 8 |

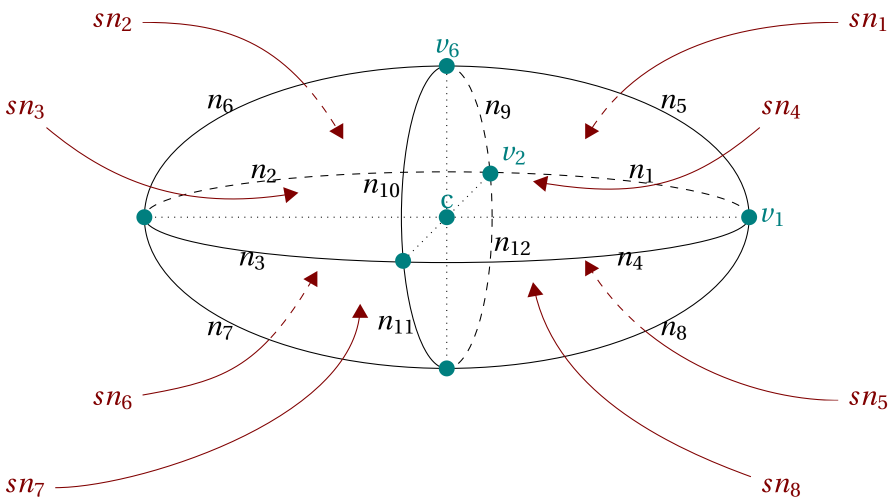
It also offers:

- some accessors
- implementation of inherited virtual functions concerning cubes:

```
virtual void computeMB();
virtual std::vector<const Point*> boundNodes() const;
virtual std::vector<Point*> nodes();
virtual std::vector<const Point*> nodes() const;
virtual std::vector<std::pair<ShapeType,std::vector<const Point*> > > curves() const;
virtual std::vector<std::pair<ShapeType,std::vector<const Point*> > > surfs() const;
```

### 4.1.27 The `Ellipsoid` class

To define an ellipsoid, you do the same way as for an ellipse, namely defining a center and 3 apogees ($c$, $p1$, $p2$ and $p_6$ in the following figure):



You can also define an ellipsoid from its center and either the axis or the semi-axis lengths, when axes are x-axis, y-axis and z-axis.

```
class Ellipsoid : public Volume
{
  protected:
    Point p_, v_;
    real_t xradius_, yradius_, zradius_;
    bool isAxis_;
    std::vector<number_t> n_;
    std::vector<real_t> h_;
    dimen_t nboctants_;
    dimen_t type_;
```

It offers constructors, taking from 4 to 9 `Parameter`. Authorized keys and what they do are:

| attribute | key to use to define it | optional | default value |
|---|---|---|---|
| p_, v_ | (**_center**, **_v1**, **_v2**, **_v6**)<br>or (**_center**, **_xlength**, **_ylength**, **_zlength**)<br>or (**_center**, **_xradius**, **_yradius**, **_zradius**) | no | no |
| n_ | **_nnodes** | yes | 2 |
| h_ | **_hsteps** | yes | no |
| domName_ | **_domain_name** | yes | "" |
| sideNames_ | **_side_names** | yes | "" |
| nboctants_ | **_nboctants** | yes | 8 |
| type_ | **_type** | yes | 1 |

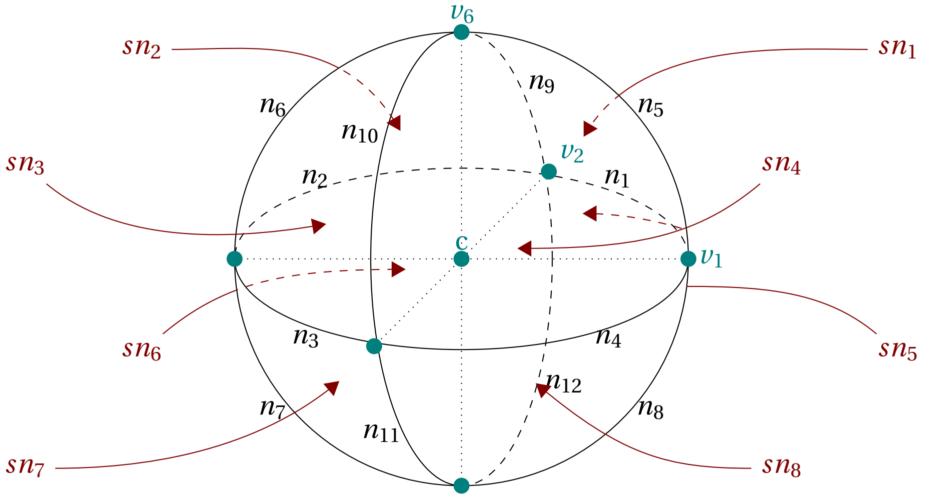
It also offers:

- some accessors
- implementation of inherited virtual functions concerning ellipsoids:

```
virtual void computeMB();
virtual std::vector<const Point*> boundNodes() const;
virtual std::vector<Point*> nodes();
virtual std::vector<const Point*> nodes() const;
virtual std::vector<std::pair<ShapeType,std::vector<const Point*> > > curves() const;
virtual std::vector<std::pair<ShapeType,std::vector<const Point*> > > surfs() const;
```

### 4.1.28 The `Ball` class

To define a ball, you do the same way as for an ellipsoid.



It offers constructors, taking from 2 to 9 `Parameter`. Authorized keys and what they do are:

| attribute | key to use to define it | optional | default value |
|---|---|---|---|
| p_, v_ | (**_center**, **_v1**, **_v2**, **_v6**)<br>or (**_center**, **_radius**)<br>or (**_origin**, **_radius**) | no | no |
| n_ | **_nnodes** | yes | 2 |
| h_ | **_hsteps** | yes | no |
| domName_ | **_domain_name** | yes | "" |
| sideNames_ | **_side_names** | yes | "" |
| nboctants_ | **_nboctants** | yes | 8 |
| type_ | **_type** | yes | 1 |

It also offers:

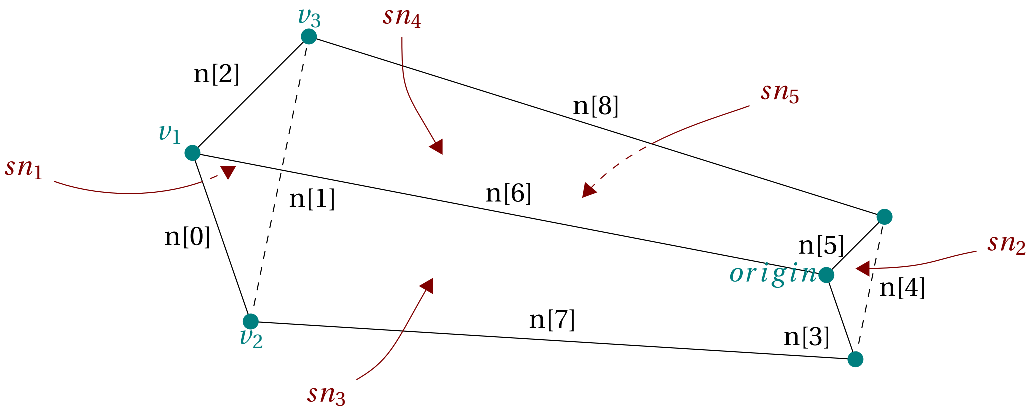
- some accessors
- implementation of inherited virtual functions concerning balls:

```
virtual void computeMB();
virtual std::vector<const Point*> boundNodes() const;
virtual std::vector<Point*> nodes();
virtual std::vector<const Point*> nodes() const;
virtual std::vector<std::pair<ShapeType,std::vector<const Point*> > > curves() const;
virtual std::vector<std::pair<ShapeType,std::vector<const Point*> > > surfs() const;
```

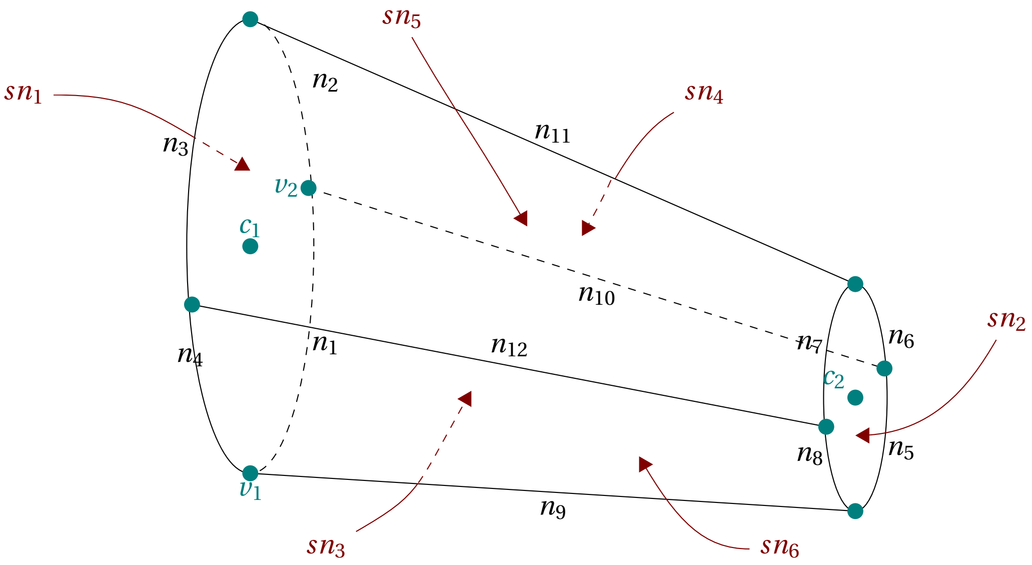
### 4.1.29 The `Trunk` class

A trunk is a generalized truncated cone. To define a trunk, you need to give a surface, namely a polygonal surface or a elliptical surface. To define the other surface, you just need to give a point of this surface ($origin$), and the scale factor according to the first surface.

For a trunk with polygonal basis, $origin$ is the equivalent of the first vertex of the surface you give, as you can see on the following figure of a trunk with triangular basis. The triangle being defined by its vertices $p_1$, $p_2$ and $p_3$, $origin$ is the equivalent of $p_1$:



For a trunk with elliptical basis, $origin$ is the center of the second basis, as you can see on the following figure of a trunk with elliptical basis.



```
class Trunk: public Volume
{
  protected:
    Surface * basis_;
    real_t scale_;
    std::vector<Point> p_;
    std::vector<number_t> n_;
    std::vector<real_t> h_;
    Point origin_, center1_, p1_, p2_;
    bool isElliptical_, isN_;
```

It offers constructors, taking from 3 to 8 `Parameter`. Authorized keys and what they do are:

| attribute | key to use to define it | optional | default value |
|---|---|---|---|
| p_ | (**_center1**, **_v1**, **_v2**, **_center2**, **_scale**)<br>or (**_basis**, **_origin**, **_scale**) | no | no |
| n_ | **_nnodes** | yes | 2 |
| h_ | **_hsteps** | yes | no |
| domName_ | **_domain_name** | yes | "" |
| sideNames_ | **_side_names** | yes | "" |

It also offers:

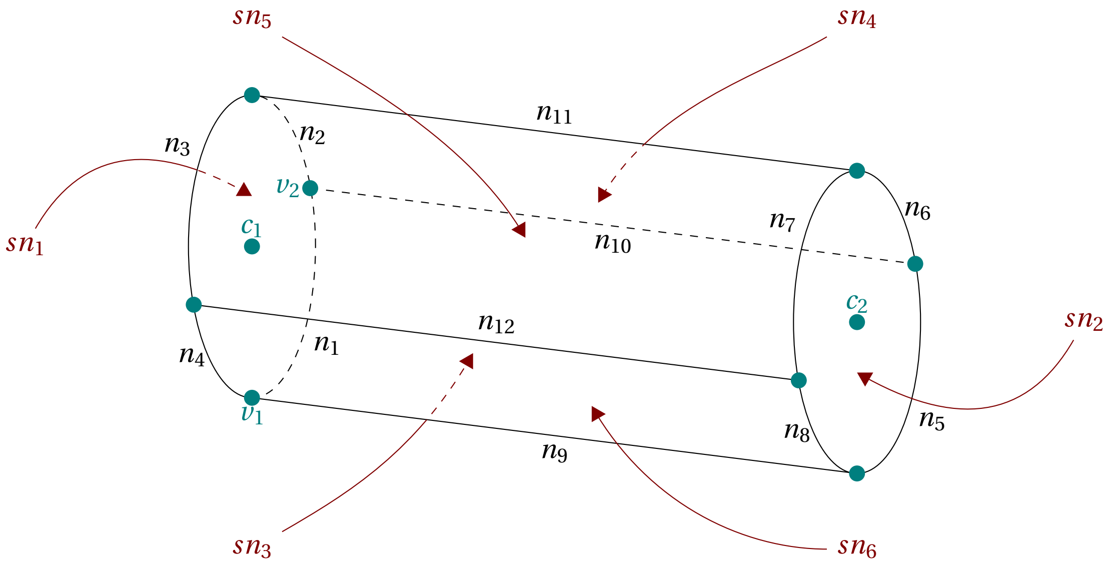
- some accessors
- implementation of inherited virtual functions concerning trunks:

```
virtual void computeMB();
virtual std::vector<const Point*> boundNodes() const;
virtual std::vector<Point*> nodes();
virtual std::vector<const Point*> nodes() const;
virtual std::vector<std::pair<ShapeType,std::vector<const Point*> > > curves() const;
virtual std::vector<std::pair<ShapeType,std::vector<const Point*> > > surfs() const;
```

### 4.1.30 The `Cylinder` class

A cylinder is a truncated cone whose apex is at infinite distance. So it is the geometry defined by the extrusion of a surface by translation.

```
class Cylinder : public Trunk
{
  protected:
    //! direction vector
    Point dir_;
```



It offers constructors, taking from 2 to 7 `Parameter`. Authorized keys and what they do are:

| attribute | key to use to define it | optional | default value |
|---|---|---|---|
| p_ | (**_center1**, **_v1**, **_v2**, **_center2**)<br>or (**_basis**, **_direction**) | no | no |
| n_ | **_nnodes** | yes | 2 |
| h_ | **_hsteps** | yes | no |
| domName_ | **_domain_name** | yes | "" |
| sideNames_ | **_side_names** | yes | "" |

It also offers:

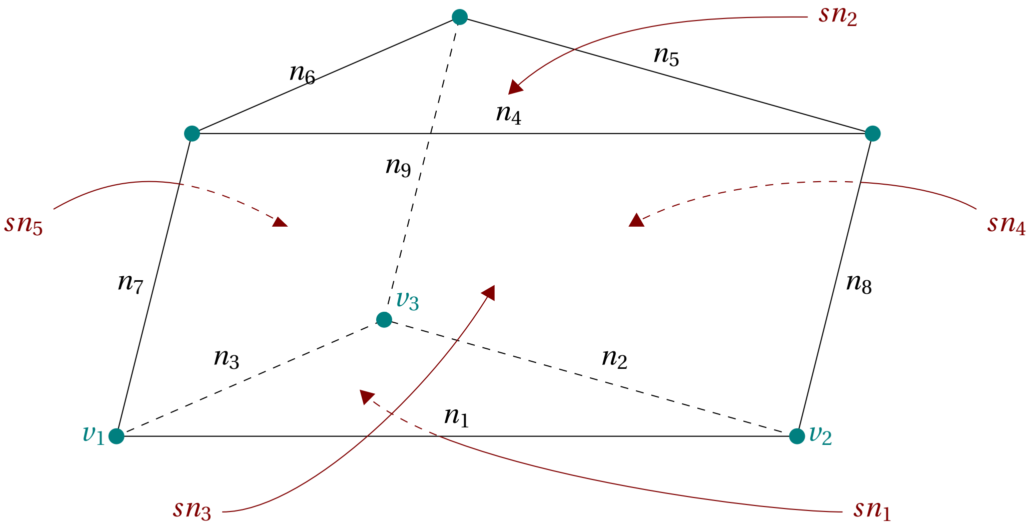
- some accessors
- implementation of inherited virtual functions concerning cylinders:

```
virtual void computeMB();
virtual std::vector<const Point*> boundNodes() const;
virtual std::vector<Point*> nodes();
virtual std::vector<const Point*> nodes() const;
virtual std::vector<std::pair<ShapeType,std::vector<const Point*> > > curves() const;
virtual std::vector<std::pair<ShapeType,std::vector<const Point*> > > surfs() const;
```

### 4.1.31 The Prism class

A prism is by definition a cylinder whose basis is a polygonal surface. Often a prism refers to a cylinder with triangular basis (as the finite element cell).

```
class Prism: public Cylinder
{
  private:
    bool isTriangular_;
    Point p3_;
```



It offers constructors, taking from 2 to 7 Parameter. Authorized keys and what they do are:

| attribute | key to use to define it | optional | default value |
|---|---|---|---|
| p_ | (**_v1**, **_v2**, **_v3**, **_direction**)<br>or (**_basis**, **_direction**) | no | no |
| n_ | **_nnodes** | yes | 2 |
| h_ | **_hsteps** | yes | no |
| domName_ | **_domain_name** | yes | "" |
| sideNames_ | **_side_names** | yes | "" |

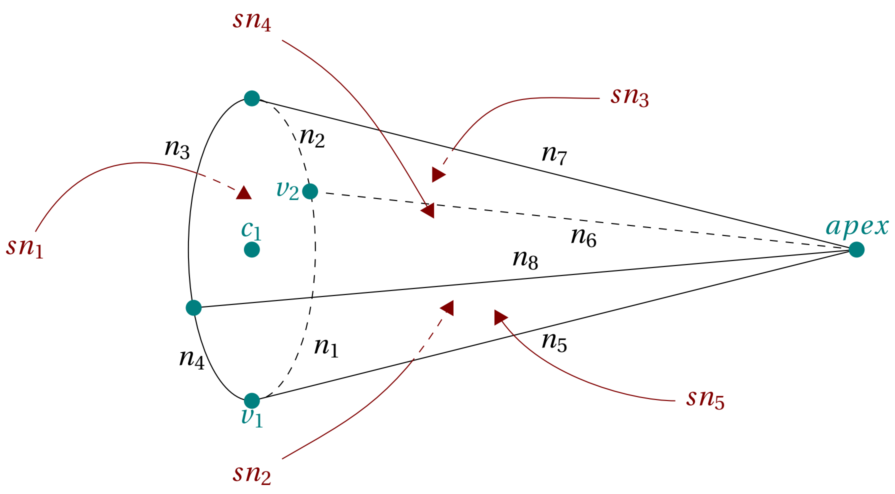
It also offers:

- some accessors
- implementation of inherited virtual functions concerning prisms:

```
virtual void computeMB();
virtual std::vector<const Point*> boundNodes() const;
virtual std::vector<Point*> nodes();
virtual std::vector<const Point*> nodes() const;
virtual std::vector<std::pair<ShapeType,std::vector<const Point*> > > curves() const;
virtual std::vector<std::pair<ShapeType,std::vector<const Point*> > > surfs() const;
```

### 4.1.32 The Cone class

A cone is defined by a surface and an apex. As for trunks and cylinders, you can also define directly a cone with elliptical basis.



It offers constructors, taking from 3 to 7 `Parameter`. Authorized keys and what they do are:

| attribute | key to use to define it | optional | default value |
|---|---|---|---|
| p_ | (**_center1**, **_v1**, **_v2**, **_apex**)<br>or (**_basis**, **_apex**) | no | no |
| n_ | **_nnodes** | yes | 2 |
| h_ | **_hsteps** | yes | no |
| domName_ | **_domain_name** | yes | "" |
| sideNames_ | **_side_names** | yes | "" |

It also offers:

- some accessors

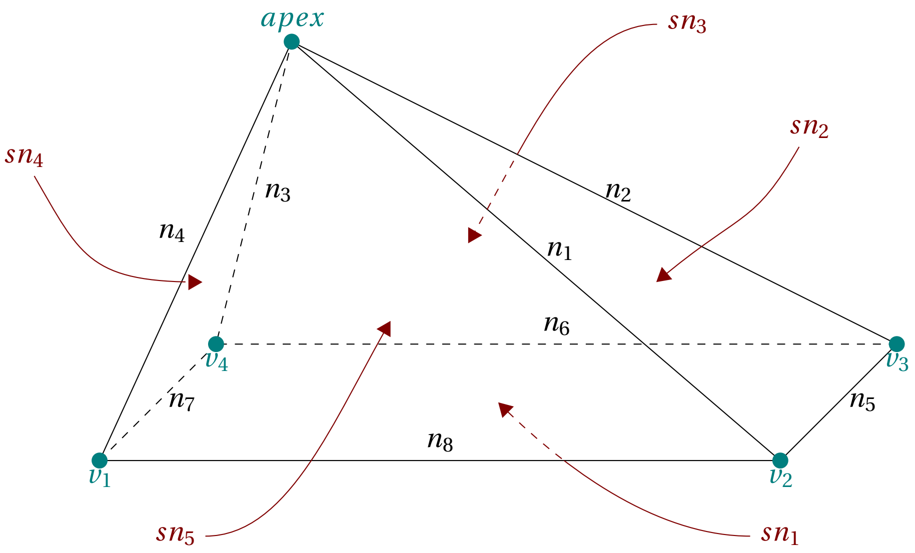
- implementation of inherited virtual functions concerning cones:

```
virtual void computeMB();
virtual std::vector<const Point*> boundNodes() const;
virtual std::vector<Point*> nodes();
virtual std::vector<const Point*> nodes() const;
virtual std::vector<std::pair<ShapeType,std::vector<const Point*> > > curves() const;
virtual std::vector<std::pair<ShapeType,std::vector<const Point*> > > surfs() const;
```

### 4.1.33 The Pyramid class

A pyramid is a cone with a polygonal basis. Often a pyramid refers to a cone with quadrangular basis (as the finite element cell).

```
class Pyramid: public Cone
{
  private:
    bool isQuadrangular_;
    Point p3_, p4_;
```



It offers constructors, taking from 2 to 8 Parameter. Authorized keys and what they do are:

| attribute | key to use to define it | optional | default value |
|---|---|---|---|
| p_ | (**_v1**, **_v2**, **_v3**, **_v4**, **_apex**)<br>or (**_basis**, **_apex**) | no | no |
| n_ | **_nnodes** | yes | 2 |
| h_ | **_hsteps** | yes | no |
| domName_ | **_domain_name** | yes | "" |
| sideNames_ | **_side_names** | yes | "" |

It also offers:

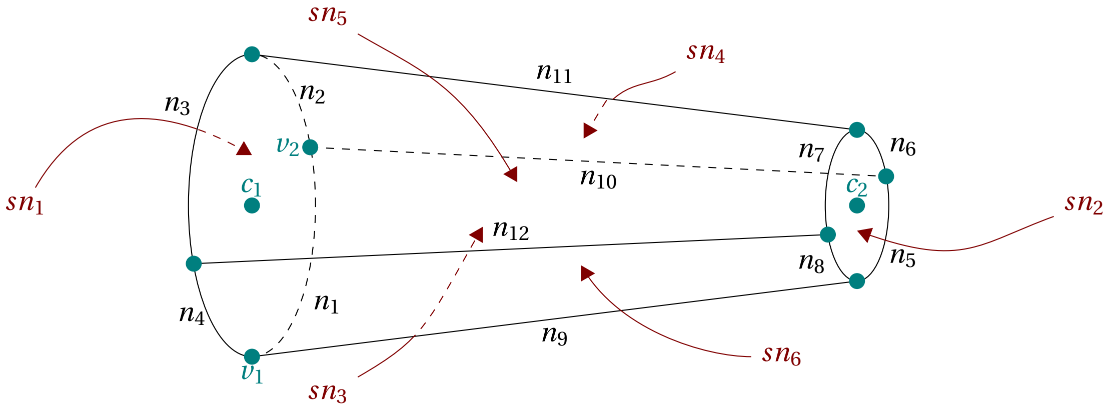
- some accessors
- implementation of inherited virtual functions concerning pyramids:

```
virtual void computeMB();
virtual std::vector<const Point*> boundNodes() const;
virtual std::vector<Point*> nodes();
virtual std::vector<const Point*> nodes() const;
virtual std::vector<std::pair<ShapeType,std::vector<const Point*> > > curves() const;
virtual std::vector<std::pair<ShapeType,std::vector<const Point*> > > surfs() const;
```

### 4.1.34 The RevTrunk class

A revolution trunk is a right trunk with circular basis. RevTrunk offers you more geometry abilities. Indeed, you can decide to add extensions at ends of the revolution trunk. Extensions can be: none, flat, ellipsoid, or cone.

```
class RevTrunk: public Trunk
{
  protected:
    real_t radius1_, radius2_;
    number_t nbSubDomains_;
    GeometricEndShape endShape1_;
    real_t distance1_;
    GeometricEndShape endShape2_;
    real_t distance2_;
    dimen_t type_;
```



It offers constructors, taking from 4 to 13 Parameter. Authorized keys and what they do are:

| attribute | key to use to define it | optional | default value |
|---|---|---|---|
| p_ | (**_center1**, **_center2**, **_radius1**, **_radius2**) | no | no |
| endShape1_ | **_end1_shape** | yes | _gesflat |
| endShape2_ | **_end2_shape** | yes | _gesFlat |
| distance1_ | **_end1_distance** | yes | 0. |
| distance2_ | **_end2_distance** | yes | 0. |
| n_ | **_nnodes** | yes | 2 |
| h_ | **_hsteps** | yes | no |
| domName_ | **_domain_name** | yes | "" |
| sideNames_ | **_side_names** | yes | "" |
| nbSubDomains_ | **_nbsubdomains** | yes | 1 |
| type_ | **_type** | yes | 1 |

It also offers:

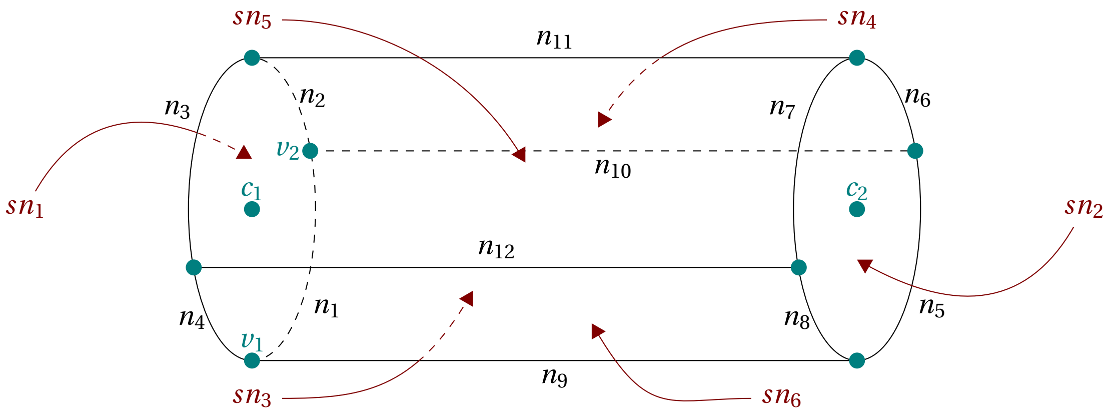
- some accessors

- implementation of inherited virtual functions concerning revolution trunks:

```
virtual void computeMB();
virtual std::vector<const Point*> boundNodes() const;
virtual std::vector<Point*> nodes();
virtual std::vector<const Point*> nodes() const;
virtual std::vector<std::pair<ShapeType,std::vector<const Point*> > > curves() const;
virtual std::vector<std::pair<ShapeType,std::vector<const Point*> > > surfs() const;
```

### 4.1.35 The RevCylinder class

A revolution cylinder is a revolution trunk where both radiuses are equal. So, we need centers of both bases, and the radius. As `RevTrunk`, `RevCylinder` offers you the ability to add extensions at ends of the revolution cylinder.



It offers constructors, taking from 3 to 12 `Parameter`. Authorized keys and what they do are:

| attribute | key to use to define it | optional | default value |
|---|---|---|---|
| p_ | (**_center1**, **_center2**, **_radius**) | no | no |
| endShape1_ | **_end1_shape** | yes | _gesflat |
| endShape2_ | **_end2_shape** | yes | _gesFlat |
| distance1_ | **_end1_distance** | yes | 0. |
| distance2_ | **_end2_distance** | yes | 0. |
| n_ | **_nnodes** | yes | 2 |
| h_ | **_hsteps** | yes | no |
| domName_ | **_domain_name** | yes | "" |
| sideNames_ | **_side_names** | yes | "" |
| nbSubDomains_ | **_nbsubdomains** | yes | 1 |
| type_ | **_type** | yes | 1 |

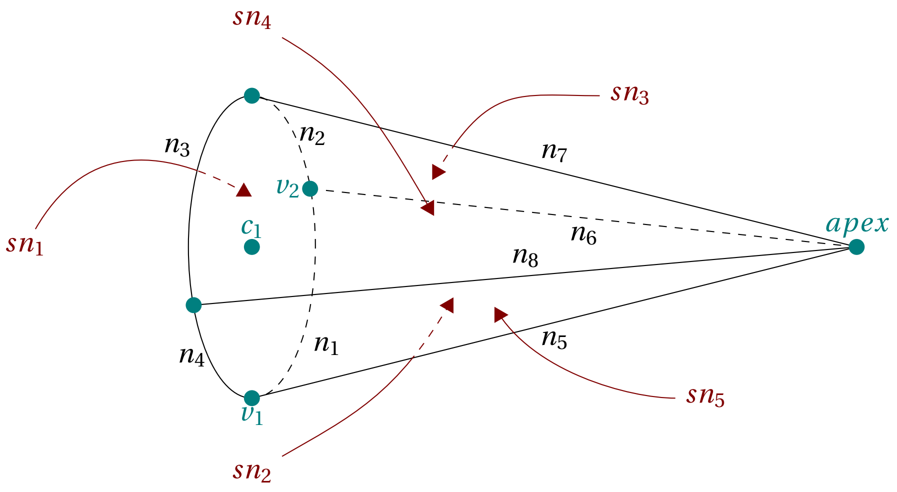
It also offers:

- some accessors
- implementation of inherited virtual functions concerning revolution cylinders:

```
virtual void computeMB();
virtual std::vector<const Point*> boundNodes() const;
virtual std::vector<Point*> nodes();
virtual std::vector<const Point*> nodes() const;
virtual std::vector<std::pair<ShapeType,std::vector<const Point*> > > curves() const;
virtual std::vector<std::pair<ShapeType,std::vector<const Point*> > > surfs() const;
```

### 4.1.36 The RevCone class

A revolution cone is a revolution trunk where second radius is equal to 0. As RevTrunk, RevCone offers you more the ability to add an extension to the basis of a revolution cone.



It offers constructors, taking from 3 to 10 Parameter. Authorized keys and what they do are:

| attribute | key to use to define it | optional | default value |
|---|---|---|---|
| p_ | (**_center**, **_radius**, **_apex**) | no | no |
| endShape1_ | **_end_shape** | yes | _gesflat |
| distance1_ | **_end_distance** | yes | 0. |
| n_ | **_nnodes** | yes | 2 |
| h_ | **_hsteps** | yes | no |
| domName_ | **_domain_name** | yes | "" |
| sideNames_ | **_side_names** | yes | "" |
| nbSubDomains_ | **_nbsubdomains** | yes | 1 |
| type_ | **_type** | yes | 1 |

It also offers:

- some accessors
- implementation of inherited virtual functions concerning revolution cones:

```
virtual void computeMB();
virtual std::vector<const Point*> boundNodes() const;
virtual std::vector<Point*> nodes();
virtual std::vector<const Point*> nodes() const;
virtual std::vector<std::pair<ShapeType,std::vector<const Point*> > > curves() const;
virtual std::vector<std::pair<ShapeType,std::vector<const Point*> > > surfs() const;
```

### 4.1.37 The SetOfElems class

## 4.2 Mesh management

The Mesh class handles mesh description, that is a collection of mesh elements. Mesh objects are built either from internal meshing tools or from mesh files provided by external meshing tools as GMSH for instance. To avoid complexity to end users, we decide to have a unique mesh class with no inheritance. It means that each meshing tool should be a member function of the Mesh class. These member functions are distributed in various files (see the Meshing tools section).

Basically, a mesh is a collection of points (vertices and intermediate points), of geometric elements (GeomElement) to carry the computation domain partition, of geometric domains (Domain): a list of elements or a list of sides of elements. Note that curved elements are supported using geometric interpolation of order greater than one. This Mesh class supports also mesh of surface in 3D space and mesh of line in 2D space. Besides the basic geometric data, it is also able to manage global list of sides (say faces of a 3D mesh, edges of a 2D mesh) or global list of sides of sides (edges of a 3D mesh). By default these lists are not constructed.

General informations on a mesh such as mesh name, space dimension, name of variables, bounding box are collected in the Geometry class. In future, this class should be developed to handle other informations, in particular boundary parametrisations useful to describe in an analytical way the domain to mesh, allowing to provide high order mesh and refinement meshing tools.

### 4.2.1 The Mesh class

```
class Mesh
{
 public :
  Geometry* geometry_p;                     // global geometric information
  std::vector<Point> nodes;                 // list of all mesh nodes
  Number lastIndex_;                        // last index of GeomElements

 protected :
  String name_;                             // name for documentation purposes
  String comment_;                          // comment documentation purposes
  std::vector<GeomElement*> elements_;      // list of geometric elements (MeshElement)
  std::vector<GeomDomain*> domains_;        // list of geometric domains
  std::vector<Number> vertices_;            // list of vertices indexed by their number in nodes
      vector
  bool isMadeOfSimplices_;                  // only segments, triangles or tetrahedra
  Dimen order_;                             // order of the mesh = max of element orders
  std::vector<GeomElement*> sides_;         // list of sides (edges in 2D, face in 3D), built if
      required
  std::vector<GeomElement*> sideOfSides_;   // list of sides of sides (edges in 3D), built if
      required
  std::vector<std::vector<GeoNumPair> > vertexElements_; // for each vertex v, list of elements
      having vertex v, built if required
  mutable Mesh* firstOrderMesh_p;           // underlying first order mesh when mesh has elements
      of order greater than one
...
```

GeomElement class is described in detail in section 4.5. In few words, the GeomElement class stores in a MeshElement object the numbering vectors of a mesh element (node numbers, vertex numbers, side numbers, side of side numbers) and a pointer to the reference element (RefElement) supporting the geometric interpolation of the element (define the map to reference geometric element). In case of a side element, the GeomElement class stores the parent sides and the side numbers. Note that in that case, MeshElement object does not necessarily exist!

Regarding meshing tools, the Mesh class provides various constructor : one reading a mesh file, two general constructors from any geometry, a constructor meshing one reference element, a constructor extruding a 1D/2D mesh and a constructor converting mesh elements to an other type:

```
Mesh();
Mesh(const String& filename, const String&, IOFormat mft = _undefFormat);
Mesh(const Mesh&);
~Mesh();
```

```
Mesh(const Geometry& g, Number order = 1, MeshGenerator mg = _defaultGenerator,
      const String& name = ""); // for 1D geometry
Mesh(const Geometry& g, ShapeType sh, Number order = 1, MeshGenerator mg = _defaultGenerator,
     const String& name = ""); // for 2D and 3D geometries
Mesh(ShapeType shape); // for reference element
Mesh(const Mesh& ms, const Point& O, const Point& d , number_t nbl, number_t namingDomain=0,
     number_t namingSection=0, number_t namingSide=0, const string_t& meshName="")   //for
     extruded mesh
Mesh(const Mesh& mesh, ShapeType sh, const string_t name=""); // for element converter
```

See subsection 4.2.2 for an exhaustive list of meshing tools.

As most of members are protected, there are useful accessors:

```
const std::vector<GeomElement*>& elements() const;
const std::vector<Domain*>& domains() const;
const std::vector<GeomElement*>& sides()const;
const std::vector<GeomElement*>& sideOfSides()const;
const std::vector<Number>& vertices()const;
const String& name() const;
bool isMadeOfSimplices()const;
const GeomElement& element(Number i) const;
const Domain& domains(Number i) const;
const GeomElement& side(Number i) const;
const GeomElement& sideOfSide(Number i) const;
const Number vertex(Number i) const;
const Point& vertexPoint(Number i) const;
Dimen spaceDim() const ;
Dimen meshDim() const;
Number nbOfElements() const;
Number nbOfDomains() const;
Number nbOfSides() const;
Number nbOfSideOfSides() const;
Number nbOfVertices() const;
Number nbOfNodes() const;
```

There are all constant and some are useful shortcuts.

The Mesh class provides four important member functions to complete on demand the construction of a mesh: functions to build the list of sides, the list of sides of sides and the list of vertex elements and a function to compute element orientation (sign of jacobian determinant) and the measure of element and its sides:

```
void buildSides();
void buildSideOfSides();
void buildVertexElements();
void buildGeomData();
```

Note that buildSides and buildSideOfSides functions update some data of GeomElements.

Finally, the class has usual printing facilities:

```
void print(std::ostream &) const;
friend std::ostream& operator<<(std::ostream&, const Mesh&);
```

### Example

We give a basic example of using the Mesh class. It concerns the meshing of the rectangle $[0,1] \times [1,3]$ with regular P1 geometric elements (20 by 40) where the boundary $[0,1] \times \{1\}$ is named Gamma_1 and the boundary $\{0\} \times [1,3]$ is named Gamma_2:

```
std::vector<String> sidenames(4,"");sidenames[0]="Gamma_1";sidenames[2]="Gamma_2";
Mesh mesh2d(Rectangle(0,1,1,3),_triangle,20,40,sidenames,"P1 mesh of [0,1]x[1,3]");
mesh2d.buildSides();    //build sides list
verboseLevel(3);std::cout<<mesh2d;
```

It produces the following output:

```
Mesh'P1 mesh of [0,1]x[1,3]'
  space dimension : 2, element dimension : 2
  Geometry rectangle [0,1]x[1,3] of dimension 2, BoundingBox [0,1]x[1,3], names of variable : x y
  number of elements : 1600, number of vertices : 861, number of nodes : 861, number of domains : 3 ( Omega Gamma_1 Gamma_2 )
list of elements (1600) :
geometric element 1 : triangle_Lagrange_1, orientation +1 measure = 0.00125
   nodes : 2 ->(0.05, 0) 22 ->(0, 0.05) 1 ->(0, 0)
   vertices : 2 ->(0.05, 0) 22 ->(0, 0.05) 1 ->(0, 0)
   measure of sides = 0.0707107 0.05 0.05
   sides : 61 21 1    sideOfSides : unset   adjacent elements : 2
geometric element 2 : triangle_Lagrange_1, orientation +1 measure = 0.00125
   nodes : 22 ->(0, 0.05) 2 ->(0.05, 0) 23 ->(0.05, 0.05)
   vertices : 22 ->(0, 0.05) 2 ->(0.05, 0) 23 ->(0.05, 0.05)
   measure of sides = 0.0707107 0.05 0.05
   sides : 61 62 63    sideOfSides : unset   adjacent elements : 1 3 41
geometric element 3 : triangle_Lagrange_1, orientation +1 measure = 0.00125
   nodes : 3 ->(0.1, 0) 23 ->(0.05, 0.05) 2 ->(0.05, 0)
   vertices : 3 ->(0.1, 0) 23 ->(0.05, 0.05) 2 ->(0.05, 0)
   measure of sides = 0.0707107 0.05 0.05
   sides : 64 62 2    sideOfSides : unset   adjacent elements : 2 4
...
geometric element 1600 : triangle_Lagrange_1, orientation +1 measure = 0.00125
   nodes : 860 ->(0.95, 2) 840 ->(1, 1.95) 861 ->(1, 2)
   vertices : 860 ->(0.95, 2) 840 ->(1, 1.95) 861 ->(1, 2)
   measure of sides = 0.0707107 0.05 0.05
   sides : 2458 2459 2460    sideOfSides : unset   adjacent elements : 1599
list of vertices (861) :
1 -> (0, 0)
2 -> (0.05, 0)
3 -> (0.1, 0)
...
861 -> (1, 2)
list of nodes (861) :
1 -> (0, 0)
2 -> (0.05, 0)
3 -> (0.1, 0)
...
861 -> (1, 2)
list of sides (2460) :
side 1 -> geometric side element 1601 : side 3 of element 1
side 2 -> geometric side element 1602 : side 3 of element 3
side 3 -> geometric side element 1603 : side 3 of element 5
...
side 2460 -> geometric side element 4059 : side 3 of element 1600
list of sides of sides (0) : unset
list of domains (3) :
 Domain 'Omega' of dimension 2 from mesh 'P1 mesh of [0,1]x[1,3]'
geometric element 1 : triangle_Lagrange_1, orientation +1 measure = 0.00125
geometric element 2 : triangle_Lagrange_1, orientation +1 measure = 0.00125
geometric element 3 : triangle_Lagrange_1, orientation +1 measure = 0.00125
...
geometric element 1600 : triangle_Lagrange_1, orientation +1 measure = 0.00125
 Domain 'Gamma_1' of dimension 1 from mesh 'P1 mesh of [0,1]x[1,3]'
geometric side element 1601 : side 3 of element 1
geometric side element 1602 : side 3 of element 3
geometric side element 1603 : side 3 of element 5
...
geometric side element 1620 : side 3 of element 39
 Domain 'Gamma_2' of dimension 1 from mesh 'P1 mesh of [0,1]x[1,3]'
geometric side element 1621 : side 2 of element 1
geometric side element 1622 : side 2 of element 41
geometric side element 1623 : side 2 of element 81
...
geometric side element 1660 : side 2 of element 1561
```

### 4.2.2 Meshing tools

In this section, we will study in details how work the `Mesh` constructors from `Geometry`.

```
Mesh(const Geometry& g, Number order = 1, MeshGenerator mg = _defaultGenerator, const String&
    name = ""); // constructor from 1D geometry
Mesh(const Geometry& g, ShapeType sh, Number order = 1, MeshGenerator mg = _defaultGenerator,
    const String& name = ""); // constructor from 2D and 3D geometries
```

The `MeshGenerator` argument can have the following values :

```
enum MeshGenerator
{
  _defaultGenerator=0,
  _structured, structured=_structured,
  _subdiv, subdiv=_subdiv,
  _gmsh, gmsh=_gmsh
};
```

We will now look at the behavior of the different generators :

#### Structured meshes

The "structured" generator works only on `Segment`, `Rectangle`, and `Parallelepiped` geometries, and for P1, Q1, prisme 1 or pyramid 1 finite elements. In this way, you call the following underlying methods :

```
void meshP1Segment(const Segment&, Number, const std::vector<String>&, const String& na="");
void meshP1Parallelogram(Parallelogram&, number_t, number_t, const std::vector<string_t>&,
                         set<MeshOption> mos=set<MeshOption>());
void meshQ1Parallelogram(Parallelogram&, number_t, number_t, const std::vector<string_t>&);
void meshP1Parallelepiped(const Parallelepiped& , Number, Number, Number, const
    vector<String_t>&,const String& na="");
void meshQ1Parallelepiped(const Parallelepiped& , Number, Number, Number, const
    vector<String>&,const String& na="");
void meshPr1Parallelepiped(Parallelepiped& , number_t, number_t, number_t, const
    vector<string_t>&,const string_t& na="");
void meshPy1Parallelepiped(Parallelepiped& , number_t, number_t, number_t, const
    vector<string_t>&,const string_t& na="");
```

The mesh options allowed in `meshP1Parallelogram` are related to the splitting of elementary parallelograms in two triangles : `_leftSplit` to split along the lines $x+y=c$ (default), `_rightSplit` to split along the lines $x-y=c$, `_alternateSplit` to split alternately along the lines $x+y=c$ and $x-y=c$, and `_randomSplit` to split in a random way.

#### Meshes with *subdivision* algorithm

The subdivision algorithm enables to mesh a wide set of geometries with triangles, quadrangles, tetrahedrons or hexahedrons: `Ball`, `Cube`, `RevCylindricVolume` and `SetOfElems`. This algorithm takes into account 2 main parameters : `nbsubdiv` and `order`. The first one controls the number of subdivisions to be done (mesh refinement), and the second one is the polynomial order of approximation of the geometry, which can take any (positive integer) value.

To use subdivision algorithm, dedicated constructors for the geometries are available:

```
Cube(Real x, Real y, Real z, Real edgeLen = 1., int nboctants=1, number_t nbsubdiv=0);
Cube(const Point& p1, const Point& p2, const Point& p3, const Point& p4, int nboctants, number_t
    nbsubdiv);
Cube(Real x, Real y, Real z, Real edgeLen, Real theta1, Dimen axis1, int nboctants=1, number_t
    nbsubdiv=0);
Cube(Real x, Real y, Real z, Real edgeLen, Real theta1, Dimen axis1, Real theta2, Dimen axis2,
    int nboctants=1, number_t nbsubdiv=0);
```

```
Cube(Real x, Real y, Real z, Real edgeLen, Real theta1, Dimen axis1, Real theta2, Dimen axis2,
    Real theta3, Dimen axis3, int nboctants=1, number_t nbsubdiv=0);
Ball(Real x, Real y, Real z, Real radius = 1., int nboctants=8, number_t nbsubdiv=0, number_t
    type=1);
Ball(Real x, Real y, Real z, Real radius, Real theta1, Dimen axis1, int nboctants=8, number_t
    nbsubdiv=0, number_t type=1);
Ball(Real x, Real y, Real z, Real radius, Real theta1, Dimen axis1, Real theta2, Dimen axis2, int
    nboctants=8, number_t nbsubdiv=0, number_t type=1);
Ball(Real x, Real y, Real z, Real radius, Real theta1, Dimen axis1, Real theta2, Dimen axis2,
    Real theta3, Dimen axis3, int nboctants=8, number_t nbsubdiv=0, number_t type=1);
RevCylindricVolume(Point p1, Point p2, Real radius, int nbslices=0, number_t nbsubdiv=0, number_t
    type=1, CylinderEndShape endShape1=_cesFlat, CylinderEndShape endShape2=_cesFlat, Real
    distance1=0., Real distance2=0.);
SetOfElems(const std::vector<Point>& pts, const std::vector<std::vector<number_t> >& tri, const
    std::vector<std::vector<number_t> >& bound, const number_t nbsubdiv=1);
```

The parameter `nboctants` determines which part of the geometry is to be meshed ; it is clarified in the following figures :

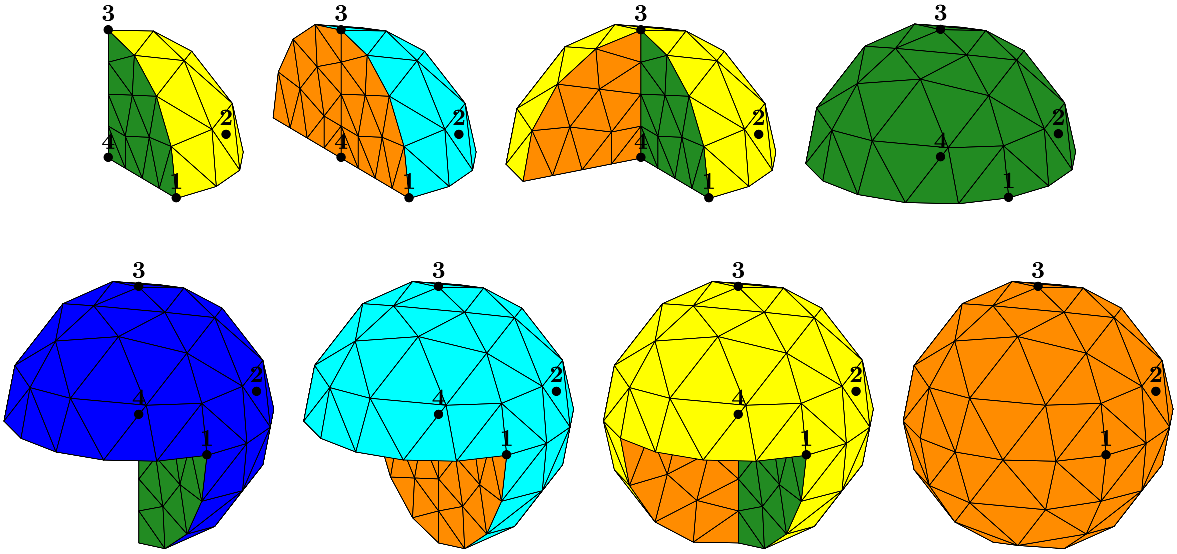


Figure 4.4: Meshes of the different portions of the sphere according to the number of octants.

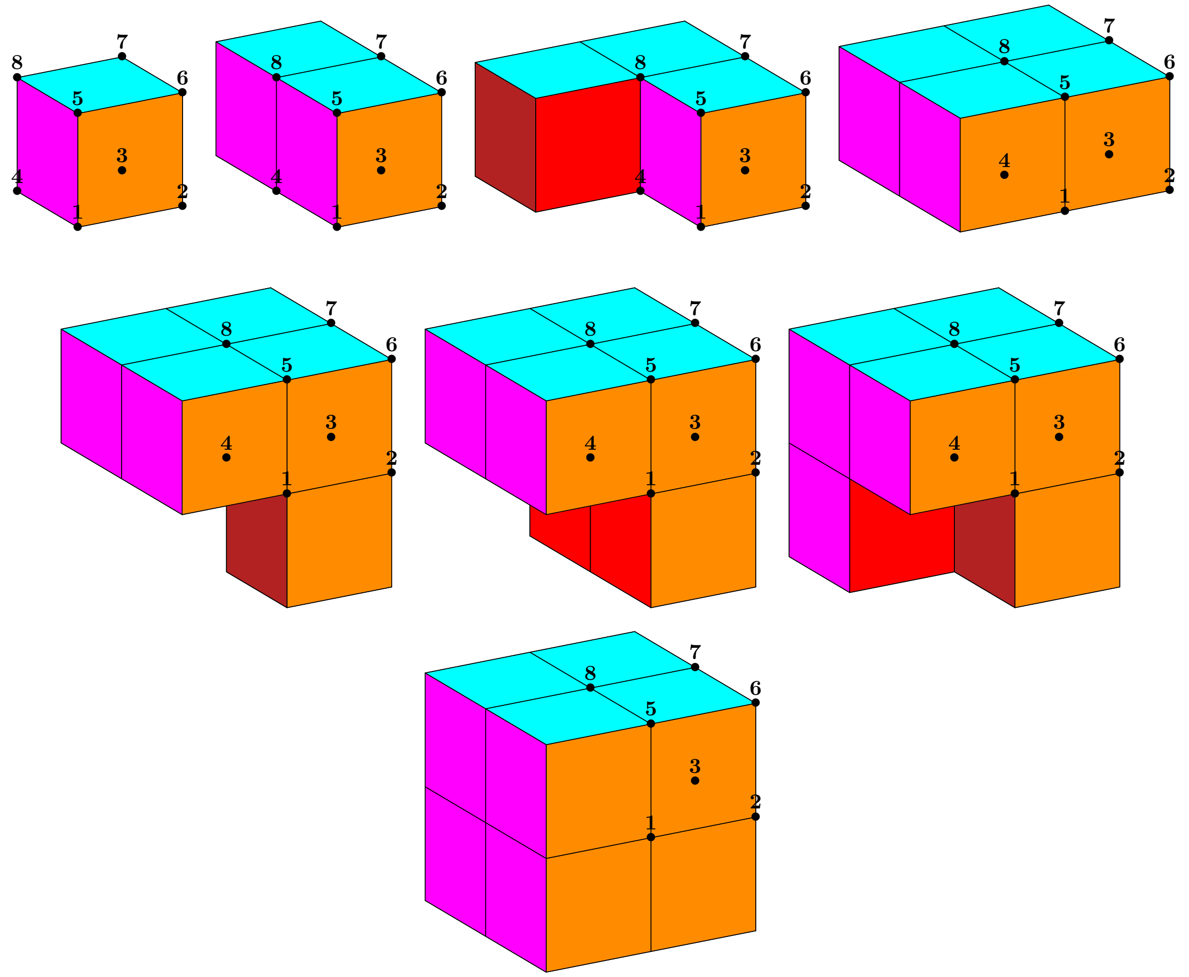


Figure 4.5: Meshes of the different portions of the cube according to the number of octants.

In this way, you call the following underlying methods :

```
void subdvMesh(Ball& sph, const ShapeType shape, const int nboctants, const number_t nbsubdiv=0,
     const number_t order=1, const number_t type=1, const string_t& name = "", const string_t&
     TeXFilename = "");
void subdvMesh(Cube& cub, const ShapeType shape, const int nboctants, const number_t nbsubdiv=0,
     const number_t order=1, const string_t& name = "", const string_t& TeXFilename = "");
void subdvMesh(RevTrunk& cyl, const ShapeType shape, const number_t nbSubDomains=1, const
     number_t nbsubdiv=0, const number_t order=1, const number_t type=1, const string_t& name =
     "", const string_t& TeXFilename = "");
void subdvMesh(Disk& carc, const ShapeType shape, const number_t nbsubdiv, const number_t order,
     const number_t type, const string_t& name, const string_t& TeXFilename);
void subdvMesh(const std::vector<Point>& pts, const std::vector<std::vector<number_t> >& elems,
     const std::vector<std::vector<number_t> >& bounds, const ShapeType shape, const number_t
     nbsubdiv=0, const number_t order=1, const string_t& name = "", const string_t& TeXFilename =
     "");
```

### Meshes with nested calls to Gmsh

This generator enables to mesh whatever geometry, canonical, "composite" or "loop". To use it, you need Gmsh installed on your computer before XLiFE++ is installed, in order to be detected. You can define meshes as if it was Gmsh directly, so that finite elements up to order 5 are allowed here.
In this way, you call the underlying external functions :

```
void Mesh::saveToGeo(Geometry& g, number_t order, const string_t& filename);
void Mesh::saveToGeo(Geometry& g, ShapeType sh, number_t order, const string_t& filename);
void saveSegmentToGeo(Segment& s, ShapeType sh, std::ofstream& fout, std::vector<PhysicalData>&
    pids, bool withLoopsStorage = true, bool withSideNames = true);
void saveEllArcToGeo(EllArc& a, ShapeType sh, std::ofstream& fout, std::vector<PhysicalData>&
    pids, bool withLoopsStorage = true, bool withSideNames = true);
void saveCircArcToGeo(CircArc& a, ShapeType sh, std::ofstream& fout, std::vector<PhysicalData>&
    pids, bool withLoopsStorage = true, bool withSideNames = true);
void savePolygonToGeo(Polygon& p, ShapeType sh, std::ofstream& fout, std::vector<PhysicalData>&
    pids, bool withLoopsStorage = true, bool withSideNames = true);
void saveTriangleToGeo(Triangle& t, ShapeType sh, std::ofstream& fout, std::vector<PhysicalData>&
    pids, bool withLoopsStorage = true, bool withSideNames = true);
void saveQuadrangleToGeo(Quadrangle& q, ShapeType sh, std::ofstream& fout,
    std::vector<PhysicalData>& pids, bool withLoopsStorage = true, bool withSideNames = true);
void saveEllipseToGeo(Ellipse& e, ShapeType sh, std::ofstream& fout, std::vector<PhysicalData>&
    pids, bool withLoopsStorage = true, bool withSideNames = true);
void savePolyhedronToGeo(Polyhedron& p, ShapeType sh, std::ofstream& fout,
    std::vector<PhysicalData>& pids, bool withLoopsStorage = true, bool withSideNames = true);
void saveTetrahedronToGeo(Tetrahedron& t, ShapeType sh, std::ofstream& fout,
    std::vector<PhysicalData>& pids, bool withLoopsStorage = true, bool withSideNames = true);
void saveHexahedronToGeo(Hexahedron& h, ShapeType sh, std::ofstream& fout,
    std::vector<PhysicalData>& pids, bool withLoopsStorage = true, bool withSideNames = true);
void saveEllipsoidToGeo(Ellipsoid& e, ShapeType sh, std::ofstream& fout,
    std::vector<PhysicalData>& pids, bool withLoopsStorage = true, bool withSideNames = true);
void saveTrunkToGeo(Trunk& t, ShapeType sh, std::ofstream& fout, std::vector<PhysicalData>& pids,
    bool withLoopsStorage = true, bool withSideNames = true);
void saveCylinderToGeo(Cylinder& c, ShapeType sh, std::ofstream& fout, std::vector<PhysicalData>&
    pids, bool withLoopsStorage = true, bool withSideNames = true);
void saveConeToGeo(Cone& c, ShapeType sh, std::ofstream& fout, std::vector<PhysicalData>& pids,
    bool withLoopsStorage = true, bool withSideNames = true);
void saveRevTrunkToGeo(RevTrunk& t, ShapeType sh, std::ofstream& fout, std::vector<PhysicalData>&
    pids, bool withLoopsStorage = true, bool withSideNames = true);
void saveRevCylinderToGeo(RevCylinder& c, ShapeType sh, std::ofstream& fout,
    std::vector<PhysicalData>& pids, bool withLoopsStorage = true, bool withSideNames = true);
void saveRevConeToGeo(RevCone& c, ShapeType sh, std::ofstream& fout, std::vector<PhysicalData>&
    pids, bool withLoopsStorage = true, bool withSideNames = true);
```

### Meshes from extrusion

The extrusion constructor can extrude any 1D or 2D mesh in the $\vec{OD}$ direction using $nbl$ layers of same width (regular extrusion). More precisely, any point $M$ of the section mesh is extruded in $nbl$ points :

$$M_k = M + O + k * \vec{OD}.$$

When a 1D section, extruded mesh is made with quadrangles. When a 2D triangular mesh section, extruded mesh is made with prisms and when a 2D quadrangular mesh section, extruded mesh is made with hexahedra.

```
Mesh(const Mesh& ms, const Point& O, const Point& D , number_t nbl,
     number_t namingDomain=0, number_t namingSection=0, number_t namingSide=0,
     const string_t& meshName=""); //constructor
void buildExtrusion(const Mesh& ms, const Point& O, const Point& D,
    number_t nbl, number_t namingDomain, number_t namingSection,
    number_t namingSide, const string_t& meshName); //effective
```

The boundary domains created by the extrusion process come from the boundary domains of the original section. This process is controlled by the 3 parameters `namingDomain`, `namingSection`, `namingSide` taking one of of the values 0, 1 or 2, with the following rules:

- 0 : domains are not created
- 1 : one extruded domain is created for any domain of the original section
- 2 : for each layer, one extruded domain is created for any domain of the original section

Be cautious, the side domains of extruded domain are created from side domains of the given section. Thus, if the given section has no side domains, the extruded domains will have no side domains! The naming convention is the following:

- Domains and side domains keep their name with the extension "_e" or "_e1", "_e2", ..., "_en"
- Section domains have the name of original domains with the extension "_0",...,"_n"
- When `namingDomain=0`, the full domain is always created and named "Omega".

The figure 4.6 illustrates the naming rules of domains.

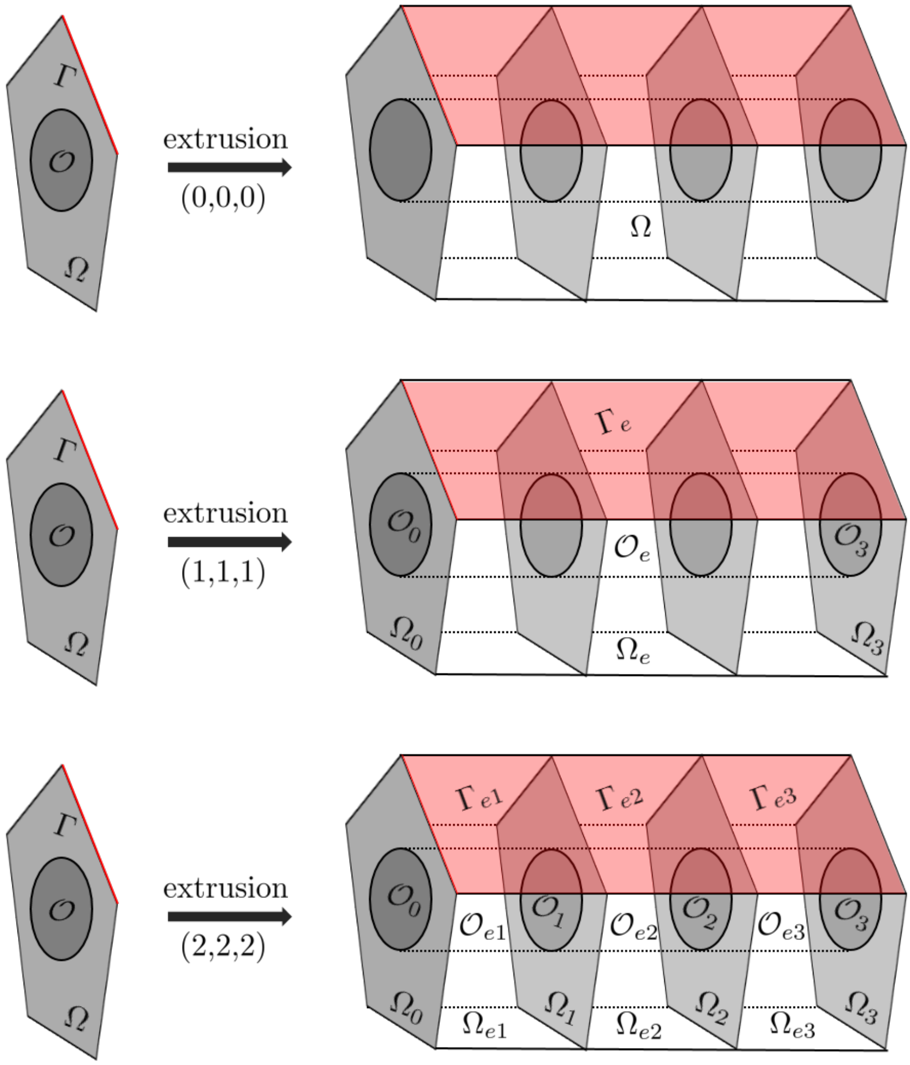


Figure 4.6: Mesh extrusion, domains naming

Note that the `meshPr1Parallelepiped` function uses this extrusion process.

### Meshes from element splitting

Sometimes it may be useful to split elements into elements of an other type, for instance to produce mesh of pyramids that are not provided by standard meshing softwares.To do this, a general constructor is offered :

```
Mesh(const Mesh& mesh, ShapeType sh, const string_t name="");
```

that calls the effective functions that processes the splitting.

Up to now, only one splitting function is available:

```
void buildPyramidFromHexadron(const Mesh& hexMesh, const string_t& meshName="");
```

that produces a pyramid mesh from an hexahedron mesh.

Note that the meshPy1Parallelepiped function uses this splitting function.

| | |
|---|---|
| library : | **geometry** |
| header : | **Mesh.hpp** |
| implementation : | **Mesh.cpp, subdivision/SubdvMesh.cpp** |
| unitary tests : | **test_Mesh.cpp** |
| header dependences : | **config.h, utils.h, GeomElement.hpp, Domain.hpp, Geometry.hpp** |

## 4.3 OpenCascade extension

Open Cascade Technology (OCT) [1] is a third party open source library dedicated to 3D CAD data. It is a powerful library dealing with canonical geometries but providing complex geometrical operations (union, intersection, difference of geometries, fillet, chamfer,... ). The standard geometry engine of XLiFE++ provides only union or difference in the case of one geometry included in an other one (if detection is easy). So to go further, XLiFE++ provides an interface to OCT. Obviously, OCT must be installed and activated in XLiFE++ (cmake option).

When OCT is activated, the macro XLIFEPP_WITH_OPENCASCADE is defined to protect any OCT specific code.

OCT library provides a very large number of classes but the central one is TopoDS_Shape encapsulating any geometry, no matter how complex. Any OCT shape is described following the boundary representation (brep) : hierarchical representation of vertices, edges(curve), wires (edge union), faces (from wire or edges), shells (face union), solids (from shell or faces) , solids union. We do not give here more details, but developer interesting in OCT interface, should have look the OCT documentation.

The purpose of the OpenCascade interface is to provide to XLiFE++ some new geometries that the standard geometrical engine is not able to manage (in particular intersection of canonical geometries). Besides, OCT geometries must be accessible in XLiFE++ for some calculus involving the parametrization of geometries (mesh being not sufficient).

### 4.3.1 The OCData class

To any Geometry may be attached an OCData object (pointer to):

```
...
#ifdef XLIFEPP_WITH_OPENCASCADE
 protected:
 mutable OCData *ocData_; //class handled main OC TopoDS_Shape and related data
#endif
```

with the OCData class :

[1] trademark @Open Cascade, https://www.opencascade.com/

```
class OCData
{ private:
  TopoDS_Shape* OCShape_;     //main OC object representing any shape
  TDocStd_Document* OCDoc_;   //additional properties related to OC shape
  ...
};
```

TDocStd_Document is an OCT class managing additional properties of TopoDS_Shape objects. In the context of XLiFE++, it is used to relate discretization parameters (hstep, nnode) and domain or side domain names to TopoDS_Shape objects.

The OCData object is not allocated until a geometric function requiring OCT capabilities has been invoked.

The OCData class provides a basic constructor, a constructor from Geometry, the copy constructor, the assign operator and the destructor:

```
OCData(TopoDS_Shape* ocshape=0, TDocStd_Document* ocdoc=0);
OCData(const Geometry& shape);
OCData(const OCData&);
OCData& operator=(const OCData&);
~OCData();
```

The constructor from Geometry is the most important. It calls the member function

```
void buildOCShape(const Geometry&);
```

that really creates OCT shapes regarding Geometry objects. This function creates the TDocStd_Document too using the other functions

```
void buildOCDocG(const Geometry&);
void buildOCDoc(const Curve&);
```

Tracking OCT shapes to relate them to names and discretization properties is a hard work. It should be revisited to simplify it!

The OCData class provides also some accessors, print tools and export functions to brep and step files:

```
[const] TopoDS_Shape& topoDS() [const];
[const] TDocStd_Document& OCDoc() [const];
ShapeDocPair asShapeDocPair() const;
bool isNull() const {return OCShape_==0;}
bool hasDoc() const {return OCDoc_!=0;}
void transform(const Transformation& t);
void print(std::ostream&, bool recursive=true) const;
void print(CoutStream&, bool recursive=true) const;
void printDoc(std::ostream& out) const;
void saveToStep(const string_t&) const;
void saveToBrep(const string_t&) const;
```

### 4.3.2 Meshing OCT geometries

As Gmsh deals with brep files (using OCT too), XLiFE++ exports OCT geometries to Gmsh in the following way:

- export the OCT geometry to the brep file *xlifepp.brep*

- create the geo script file *xlifepp.geo* containing as first line `Merge "xlifepp.brep";` and then other geo commands relating to step discretization and domain naming. It looks like

  ```
  Merge "xlifepp.brep";
  Characteristic Length{1} = 0.1;
  Characteristic Length{2} = 0.1;
  Characteristic Length{3} = 0.1;
  Characteristic Length{4} = 0.1;
  Physical Line("Gamma") = {2,4};
  Physical Line("Sigma1") = {1};
  Physical Line("Sigma2") = {3};
  Physical Surface("Square") = {1};
  ```

  This job is done by the function

  ```
  void saveToBrepGeo(Geometry&, ShapeType, number_t, std::set<MeshOption>,
                     const string_t& geofile, const string_t& brepfile) ;
  ```

- run GMSH with the script *xlifepp.geo* in non interactive mode, creating the mesh file *xlifepp.msh*,
- load the mesh file *xlifepp.msh* into a `Mesh` object.

The last two steps are not specific to the OCT extension.

To invoke the gmsh OCT meshing process, users have to specify the option `_gmshOC` as mesh generator in Mesh constructors. Note, that if no OCT functions has been previously called, the mesh command will construct recursively all OC objects related to all geometries involved.

### 4.3.3 OCT interactions in `Geometry` class

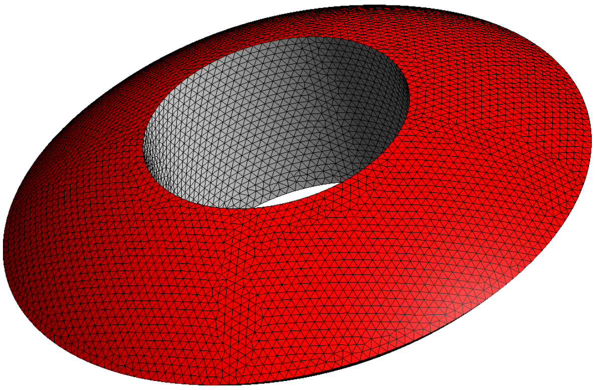
As mentioned above, `Geometry` object may instantiate `OCData` object. There are particular member functions to interact with this `OCData` object. They are defined with the macro protection `XLIFEPP_WITH_OPENCASCADE` and are all implemented in the file *opencascade.cpp* for header dependence reasons:

```
public:
 void initOC();
 void clearOC();
 void cloneOC(const Geometry&);
 [const] OCData& ocData() [const];    //built on fly if not allocated
 const TopoDS_Shape& ocShape() const; //built on fly if not allocated
 bool hasDoc() const;
 void buildOCData() const;            //built on fly if not allocated
 void ocTransformP(const Transformation&);

 void printOCInfo(CoutStream&) const;
 void printOCInfo(std::ostream&) const;
 void loadFromBrep(const string_t& file, const Strings& domNames=Strings(),
                   const Strings& sideNames=Strings(), const Reals& hsteps=Reals());

 void setOCName(OCShapeType oct,const std::vector<number_t>&, const string_t&);
 void setOCName(OCShapeType oct,number_t num, const string_t& na);
 void setOCHstep(const std::vector<number_t>& nums, real_t hstep);
 void setOCHstep(number_t num, real_t hstep);
 void setOCNnode(const std::vector<number_t>& nums, number_t nnode);
 void setOCNnode(number_t num, number_t nnode);

 Geometry& operator^=(const Geometry& g); //!< build of common part
 friend Geometry operator^(const Geometry& g1, const Geometry& g2);
```

If you intend to add new functionalities involving new OCT classes, do not forget to add the corresponding OCT include files to the *opencascade.h* file.

The following example illustrates how users deal with OCT extension :

```
Sphere S1(_center=Point(1.,0,0.),_radius=1,_hsteps=0.02,
          _domain_name="sphere",_side_names="Sigma");
Sphere S2=translate(S1,1.5,0.,0.);
RevCylinder C(_center1=Point(1,0.,0),_center2=Point(2.5,0.,0.),_radius=0.3,_hsteps=0.02,
              _domain_name="cylinder",_side_names="Gamma");
Geometry G = (S1^S2)-C;
Mesh M(G,tetrahedron,1,_gmshOC);
```



| | |
|---:|---|
| library : | **geometry** |
| header : | **OpenCascade.hpp** |
| implementation : | **OpenCascade.cpp** |
| unitary tests : | **test_OpenCascade.cpp** |
| header dependences : | **config.h, utils.h, opencascade.h, geometry1D.hpp, geometry2D.hpp, geometry3D.hpp, Mesh.hpp** |

## 4.4 Domain management

Main objects in variational formulation are integrals over a geometrical domain. Geometrical domains can be any subset of any dimension of the computational geometrical domain, usually given by a mesh. But they can also be defined from analytical parametrisations. Besides, it me bay useful to consider unions of domains and sometimes, intersections of domains. Such "composite" domains are involved when evaluating linear combination of integrals over different domains. To deal with all this kind of geometrical domains, the following classes are provided:

- `MeshDomain` class to deal with domain defined from a list of mesh elements,
- `CompositeDomain` class to deal with domain defined as an union or an intersection of MeshDomains,
- `AnalyticalDomain` class to deal with domain defined from parametrisations (not yet implemented).
- `PointsDomain` class to deal with domain managing only a list of Points (cloud)

These classes inherit from the `GeomDomain` base class.
In order for the end user to deal with only a single class (`GeomDomain`), we use the "abstract/non abstract" pattern: `GeomDomain` has a `GeomDomain*` member attribute that points either to a child (end user object) or to

itself (child object). Constructors of GeomDomain class construct child objects and member functions (either virtual or not) are interfaces with children.

### 4.4.1 The GeomDomain base class

The GeomDomain base class has only two pointers as member attributes, one for general information and the other for child

```
class GeomDomain
{protected :
   DomainInfo* domainInfo_p;     // pointer to domain information class
   GeomDomain* domain_p;         // pointer to its child or itself if a child
   static std::vector<const GeomDomain*> theDomains; // list of all domains
   ...
```

where DomainInfo is the simple class:

```
class DomainInfo
{public :
   String name;          // name of domain
   Dimen dim;            // dimension of domain (the max when compositeDomain)
   DomainType domType;   // type of domain
   const Mesh* mesh_p;   // pointer to mesh
   String description;   // additionnal information
  DomainInfo(const String&, Dimen, DomainType, const Mesh*, const String& = "");
};
```

The type of domain is defined by the enumeration:

```
enum DomainType {_undefDomain = 0, _analyticDomain, _meshDomain,
                 _compositeDomain, _pointsDomain}
```

In order to not have clones of domains, created domains are listed in the static vector theDomains.

> There is no reason to instantiate child objects without using base class constructors like. Thus, only base class objects are collected in the static vector theDomains and not child objects!

The GeomDomain base class provides a basic constructor and child constructors like that construct a child object in memory and store its pointer in the domain_p attribute:

```
GeomDomain(const String & na="",dimen_t d=0, const Mesh* m=0);
GeomDomain(const Mesh&, const String&, Dimen, const String& =""); //build meshdomain
GeomDomain(SetOperationType sot,
           const GeomDomain&,const GeomDomain&,
           const String & na="");    //build composite domain with two domains
GeomDomain(SetOperationType sot,
           const std::vector<const GeomDomain*>&,
           const String & na="");   //build composite domain with n domains
~GeomDomain();                      //destructor
```

The set operations available are listed in the SetOperationType enumeration:

```
enum SetOperationType{_union, _intersection};
```

The class has the following accessors, some to access to DomainInfo attributes, the others to access to child attributes through polymorphism behaviour:

```
const String& name() const;
Dimen dim() const;
```

```
const DomainType domType() const;
const Mesh* mesh() const;
const String& description() const;
virtual const MeshDomain* meshDomain() const;             // non const also
virtual const CompositeDomain* compositeDomain() const;    // non const also
virtual const AnalyticalDomain* analyticalDomain() const; // non const also
```

For instance, the virtual accessor `meshDomain()` has the following implementation in the base class:

```
const MeshDomain* GeomDomain::meshDomain() const
{if(domain_p!=this) return domain_p->meshDomain();
 error("domain_notmesh");
 return 0;
}
```

and the `meshDomain()` function in the `MeshDomain()` child class is:

```
const MeshDomain* MeshDomain::meshDomain() const {return this;}
```

Besides, some useful member functions are provided

```
void rename(const String&) ;          //rename domain
void addSuffix(const String&);        //add a suffix to domain name
Dimen spaceDim() const;               //return the space dimension
const String domTypeName() const;     //return domain type name
virtual bool isUnion() const;         //true if union
virtual bool isIntersection() const; //true if intersection
virtual bool include(const GeomDomain&) const; //true if includes a domain
virtual Number numberOfElements() const;  // number of geometric elements
virtual GeomElement* element(Number); //access to k-th element (k>=1)
virtual void setMaterialId(Number);    //set material id (>0) for all elements
virtual void setDomainId(Number);      //set a domain id for all elements
virtual void clearGeomMapData();       //clear geometric data
virtual const GeomDomain* largestDomain(std::vector<const GeomDomain*>) const;
```

There are some static member functions to search domains in the domain list and to print the domain list:

```
static const GeomDomain* findDomain(const GeomDomain*);
static const GeomDomain* findDomain(SetOperationType,
                                    const std::vector<const Domain*>&);
static void printTheDomains(std::ostream&);
```

To manage the union of domains, the following functions are proposed:

```
const GeomDomain* geomUnionOf(std::vector<const GeomDomain*>&);
GeomDomain& merge(const std::vector<GeomDomain*>&, const String& name); //merge n domains
GeomDomain& merge(GeomDomain&, GeomDomain&, const String& name);    //merge 2 domains
...
```

The `geomUnionOf` function constructs (or identifies) the symbolic union of domains, say in the meaning of composite domains, whereas `merge` functions create a true union of domains by merging list of elements.

There are some tools to set the normal orientations (see `MeshDomain` class for some explanations):

```
virtual void setNormalOrientation(OrientationType, const GeomDomain&) const;
virtual void setNormalOrientation(OrientationType, const Point&) const;
virtual void setNormalOrientation(OrientationType = _undefOrientationType,
                           const GeomDomain* gp=0, const Point* p=0) const;
```

Finally, the class provides print facilities:

```
virtual void GeomDomain::print(std::ostream&) const;
std::ostream& operator<<(std::ostream&,const GeomDomain&);
```

### 4.4.2 The `MeshDomain` child class

The `MeshDomain` child class handles a domain defined as a list of mesh elements, say a lis tof `GeomElement` objects that is a basic stone of a mesh.

```
class MeshDomain : public GeomDomain
{ public :
    vector<GeomElement*> geomElements; //list of geometric elements
  ...
```

It manages other important informations :

```
protected :
  MeshDomain* parent_p;            //parent mesh domain if submesh domain
public :
  set<ShapeType> shapeTypes;       //list of element shape types in mesh domain
  const MeshDomain* extensionof_p; //side domain pointer extension pointer
  mutable pair<OrientationType, const GeomDomain*> normalOrientationRule;  //orientation rule
```

`shapeTypes` is the list of element shape types contains at least one item and more than one if the mesh domain is a mixture of different elements. For instance if there are some triangles and quadrangles, the `shapeTypes` list has two items (`_triangle`,`_quadrangle`).
The `MeshDomain` pointer `parent_p` gives a link to its parent domain when it is a side domain.
The `MeshDomain` pointer `extensionof_p` gives a link to its "child" when domain is an extension of a side domain. The extension of a side domain is the set of elements having a side (edge/face) located on the side domain. Such domains are required to compute boundary terms that involves non tangential derivative, for instance:

$$\int_\Gamma \partial_x u\, v.$$

`normalOrientationRule` stores informations about the way the normals of a manifold domain are oriented :

- an orientation type from the enumeration

```
enum OrientationType{_undefOrientationType, _towardsInfinite,
                     _outwardsInfinite, _towardsDomain, _outwardsDomain};
```

- a `GeomDomain` pointer providing the domain involved when `_towardsDomain` or `_outwardsDomain` is selected

> When not specified, `_towardsInfinite` is chosen for an immersed manifold and `_outwardsDomain` for a boundary (may be hazardous when the boundary is an interface).

Two structures useful to locate element from point, may be also constructed if they are required:

```
mutable std::map<Point,std::list<GeomElement*> > vertexElements;
mutable KdTree<Point> kdtree;
```

The first one gives for any vertex of the domain, the list of elements having this vertex and the second is a kdtree structure (tree of points) allowing to get in a short time the vertex closest to a given point. These structures are built on the fly by interpolation tools.

The class manages also some flags to know what quantities are already computed :

```
mutable bool orientationComputed;
mutable bool jacobianComputed;
mutable bool diffEltComputed;
mutable bool normalComputed;
mutable bool inverseJacobianComputed;
```

This class provides a single basic constructor and the member functions related to virtual member functions of the `GeomDomain` base class:

```
MeshDomain(const Mesh&,const String&,Dimen);
MeshDomain* meshDomain();
const MeshDomain* meshDomain() const;
```

Some accessors and basic tools are provided:

```
MeshDomain* parent() const {return parent_p;};
void setShapeTypes();
virtual MeshDomain* meshDomain();
virtual const MeshDomain* meshDomain() const;
virtual bool isUnion() const;
virtual bool isIntersection() const;
bool isSideDomain() const;
virtual Number numberOfElements() const;
virtual GeomElement* element(Number);
virtual void setMaterialId(Number);
virtual void setDomainId(Number);
```

The `setMaterialId` and `setDomainlId` end user functions propagates Ids to all geometric elements of the domain. It is the way to get some physical information in FE computation at a low level.

There are more specific tools related to mesh domains:

```
//node access
std::set<Number> nodeNumbers() const;
std::vector<Point> nodes() const;
//set functions
virtual bool include(const GeomDomain&) const;
bool include(const MeshDomain& d) const;
bool isUnionOf(const std::vector<const GeomDomain*>&)const;
const GeomDomain* largestDomain(std::vector<const GeomDomain*>)const;
//Geometric tool
void setNormalOrientation(OrientationType, const GeomDomain& ) const;
void setNormalOrientation(OrientationType, const Point&) const;
void setNormalOrientation(OrientationType = _undefOrientationType,
                          const GeomDomain* gp=0, const Point* p=0) const;
void setOrientationForManifold(OrientationType = _towardsInfinite,
                               const Point* P=0) const;
void setOrientationForBoundary(OrientationType ort =_outwardsDomain,
                               const GeomDomain*  =0) const;
void reverseOrientations() const;
void buildGeomData() const;
void clearGeomMapData();
//create domain extension
const GeomDomain* extendDomain() const;
//tools to locate element
void buildVertexElements() const;
void buildKdTree() const;
GeomElement* locate(const Point&) const;
```

The `buildGeomData` function constructs measure and orientation of the elements of the domain.

The orientation of an element is the sign $s$ such that the normal computed times $s$ is the desired normal. When domain is a side domain, the orientations are either constructed using a tracking algorithm (setOrientationForManifold) or using a "volumic" algorithm (setOrientationForBoundary) when the side domain is the boundary of a "volumic" domain. In case of an open manifold (e.g screen) the global orientation is correct but unpredictable.It may be controlled by specifying an "interior" point. Contrary to most FE softwares, XLIFE++ does not assume that the numbering of nodes provided by meshing tools gives the outward normals! So the normal are always oriented by XLIFE++.

> The computation of normal vector orientations is not done when mesh is generated or loaded but it is done during the construction of a space involving a manifold or during the computation of a Term involving normal vectors.

Users can access to the normal at a point using the following function:

```
Vector<real_t> getNormal(const Point& x, OrientationType ort =
                _undefOrientationType, const GeomDomain& dom = GeomDomain()) const;
```

The locate function is a powerful tool that returns one of the elements including a given point (null pointer if no element). It is used in all interpolation operations. It is wellknown that this operation is time expansive. This is the reason why additional structures vertexElements and kdtree may be constructed if point location is required. This structures are constructed only once by buildVertexElements and buildKdTree functions at the first call of locate. The time to locate a point is generally (may be worth) in $log(n)$ ($n$ the number of vertices).

Some print/export stuff is available:

```
virtual void print(std::ostream&) const;
friend std::ostream& operator<<(std::ostream&, const MeshDomain&);
void saveNormalsToFile(const string_t&, IOFormat iof=_vtk) const;
```

### 4.4.3 The CompositeDomain child class

The CompositeDomain child class describes set operations (union and intersection) of geometrical domains (Domain objects). It is an abstact description that it means that elements lists of MeshDomain objects are not merged or intersected!

```
class CompositeDomain : public GeomDomain
{protected :
  SetOperationType setOpType_;              //type of the set operation
  std::vector<const Domain*> domains_;      //list of domains
      ...
```

SetOperationType enumerates _union and _intersection values.

This class provides a single basic constructor, an accessor to the set operation and the member functions related to virtual member functions of the GeomDomain base class:

```
CompositeDomain(SetOperationType, const std::vector<const GeomDomain*>&,const String&);
SetOperationType setOpType() const;
const std::vector<const GeomDomain*>& domains() const;
CompositeDomain* compositeDomain();
const CompositeDomain* compositeDomain();
bool isUnion() const;
bool isIntersection() const;
std::vector<const GeomDomain *> basicDomains() const;    //recursive
virtual Number numberOfElements() const;
void print(std::ostream&) const;
```

The basicDomains() function is recursive and provides the list of all basic domains, that are domains which are not composite domains.

### 4.4.4 The PointsDomain child class

This class deals with domain only defined by a list of points (cloud):

```
class PointsDomain : public GeomDomain
{
public :
 std::vector<Point> points;
 PointsDomain(const std::vector<Point>&, const String& = "");
 PointsDomain* pointsDomain();
 const PointsDomain* pointsDomain() const;
 const Point& point(Number n) const;
 Point& point(Number n);
 virtual bool include(const GeomDomain&) const;
 virtual void print(std::ostream&) const;
};
```

It may be useful but it is not used in core of the library!

### 4.4.5 The AnalyticalDomain child class

This class has not be yet implemented (here for future usage).

### 4.4.6 The Domains class

Domains is an alias of PCollection<GeomDomain> class that manages a collection of GeomDomain, in fact a std::vector<GeomDomain*> (see the definition of PCollection). It may be used as following:

```
Strings sn("Gamma1","Gamma2","Gamma3","Gamma4");
Mesh mesh2d(Rectangle(_xmin=0,_xmax=0.5,_ymin=0,_ymax=1,_nnodes=Numbers(3,6),
            _domain_name="Omega",_side_names=sn),_triangle,1,_structured);
Domain omega=mesh2d.domain("Omega"),
       gamma1=mesh2d.domain("Gamma1"), gamma2=mesh2d.domain("Gamma2"),
       gamma3=mesh2d.domain("Gamma3"),gamma4=mesh2d.domain("Gamma4");
Domains ds3(gamma1,gamma2,gamma3);
Domains ds4;
for(Number i=0;i<4;i++) ds4<<mesh2d.domain(i+1);
Domains ds5(5);
for(Number i=1;i<=5;i++) ds5(i)=mesh2d.domain(i-1);
```

> If C++11 is available (the library has to be compiled with C++11), the following syntax is also working:
>
> ```
> Domains dsi={gamma1,gamma2,gamma3};
> ```

### 4.4.7 The DomainMap class

Transporting a point from one domain to an other one may be useful, in particular to relate two domains, for instance when dealing with a periodic condition or when interpolating a mesh to an other. XLiFE++ provides the DomainMap class that allows to associate a function (the map) to a pair of domains:

```
protected:
 const GeomDomain* dom1_p; // start domain
 const GeomDomain* dom2_p; // end domain
```

```
 Function map1to2_;         // map function from domain1 to domain2
public:
 bool useNearest;           // use nearest method instead of locate method after mapping
 string_t name;             // a unique name
```

The following constructors, destructor and accessors are proposed:

```
DomainMap();   // private
DomainMap(const GeomDomain&, const GeomDomain&, const Function&, bool nearest=false);
DomainMap(const GeomDomain&, const GeomDomain&, const Function&, const string_t&,
          bool nearest=false);
~DomainMap();
const GeomDomain& dom1() const;   // returns start domain
const GeomDomain& dom2() const;   // returns end domain
const Function& map1to2() const; // returns map function
```

DomainMap objects are usually shadowed to the users. They are collected in a static map (list of DomainMap pointers indexed by their names):

```
static std::map<string_t, DomainMap *> theDomainMaps; // list of existing maps indexed by name
static void clearGlobalVector();                      // delete all map objects
static void removeMaps(const GeomDomain&);    // delete and remove maps involving a given domain
```

To deal with domain maps, users have access to the following functions

```
void defineMap(const GeomDomain&, const GeomDomain&, const Function&, bool nearest=false);
void defineMap(const GeomDomain&, const GeomDomain&, const Function&, const string_t&,
               bool nearest=false);
const DomainMap* domainMap(const GeomDomain&, const GeomDomain&);
const Function* findMap(const GeomDomain&, const GeomDomain&);
const Function* buildMap(const GeomDomain&, const GeomDomain&);
Vector<real_t> domainTranslation(const Point&, Parameters& pa = defaultParameters);
```

If no name is provided by the defineMap, a default name is created : "dom1.name –> dom2.name". The DomainMap must be unique. If not an error is raised during its construction/definition.

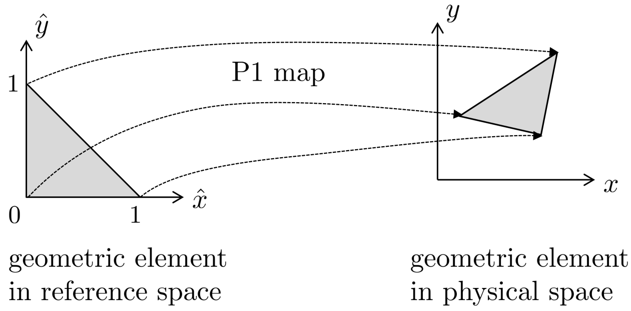
Several FE computation functions require some maps between domains. They query the global DomainMap to find a map that relates a pair of domains (findMap function). So the map has to be defined before! In the particular case where the two domains are in translation (same shape, boundary points in translation), the map is constructed on the fly using the functions builddMap and domainTranslation.

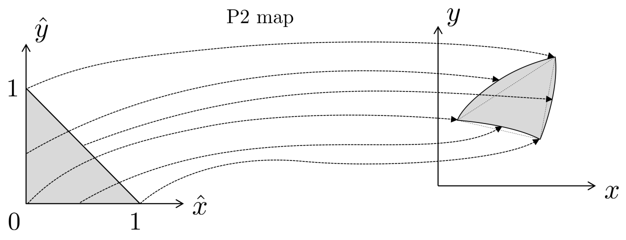
☠ Up to now, FE computation functions do not deal with the name of the map but only with a domain pair. As a consequence, if several maps are related to the same pair of domains, the first one in the map will be used! In future, this behavior should be improved.

| | |
|---|---|
| library : | **geometry** |
| header : | **GeomDomain.hpp, DomainMap.hpp** |
| implementation : | **GeomDomain.cpp, DomainMap.cpp** |
| unitary tests : | **test_Domain.cpp** |
| header dependences : | **config.h, utils.h** |

## 4.5 Geometric element

The atomic object of a mesh is a geometric element, that is a segment, a polygon or a polyhedron of physical space with flat or curved faces or edges. A general way to describe it, consists in giving a polynomial interpolation and a reference geometric element in reference space. Thus, a geometric element is the image by the map of a reference geometric element. This map is defined from the polynomial interpolation and some nodes of the geometric element: vertices and extra points regarding the order of the polynomial interpolation.





Geometric elements are the geometric supports of finite element. In other words, a finite element is defined from a geometric element and an interpolation (different from interpolation used in geometric element!), see `Element` class in *space* library.

As some finite elements may be required on a boundary of domain, geometric element can be a side of geometric element and even a side of side. It is the reason why a geometric element can possibly manage side informations (parent and side number).

### 4.5.1 The `GeomElement` class

The `GeomElement` class has only four protected members:

```
class GeomElement
{protected :
   const Mesh* mesh_p;                         //pointer to the mesh
   Number number_;                             //unique id number
   MeshElement* meshElement_p;                 //pointer to a MeshElement
   std::vector<GeoNumPair> parentSides_;       //if a side element
   ...
```

The most important member `meshElement_p` is a pointer to a `MeshElement` object collecting real geometric informations (nodes, numbering, reference element, map data, ...). This class is detailed in the next section.

Besides, it manage some additional informations :

```
Number materialId;     // material id (default= 0)
Number domainId;       // domain id (default=0)
Real theta, phi;       // angles to describe local curvature (default 0,0)
```

`GeoNumPair` is an alias for storing a pair of parent geometric element and a side number:

```
typedef std::pair<GeomElement*,Number> GeoNumPair;
```

When the geometric element is a side of a geometric element, parentSides_ is not empty and by default, the meshElement_p is null. Note that it is possible to build it. Of course, when geometric element is not a side element (say plain element), parentSides_ is empty.

This class provides few public constructors, an assignment operator and a destructor:

```
GeomElement(const Mesh* m=0, Number n = 0);
GeomElement(const Mesh*, const RefElement*, Dimen, Number);  //for plain element
GeomElement(GeomElement*, Number, Number);                   //for side element
GeomElement(const GeomElement&);
GeomElement& operator =(const GeomElement&);
```

some simple accessors:

```
Number number() const;
Number& number();
bool hasMeshElement() const;
bool isSideElement() const;
```

and complex accessors working for plain or side elements, even if meshElement_p is null :

```
const MeshElement* meshElement() const;
MeshElement* meshElement();
const GeomElement* parent(Number i=0) const;
const GeoNumPair parentSide(Number i) const;
std::vector<GeoNumPair>& parentSides();
Dimen elementDim() const;
const RefElement* refElement(Number s = 0) const;
const GeomRefElement* geomRefElement(Number s = 0) const;
Number numberOfVertices() const;
Number numberOfSides() const;
Number numberOfSideOfSides() const;
ShapeType shapeType(Number s = 0) const;
Number vertexNumber(Number i) const;
Number nodeNumber(Number i) const;
std::vector<Number> vertexNumbers(Number s = 0) const;
std::vector<Number> nodeNumbers(Number s = 0) const;
```

s means a side number of element and when it is null, function applies to element itself. Most of these member functions are recursive. It allows to get data for plain, side and side of side elements (side of side of side is not managed). Be cautious, these member functions does not check the integrity of data. For instance, the function meshElement() may return a null pointer (case of a side element).

For a side element, it is possible to construct, if really necessary, its MeshElement structure using the member function:

```
void buildSideMeshElement();
void deleteMeshElement();          // destroy meshElement information
```

There is an encoding function which constructs a string key with global numbers of vertices of the geometric element (s=0) or its side (s). This function is used to build global lists of sides (edge in 2D or face in 3D), of side of sides (edge in 3D) and vertices (see the Mesh class).

```
String encodeElement(Number s=0) const;
```

Related to these global lists, the following functions return temporary lists of adjacent elements by side, by side of side or by vertex:

```
GeoNumPair elementsSharingSide(Number s) const;
std::vector<GeoNumPair> elementsSharingVertex(Number v,bool o=false) const;
std::vector<GeoNumPair> elementsSharingSideOfSide(Number s, bool o=false) const;
```

When the boolean argument `o` is true, it means that elements in lists are adjacent **only** by side of side or only by vertex. When it is false, all elements are listed. Obviously, these functions work only if the global lists of sides, of side of sides and vertices have been constructed before. By default, they are not (see the `Mesh` class).

The class provides a function to test if a point belongs to element:

```
bool contains(const std::vector<Real>& p);
```

It is possible to compare `GeomElement` objects by their indices (`number_`) using the operators:

```
bool operator== (const GeomElement&, const GeomElement&);
bool operator<  (const GeomElement&, const GeomElement&);
```

For output purpose, you can split a GeomElement in first order elements, either simplices or of same shape :

```
std::vector<GeomElement*> splitP1() const;
std::vector<GeomElement*> splitO1() const;
```

Finally, the `GeomElement` class provides usual printing facilities:

```
void print(std::ostream&) const ;
friend std::ostream& operator<< (std::ostream&, const GeomElement&);
```

### 4.5.2 The `MeshElement` class

`MeshElement` is the real class storing geometric element data:

```
class MeshElement
{public:
  std::vector<Point*> nodes;                 //nodes of element
  std::vector<Number> nodeNumbers;           //global numbers of node
  std::vector<Number> vertexNumbers;         //global numbers of vertices
  std::vector<Number> sideNumbers;           //global numbers of sides
  std::vector<Number> sideOfSideNumbers;     //global numbers of side of sides
  short int orientation;                     //element orientation
  std::vector<Real> measures;                //measure of element and its sides
  GeomMapData* geomMapData_p;                //useful data for geometric map
 private:
  Number index_;                             //element index
  const Dimen spaceDim_;                     //space dimension
  const RefElement* refElt_p;          //pointer to associated Reference Element
  ...
```

The vector `nodes` gives a direct access to the node coordinates of the element (it is redundant). The numbering vectors `nodeNumbers`, `vertexNumbers`, `sideNumbers` and `sideOfSideNumbers` are related to global vectors defined in `Mesh` ; `nodes`, `vertices_`, `sides_` and `sideOfSide_`. Note that the `sideNumbers` and `sideOfSideNumbers` vectors are not built by default (see the `buildSides` and `buildSideOfSides` member functions of `Mesh` class). The `nodeNumbers` and `vertexNumbers` vectors are the same for one order polynomial geometric interpolation.

The orientation of an element is defined by default as the sign of the determinant of the jacobian of the geometric map from reference element to geometric element; this map being well defined through the `RefElement` pointer refElt_p and the geometric element nodes. But, this orientation may be changed by the function setOrientationForManifold which set the orientation in order the normal computed from jacobian be always the outward normal.

Besides, the MeshElement class manages a pointer to a GeomMapData object storing computational data related to the geometric map: jacobian matrix, its inverse, its determinant, ... see the next section.

> As it refers to some Mesh class members, MeshElement object should not be instanciated independantly of a mesh.

The class has only one basic constructor initializing the RefElement pointer, the space dimension and the element index:

```
MeshElement();
MeshElement(const RefElement*, Dimen, Number);
~MeshElement();
```

It means that numbering informations has to be given outside the constructor. Generally, this is done by meshing tools.

There are some useful accessors, most of them providing same information as those defined in the GeomElement interface class:

```
Number index() const;
Dimen spaceDim() const;
Number order() const;
Real measure(const Number s = 0) const;
const RefElement* refElement(Number s = 0) const;
const GeomRefElement* geomRefElement(Number i = 0) const;
Dimen elementDim() const;
ShapeType shapeType(Number s = 0) const;
Number vertexNumber(Number i) const;
Number nodeNumber(Number i) const;
std::vector<Number> verticesNumbers(Number s=0) const;
Number numberOfNodes() const;
Number numberOfVertices() const;
Number numberOfSides() const;
Number numberOfSideOfSides() const;
```

Besides, there are some computation functions related to geometric element:

```
void computeMeasures();
void computeMeasure();
void computeMeasureOfSides();
void computeOrientation();
bool contains(const std::vector<Real>&);
void clearGeomMapData();
```

The functions related to jacobian computations are defined in the GeomMapData class. The geomMapData_p pointer may be used to store map data and the function clearGeomMapData() deletes the GeomMapData object.

Finally, MeshElement informations are displayed with:

```
void print(std::ostream&) const;
friend std::ostream& operator<< (std::ostream&, const MeshElement&);
```

| | |
|---|---|
| library : | **geometry** |
| header : | **GeomElement.hpp** |
| implementation : | **GeomElement.cpp** |
| unitary tests : | **test_GeomElement.cpp** |
| header dependences : | **config.h, utils.h** |

## 4.6 Transformations on points, geometries and meshes

XLIFE++ allows you to apply geometrical transformations on `Point`, `Mesh`, `Geometry` and `Geometry` children objects. The main type is `Transformation`. It can be a canonical transformation or a composition of transformations.

### 4.6.1 Canonical transformations

In the following, we will consider straight lines and planes.
A straight line is fully defined by a point and a direction. The latter is a vector of components (2 or 3). This is a reason why we will write a straight line as follows : $\left(\Omega, \vec{d}\right)$
A plane is fully defined by a point and a normal vector. This is a reason why we will write a plane as follows : $[\Omega, \vec{n}]$

**Translations**

Point B is the image of point A by a translation of vector $\vec{u}$ if and only if

$$\overrightarrow{AB} = \vec{u}$$

A translation can be defined by a STL vector (size 2 or 3) or its components:

```
Vector<Real> u;
Real ux, uy, uz;
Translation t1(u), t2(ux, uy), t3(ux, uy, uz);
```

u can be omitted. If so, its default value is the 3d zero vector. uy and uz can be omitted too. If so, their default value is 0.

As the `Vector` class inherits from `std::vector` you can use it in place of `Vector` because all prototypes are based on `std::vector`.

**2d rotations**

Point B is the image of point A by the 2d rotation of center $\Omega$ and of angle $\theta$ if and only if

$$\overrightarrow{\Omega B} = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix} \overrightarrow{\Omega A}$$

A 2d rotation is defined by a point and an angle (in radians):

```
Point omega;
Real angle;
Rotation2d r(omega, angle);
```

`angle` can be omitted. If so, its default value is 0 and `omega` can be omitted too. If so, its default value is the 3d zero point.

### 3d rotations

Point B is the image of point A by the 3d rotation of axis $\left(\Omega,\vec{d}\right)$ and of angle $\theta$ (in radians) if and only if

$$\overrightarrow{\Omega B} = \cos\theta\,\overrightarrow{\Omega A} + (1-\cos\theta)\,\overrightarrow{\Omega A}\cdot\vec{n} + \sin\theta\,\vec{n}\wedge\overrightarrow{\Omega A} \quad \text{(Rodrigues' rotation formulae)}$$

where $\vec{n} = \dfrac{\vec{u}}{||\vec{u}||}$ (the unitary direction).

The direction can be defined by a STL vector or by its components:

```
Point omega;
Vector<Real> d;
Real dx, dy, dz;
Real theta;
Rotation3d r1(omega, d, theta), r2(omega, dx, dy, dz, theta);
```

In the first syntax, `angle` can be omitted. If so, its default value is 0. and `d` can also be omitted. If so, its default value is the 3d zero vector.
In the second syntax, `dz` can be omitted too. If so, its default value is 0.

### Homotheties

Point B is the image of point A by the homothety of center $\Omega$ and of factor $k$ if and only if

$$\overrightarrow{\Omega B} = k\,\overrightarrow{\Omega A}$$

```
Point omega(1.,2.,3.);
Real k=2.;
Homothety h(omega, k);
```

`factor` can be omitted. If so, its default value is 0. and `omega` can also be omitted. If so, its default value is the 3d zero vector.

### Point reflections

Point B is the image of point A by the point reflection of center $\Omega$ if and only if s

$$\overrightarrow{\Omega B} = -\overrightarrow{\Omega A}$$

It is an homothety of factor -1 and same center.

```
Point omega(1.,2.,3.);
PointReflection h(omega); // omega can still be omitted, as for homothety
```

### 2d reflections

Point B is the image of point A by the 2d reflection of axis $\left(\Omega,\vec{d}\right)$ if and only if

$$\overrightarrow{AB} = 2\overrightarrow{AH} \quad \text{where } H \text{ is the orthogonal projection of } A \text{ on } \left(\Omega,\vec{d}\right)$$

```
Point omega(1.,2.,3.);
Vector<Real> d(1.,0.,0.);
Real dx=1., dy=0.;
Reflection2d r1(omega, d), r2(omega, dx, dy);
```

In the first syntax, `d` can be omitted. If so, its default value is the 2d zero vector and `omega` can be omitted. If so, its default value is the 2d zero point.

### 3d reflections

Point B is the image of point A by the 2d reflection of plane $[\Omega,\vec{n}]$ if and only if

$$\overrightarrow{AB} = 2\overrightarrow{AH} \quad \text{where } H \text{ is the orthogonal projection of } A \text{ on } [\Omega,\vec{n}]$$

```
Point omega(1.,2.,3.);
Vector<Real> n;
Real nx, ny, nz;
Reflection3d r1(omega, n), r2(omega, nx, ny, nz);
```

In the first syntax, `n` can be omitted. If so, its default value is the 3d zero vector and `omega` can be omitted. If so, its default value is the 3d zero point.

## 4.6.2 Composition of transformations

To define a composition of transformations, you can use the operator * between canonical transformations, an is the following example:

```
Rotation2d r1(Point(0.,0.), 120.);
Reflection2d r2(Point(1.,-1.), 1.,2.5, -3.);
Translation t1(-1.,4.);
Homothety h (Point(-1.,0.), -3.2);
Transformation t = r1*h*r2*t1;
```

Composition * has to be understood as usual composition operator $\circ$ : `t(P)=r1(h(r2(t1(P))))`.

## 4.6.3 Applying transformations

### How to apply a transformation ?

In this paragraph, we will look at the `Cube` object, but you have same functions for any canonical or composite `Geometry`.

If you want to apply a transformation and modify the input object, you can use one of the following functions:

```
//! apply a geometrical transformation on a Cube
Cube& Cube::transform(const Transformation& t);
//! apply a translation on a Cube
Cube& Cube::translate(std::vector<Real> u = std::vector<Real>(3,0.));
```

```
Cube& Cube::translate(Real ux, Real uy = 0., Real uz = 0.);
//! apply a rotation 2d on a Cube
Cube& Cube::rotate2d(const Point& c = Point(0.,0.), Real angle = 0.);
//! apply a rotation 3d on a Cube
Cube& Cube::rotate3d(const Point& c = Point(0.,0.,0.), std::vector<Real> u =
    std::vector<Real>(3,0.), Real angle = 0.);
Cube& Cube::rotate3d(Real ux, Real uy, Real angle);
Cube& Cube::rotate3d(Real ux, Real uy, Real uz, Real angle);
Cube& Cube::rotate3d(const Point& c, Real ux, Real uy, Real angle);
Cube& Cube::rotate3d(const Point& c, Real ux, Real uy, Real uz, Real angle);
//! apply a homothety on a Cube
Cube& Cube::homothetize(const Point& c = Point(0.,0.,0.), Real factor = 1.);
Cube& Cube::homothetize(Real factor);
//! apply a point reflection on a Cube
Cube& Cube::pointReflect(const Point& c = Point(0.,0.,0.));
//! apply a reflection2d on a Cube
Cube& Cube::reflect2d(const Point& c = Point(0.,0.), std::vector<Real> u =
    std::vector<Real>(2,0.));
Cube& Cube::reflect2d(const Point& c, Real ux, Real uy = 0.);
//! apply a reflection3d on a Cube
Cube& Cube::reflect3d(const Point& c = Point(0.,0.,0.), std::vector<Real> u =
    std::vector<Real>(3,0.));
Cube& Cube::reflect3d(const Point& c, Real ux, Real uy, Real uz = 0.);
```

For instance,

```
Cube c;
c.translate(0.,0.,1.);
```

If you want now to create a new Cube by applying a transformation on a Cube, you should use one of the following functions instead:

```
//! apply a geometrical transformation on a Cube (external)
Cube transform(const Cube& m, const Transformation& t);
//! apply a translation on a Cube (external)
Cube translate(const Cube& m, std::vector<Real> u = std::vector<Real>(3,0.));
Cube translate(const Cube& m, Real ux, Real uy = 0., Real uz = 0.);
//! apply a rotation 2d on a Cube (external)
Cube rotate2d(const Cube& m, const Point& c = Point(0.,0.), Real angle = 0.);
//! apply a rotation 3d on a Cube (external)
Cube rotate3d(const Cube& m, const Point& c = Point(0.,0.,0.), std::vector<Real> u =
    std::vector<Real>(3,0.), Real angle = 0.);
Cube rotate3d(const Cube& m, Real ux, Real uy, Real angle);
Cube rotate3d(const Cube& m, Real ux, Real uy, Real uz, Real angle);
Cube rotate3d(const Cube& m, const Point& c, Real ux, Real uy, Real angle);
Cube rotate3d(const Cube& m, const Point& c, Real ux, Real uy, Real uz, Real angle);
//! apply a homothety on a Cube (external)
Cube homothetize(const Cube& m, const Point& c = Point(0.,0.,0.), Real factor = 1.);
Cube homothetize(const Cube& m, Real factor);
//! apply a point reflection on a Cube (external)
Cube pointReflect(const Cube& m, const Point& c = Point(0.,0.,0.));
//! apply a reflection2d on a Cube (external)
Cube reflect2d(const Cube& m, const Point& c = Point(0.,0.), std::vector<Real> u =
    std::vector<Real>(2,0.));
Cube reflect2d(const Cube& m, const Point& c, Real ux, Real uy = 0.);
//! apply a reflection3d on a Cube (external)
Cube reflect3d(const Cube& m, const Point& c = Point(0.,0.,0.), std::vector<Real> u =
    std::vector<Real>(3,0.));
Cube reflect3d(const Cube& m, const Point& c, Real ux, Real uy, Real uz = 0.);
```

For instance,

```
Cube c1;
Cube c2=translate(c1,0.,0.,1.);
```

Of course, you can not apply a 2d rotation or a 2d reflection for geometries defined by 3d points !

**What does a transformation really do ?**

Applying a transformation on an object means computing the image of each point defining the object. But it can also change names.
When you create a new object by applying a transformation on a object, names are modified. Indeed, the transformation add a suffix "_prime". It concerns geometry names and sidenames.

When you transform a `Geometry`, it also apply the transformation on the underlying bounding box.

## 4.7 Geometric map data

The `GeomMapData` class is helpful to compute and store jacobian matrices and various values related to the map from a reference element to a geometric element.

### 4.7.1 Differential calculus

**Mapping**

The map from Lagrange reference element (say $\hat{E}$) to any Lagrange geometric element (say $E$) is defined by

$$F(\hat{x}) = \sum_{k=1,q} M_k \hat{\tau}_k(\hat{x})$$

where $(M_k)_{k=1,q}$ are the nodes of geometric element $E$ and $(\hat{\tau}_k)_{k=1,q}$ are the shape functions of reference element $\hat{E}$.
Note that $\hat{E}$ and $E$ may be not in the same dimension space, think to a triangle in 3D space or a segment in 2D or 3D space. Denote $n$ the space dimension (the dimension of point $M_i$) and $p$ the dimension of element (the dimension of point of reference element and variable $\hat{x}$ too). So the map $F$ acts from $\mathbb{R}^p$ to $\mathbb{R}^n$. If the element $E$ is not degenerated (its measure as element of dimension $p$ is not null), $F$ is injective and $C^1$, by construction $E = F(\hat{E})$, thus $F$ is a diffeomorphism from $\hat{E}$ onto $E$.

For a side $S$ of element $E$, image of $\hat{S}$ by map $F$, the restriction of $F$ on $\hat{S}$ is defined by:

$$F_S(\hat{x}) = \sum_{k\,/\,M_k \in S} M_k \hat{\tau}_k(\hat{x}).$$

**Differential element in integrals**

The $n \times p$ jacobian matrix is defined by ($\hat{x} = (\hat{x}_1, ..., \hat{x}_p)$) :

$$J_{ij}(\hat{x}) = \sum_{k=1,q} (M_k)_i \partial_{\hat{x}_j} \hat{\tau}_k(\hat{x})$$

- When $n = p$ it is assumed that the Jacobian matrix is invertible (no degenerate element) and $J^{-1}$ denotes its inverse.

- When $n = p+1$, it is assumed that the columns of jacobian $(J_{.j}(\widehat{x}))_{j=1,p}$ form a basis of the tangential plane of the element at point $\widehat{x}$. There exists a $p \times p$ sub matrix of $J(\widehat{x})$ invertible, say $\widetilde{J}(\widehat{x})$.
- When $n = p+2$, only in 3D ($n = 3$ and $p = 1$), the unique column of jacobian $(J_{.1}(\widehat{x}))$ is a tangential vector of the element at point $\widehat{x}$ and at least, one component of $J_{.1}(\widehat{x})$ is not null.

Most of finite element computation are integrals over $E$ involving the mapping to the reference element ($g$ an integrable function):

$$\int_E g(x)dx = \int_{\widehat{E}} g \circ F(\widehat{x})\,\gamma(\widehat{x})\,d\widehat{x}$$

where $\gamma(\widehat{x})$ denotes the differential element defined by:

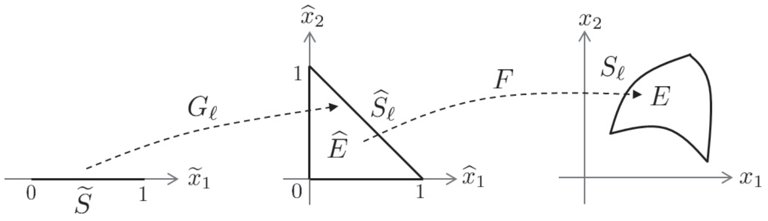
$$\gamma(\widehat{x}) = \begin{cases} |\det J(\widehat{x})| & \text{if } p = n \\ |\vec{n}(\widehat{x})| & \text{if } p = n-1 \\ |J_{.1}(\widehat{x})| & \text{if } p = n-2 = 1 \end{cases}$$

where $\vec{n}(\widehat{x})$ denotes the following normal to the element (oriented area):

$$\vec{n}(\widehat{x}) = \begin{cases} J_{.1}(\widehat{x}) \times J_{.2}(\widehat{x}) & \text{if } p = n-1 = 2 \\ J_{.1}(\widehat{x})\perp & \text{if } p = n-1 = 1 \end{cases}$$

Integrals over a side $S_\ell$ of element $E$ involve the mapping from a side reference element $\widetilde{S}$:

$$S_\ell = H_\ell(\widetilde{S}) = F \circ G_\ell(\widetilde{S})$$



where $G_\ell$ maps the side reference element $\widetilde{S}$ to the side $\ell$ of the reference element $\widehat{E}$, say $\widehat{S}_\ell$. As reference elements are flat elements, $G_\ell$ may be chosen as a first order polynomial map from $\mathbb{R}^{n-1}$ to $\mathbb{R}^n$ given by:

$$G_\ell(\widetilde{x}) = \sum_{k=1,q} \widehat{M}_{\ell k}\widetilde{\tau}_k(\widetilde{x}) \;\; (\widehat{M}_{\ell k} \text{ vertices of } \widehat{S}_\ell).$$

The mapping of the integral on side $S$ is:

$$\int_S g(x)dx = \int_{\widetilde{S}} g \circ F \circ G_\ell(\widetilde{x})\,\mu(\widetilde{x})\,d\widetilde{x}$$

where the differential element is given by:

$$\mu(\widetilde{x}) = \begin{cases} |(J_{H_\ell})_{.1} \times (J_{H_\ell})_{.2}| & \text{if } n = 3 \\ |(J_{H_\ell})_{.1}| & \text{if } n = 2 \end{cases}.$$

As $J_{H_\ell} = J_F\,J_{G_\ell}$, the differential element $\mu(\widetilde{x})$ may be written :

$$\mu(\widetilde{x}) = \begin{cases} |J_F(J_{G_\ell})_{.1} \times J_F(J_{G_\ell})_{.2}| & \text{if } n = 3 \\ |(J_F(J_{G_\ell})_{.1}| & \text{if } n = 2 \end{cases}.$$

An other way to get the differential element, consist in introducing the side reference element with the same order polynomial interpolation as the reference element and the map:

$$\widetilde{H}_\ell = \sum_{k=1,q} M_{\ell k}\widetilde{\widetilde{\tau}}_k \;\; (M_{\ell k} \text{ nodes of } S_\ell)$$

with ($\widetilde{\widetilde{\tau}}_k$) the shape functions of the side reference element, differents from ($\widetilde{\tau}_k$) if the interpolation is not of order 1. As

$$H_\ell(\widetilde{x}) = \sum_{k\,/\,M_k\in S_\ell} M_k\widehat{\tau}_k(G_\ell(\widetilde{x})) = \sum_k M_{\ell k}\widehat{\tau}_{\ell k}(G_\ell(\widetilde{x}))$$

and $\widehat{\tau}_{\ell k}(G_\ell(\widetilde{x})) = \widetilde{\widetilde{\tau}}_k$, maps $H_\ell$ and $\widetilde{H}_\ell$ are the same.
The jacobian is given by:

$$\left(J_{H_\ell}\right)_{ij} = \sum_{k=1,q} (M_{\ell k})_i \partial_{\widetilde{x}_j}\widetilde{\widetilde{\tau}}_k$$

and the differential element is given by:

$$\mu(\widetilde{x}) = \begin{cases} |(J_{H_\ell})_{.1} \times (J_{H_\ell})_{.2}| & \text{if } n=3 \\ |(J_{H_\ell})_{.1}| & \text{if } n=2 \end{cases}.$$

**Gradient**

Sometimes, differential operators may appear in integrals. For any differentiable function $h$ defined on $E$, we set $\widehat{h} = h\circ F$. The following relations holds

- "volumic" computation, $p=n$:

$$\nabla h = J(\widehat{x})^{-t}\widehat{\nabla}\widehat{h}$$

- surfacic gradient, $p=n-1=2$:

$$\nabla_S h = J(\widehat{x})T(\widehat{x})^{-1}\widehat{\nabla}\widehat{h}$$

  where $T(\widehat{x})$ is the $p\times p$ metric tensor defined by:

$$T(\widehat{x}) = J(\widehat{x})^t J(\widehat{x}).$$

  Note that $\nabla_S h$ is a $n$ vector.

- lineic gradient, $p=n-2=1$ or $p=n-1=1$:

$$\nabla_L h = \frac{\widehat{h}'}{|J_{.1}(\widehat{x})|}\frac{J_{.1}(\widehat{x}}{|J_{.1}(\widehat{x})|} = \frac{\widehat{h}'}{|J_{.1}(\widehat{x})|}\tau$$

  In this expression, $\nabla_L h$ is a $n$ vector. The scalar tangential derivative is thus given by

$$\partial_\tau h = \frac{\widehat{h}'}{|J_{.1}(\widehat{x})|}.$$

### 4.7.2 The GeomMapData class

In view of main differential calculus formulas, the GeomMapData class has the following members:

```
class GeomMapData
{private :
   const MeshElement* geomElement_p;     //current geometric element
   Point currentPoint;                   //point used in computation
 public :
   Matrix<Real> jacobianMatrix;          //jacobian matrix of map from reference element
   Matrix<Real> inverseJacobianMatrix;   //inverse jacobian matrix
   Real jacobianDeterminant;             //jacobian determinant
   Real differentialElement;             //differential element (abs(jac. det.))
   Vector<Real> normalVector;            //unit oriented normal vector at a boundary point
   Vector<Real> metricTensor;            //symetric metric tensor (t_i|t_j)
   Real metricTensorDeterminant;         //metric_tensor determinant
                    ...
};
```

This class provides three basic constructors and some computation functions:

```
GeomMapData(const MeshElement*,const Point&);
GeomMapData(const MeshElement*, std::vector<Real>::iterator);
GeomMapData(const MeshElement*);
void computeJacobianMatrix(Number side=0);
void computeJacobianMatrix(const std::vector<Real>& x, Number s=0);
Real computeJacobianDeterminant();
void invertJacobianMatrix();
void computeNormalVector();
void normalize();
void computeOrientedNormal();
void computeDifferentialElement();
Real diffElement();
Real diffElement(Number s);
void computeMetricTensor();
void computeSurfaceGradient(Real, Real, std::vector<Real>&);
```

The function `computeNormalVector` computes a normal vector from the jacobian matrix; `normalize` makes it unitary and may be reverse its sign according to an orientation done by the function `setNormalOrientation` of the `GeomDomain` class. The function `computeOrientedNormal` do the same jobs in one time.

Note that these computations requires the evaluation of the shape functions of the reference element at a given point.

The `GeomMapData` class proposes also some functions to map a point from the reference space to the physical one or the contrary and important geometrical maps related to Piola transformations:

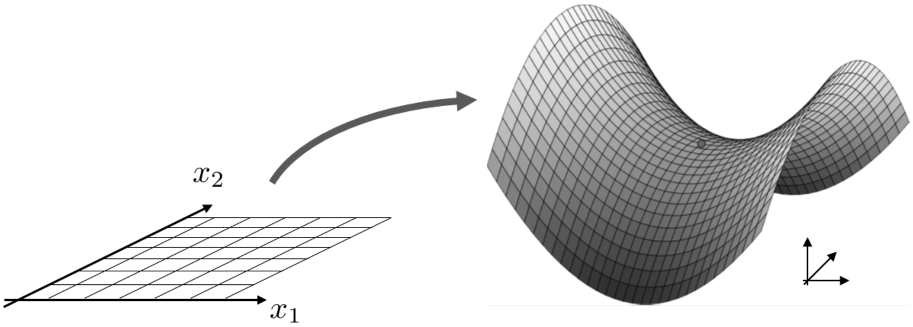
```
Point geomMap(Number side = 0);
Point geomMap(const std::vector<Real>& x, Number side = 0);
Point piolaMap(number_t side = 0);
Matrix<real_t> covariantPiolaMap(const Point& =Point());
Matrix<real_t> contravariantPiolaMap(const Point& =Point());
```

| | |
|---:|:---|
| library : | **geometry** |
| header : | **GeomMapData.hpp** |
| implementation : | **GeomMapData.cpp** |
| unitary tests : | **test_GeomElement.cpp** |
| header dependences : | **config.h, utils.h,GeomElement.hpp** |

## 4.8 Parametrization

### 4.8.1 The `Parametrization` class

The `Parametrization` class handles geometric maps that can describe either immersed curves in 2D/3D, surfaces in 3D or 1D/2D/3D mapping.



The Parametrization class manages mainly a XLiFE++ geometry describing the domain of the parameter variables $p$ (for instance $t$, $(u, v)$ or $(x_1, x_2)$) and a pointer to a function of the form:

```
Vector<real_t> (*par_fun)(const Point&, Parameters&, DiffOpType);
```

Generally the geometry is either a segment or a rectangle, but other geometries are allowed. The function describing the geometric map may deal with Parameters object (do not confuse with the parameter variables) and a differential operator (_id, _d1,_d2,_d3,_d11, d12, ...) that indicates which derivative is required. Offering first derivatives and second derivatives is not mandatory, but it allows to access to interesting geometrical quantities such as local length, curvature, ....

```
Geometry* geom_p;   // pointer to the parametrized geometry (may be 0)
Geometry* geomSupport_p;  // pointer to the geometry support of the parameter
par_fun f_p;        // pointer to the parametrization function with parameters

string_t name;      //a parametrization name useful for printing
Parameters params;  //optional parameter list passed to par_fun
dimen_t dimg;       //dimension of the geometry, set by init()
dimen_t dim;        //dimension of the arrival space, set by init()
```

Geometrical quantities can be computed (if derivatives of the map are given) but, for more efficiency, they can be also given as par_fun functions;

```
par_fun curvature_p;  //pointer to the curvature function
par_fun length_p;     //pointer to the length function
par_fun invParametrization_p;  //pointer to the inverse function
par_fun normal_p;     //pointer to the normal function
par_fun tangent_p;    //pointer to the tangent function
par_fun curabc_p;     //pointer to the curvilinear abcissa function
par_fun christoffel_p;// pointer to the Christoffel symbols function
```

par_fun functions return always a real vector even if the natural quantity is a real scalar. Be cautious, the dimension of the returned quantities depends on the parametrization type:

| | 1D→ 2D | 1D→ 3D | 2D→ 3D |
|---|---|---|---|
| length | ds | ds | ds1,ds2 |
| curvature | c | c1,c2 | c1,c2 |
| normal | n | n1,n2 | n |
| tangent | t | t2 | t1,t2 |
| curvilinear | s | s | s1,s2 |
| Christoffel | | | $\Gamma^k_{ij},\ i,j,k=1,2$ |
| inverse | x1 | x1 | x1,x2 |

When these pointers are allocated they are used in priority. Some of these functions are generally easy to compute from the derivatives (curvature, length, normal, tangent) but it is not the case for the curvilinear abscissas (given by an integral of the length) and for the inverse map that requires to solve a non linear equation.

When the curvilinear abscissa is computed, to avoid heavy re-computation, curvilinear abscissas are computed once on a fine discretization and stored in a vector:

```
mutable Vector<Vector<real_t> > curabcs_;
```

Up to now, the inverse map is not computed automatically. So if required, the function has to be given explicitely.

To offer the possibility to use symbolic functions instead of `par_fun` functions, special `par_fun` functions encapsulating `SymbolicFunction` are defined:

```
Vector<real_t> symbolic_f(const Point&, Parameters&, DiffOpType);
Vector<real_t> symbolic_invParametrization(const Point&, Parameters&, DiffOpType);
Vector<real_t> symbolic_length(const Point&, Parameters&, DiffOpType);
Vector<real_t> symbolic_curvature(const Point&, Parameters&, DiffOpType);
Vector<real_t> symbolic_curabc(const Point&, Parameters&, DiffOpType);
Vector<real_t> symbolic_normal(const Point&, Parameters&, DiffOpType);
Vector<real_t> symbolic_tangent(const Point&, Parameters&, DiffOpType);
```

The following constructors address construction from explicit or implicit geometries and `par_fun` functions:

```
Parametrization(); //default (all set to 0)
Parametrization(const Geometry&, par_fun, const Parameters&,
                const string_t& na=""); //general case
Parametrization(real_t, real_t, par_fun, const Parameters&,
                const string_t& na=""); //1D -> nD
Parametrization(real_t, real_t, real_t, real_t, par_fun, const Parameters&,
                const string_t& na=""); //2D -> nD
```

and the following constructors deal with symbolic functions:

```
Parametrization(const Geometry&, const SymbolicFunction&, const Parameters&,
                const string_t& na=""); // 1D->1D
Parametrization(const Geometry&, const SymbolicFunction&, const SymbolicFunction&,
                const Parameters&, const string_t& na="");  // 1D/2D -> 2D
Parametrization(const Geometry&, const SymbolicFunction&, const SymbolicFunction&,
                const SymbolicFunction&, const Parameters&, const string_t& na="");
                // 1D/2D/3D -> 3D
Parametrization(real_t, real_t, const SymbolicFunction&, const Parameters&,
                const string_t& na="");  //1D->1D
Parametrization(real_t, real_t, const SymbolicFunction&, const SymbolicFunction&,
                const Parameters&, const string_t& na="");// 1D->2D
Parametrization(real_t, real_t, const SymbolicFunction&, const SymbolicFunction&,
                const SymbolicFunction&, const Parameters&,
                const string_t& na="");// 1D->3D
Parametrization(real_t, real_t, real_t, real_t, const SymbolicFunction&,
                const SymbolicFunction&, const Parameters&,
                const string_t& na="");// 2D->2D
Parametrization(real_t, real_t, real_t, real_t, const SymbolicFunction&,
                const SymbolicFunction&, const SymbolicFunction&,
                const Parameters&, const string_t& na=""); //2D -> 3D
```

Besides, copy constructor, assign operator, destructor and some building tools are defined:

```
Parametrization(const Parametrization&);             // copy constructor
Parametrization& operator=(const Parametrization&); // assign operator
~Parametrization();                                  // destructor (clear pointers)

void init();            //initialization, set dim
void clearPointers();   //clear internal pointers (geometry and symbolic functions)
void copy(const Parametrization&); //copy tool
void buildSymbolic(const SymbolicFunction&);
void buildSymbolic(const SymbolicFunction&, const SymbolicFunction&);
void buildSymbolic(const SymbolicFunction&, const SymbolicFunction&,
                   const SymbolicFunction&);
```

Once `Parametrization` object is constructed, the optional `par_fun` functions may be associated to the parametrization:

```
void setinvParametrization(par_fun f) {invParametrization_p=f;}
void setLength(par_fun f)     {length_p=f;}
void setCurvature(par_fun f) {curvature_p=f;}
void setCurabc(par_fun f)     {curabc_p=f;}
void setNormal(par_fun f)     {normal_p=f;}
void setTangent(par_fun f)    {tangent_p=f;}
```

In a sawe way, some symbolic functions may be associated to the parametrization;

```
void setinvParametrization(const SymbolicFunction&);
void setinvParametrization(const SymbolicFunction&, const SymbolicFunction&);
void setLength(const SymbolicFunction&);
void setCurvature(const SymbolicFunction&);
void setCurvatures(const SymbolicFunction&, const SymbolicFunction&);
void setCurabc(const SymbolicFunction&);
void setCurabcs(const SymbolicFunction&, const SymbolicFunction&);
void setNormal(const SymbolicFunction&, const SymbolicFunction&);
void setNormal(const SymbolicFunction&, const SymbolicFunction&,
               const SymbolicFunction&);
void setNormals(const SymbolicFunction&, const SymbolicFunction&,
                const SymbolicFunction&, const SymbolicFunction&,
                const SymbolicFunction&, const SymbolicFunction&);
void setTangent(const SymbolicFunction&, const SymbolicFunction&);
void setTangent(const SymbolicFunction&, const SymbolicFunction&,
                const SymbolicFunction&);
void setTangents(const SymbolicFunction&, const SymbolicFunction&,
                 const SymbolicFunction&, const SymbolicFunction&,
                 const SymbolicFunction&,const SymbolicFunction&);
```

The following accessors are available:

```
Geometry& geometry() const {return *geom_p;};
RealPair bounds(VariableName v) const; //geometry bounds in direction (_x1,_x2,_x3)
```

The class provides methods to compute the parametrization map (using the operator `()`) and its inverse if it is defined:

```
Point operator()(const Point&, DiffOpType d=_id) const;
Point operator()(real_t t, DiffOpType d=_id) const; // 1D shortcut
Point operator()(real_t u, real_t v, DiffOpType d=_id) const; // 2D shorcut
Point toParameter(const Point&) const;
real_t toRealParameter(const Point&) const; //1D shortcut
```

In the following $f(p) = (f_1(p), f_2(p), [f_3(p)])$ denotes the point given by the parametrization at $p$. For 1D parametrization (curve), the local "lengths" $ds$ is defined as

$$ds(p) = \sqrt{(f_1'(p))^2 + (f_2'(p))^2 + [(f_3'(p))^2]}$$

and for 2D parametrization (surface) the two "lengths" are defined as

$$ds_1(p) = \sqrt{(d_1 f_1(p))^2 + (d_1 f_2(p))^2 + (d_1 f_3(p))^2}$$

$$ds_2(p) = \sqrt{(d_2 f_1(p))^2 + (d_2 f_2(p))^2 + (d_2 f_3(p))^2}$$

The class provides length functions with different arguments:

```
Vector<real_t> lengths(const Point&, DiffOpType =_id) const;         //lengths
Vector<real_t> lengths(real_t t, DiffOpType d=_id) const;            //1D shortcut
Vector<real_t> lengths(real_t u, real_t v, DiffOpType d=_id) const; //2D shortcut
real_t length(const Point& P, DiffOpType d =_id) const;              //first length
real_t length(real_t t, DiffOpType d =_id) const;                    //1D shortcut
real_t length(real_t u, real_t v, DiffOpType d =_id) const;          //2D shortcut
real_t bilength(const Point& P, DiffOpType d =_id) const;            //second length
real_t bilength(real_t t, DiffOpType d =_id) const;                  //1D shortcut
real_t bilength(real_t u, real_t v, DiffOpType d =_id) const;        //2D shortcut
```

This scheme of member functions is common to all geometric functions: 's' suffix for the general function, no suffix for the first value, 'bi' prefix for the second value if it is relevant; same 1D, 2D shortcuts. Shortcut versions are no longer written in the following.

For 1D parametrization, the curvature is given by

$$c(p)=\frac{\|f''(p)\times f'(p)\|}{\|f'(p)\|^3}$$

while for 2D parametrization (in $\mathbb{R}^3$), the main curvatures are the eigenvalues $(c_1(p),c_2(p))$ of the Weingarten's matrix

$$W(p)=\frac{1}{EG-F^2}\left[\begin{array}{cc} MF-LG & NF-LG\\ LF-ME & MF-NE\end{array}\right]$$

where $E=(d_1f(p))^2$, $F=d_1f(p)d_2f(p)$, $G=(d_2f(p))^2$, $L=d_{11}f(p).n$, $M=2d_{12}f(p).n$ and $N=d_{22}f(p).n$. The Gauss curvature and the mean curvature are given by

$$c_G(p)=c_1(p)c_2(p)\text{ and }c_m(p)=\frac{1}{2}(c_1(p)+c_2(p)).$$

```
Matrix<real_t> weingarten(const Point& t) const;                  //Weingarten matrix
Vector<real_t> curvatures(const Point&, DiffOpType =_id) const;  //curvatures (1/2)
real_t curvature(const Point& P, DiffOpType d =_id) const;        //first curvature
real_t bicurvature(const Point& P, DiffOpType d =_id) const;      //second curvature
real_t gausscurvature(const Point& P, DiffOpType d =_id) const;   //Gauss curvature
real_t meancurvature(const Point& P, DiffOpType d =_id) const;    //mean curvature
```

The curvilinear abscissa is defined for 1D parametrization as ($p$ is a scalar)

$$s(p)=\int_0^p ds(t)$$

and for 2D parametrization ($p=(u,v)$)

$$\begin{aligned} s_1(p)&=\int_0^u ds_1(t,v)dt\\ s_2(p)&=\int_0^v ds_2(u,t)dt.\end{aligned}$$

```
Vector<real_t> curabcs(const Point&, DiffOpType =_id) const; //cur. abc. (1/2)
real_t curabc(const Point& P, DiffOpType d =_id) const;       //first cur. abc.
real_t bicurabc(const Point& P, DiffOpType d =_id) const;     //second cur. abc.
```

For 1D parametrization, the tangent vector is given by

$$T=\frac{f'(p)}{\|f'(p)\|}$$

the first normal and the binormal (Frenet definition) by:

$$N = d_s T(P)/c(p) \text{ and } bN = T \times N.$$

For 2D parametrization, the normal is given by

$$N = \frac{d_1 f(p) \times d_2 f(p)}{\|d_1 f(p) \times d_2 f(p))\|}$$

and the tangent and bitangent vectors by:

$$T = \frac{d_1 f(p)}{\|d_1 f(p)\|} \text{ and } bT = T \times N.$$

The following member functions are defined:

```
Vector<real_t> normals(const Point&, DiffOpType =_id) const;          //normal vectors
Vector<real_t> normal(const Point& P, DiffOpType d=_id) const;        //first normal
Vector<real_t> binormal(const Point& P, DiffOpType d=_id) const;      //second normal
Vector<real_t> tangents(const Point&, DiffOpType =_id) const;         //tangent vectors
Vector<real_t> tangent(const Point& P, DiffOpType d=_id) const;       //first tangent
Vector<real_t> bitangent(const Point& P, DiffOpType d=_id) const;     //second tangent
```

It provides also the jacobian matrix (say $J$), the metric tensor ($G = J^t J$, symmetric matrix) stored as a 3[6]-vector:

$$(G_{11}, G_{21}, G_{22}, [, G_{31}, G_{32}, , G_{33}])$$

and the Christoffel symbols (immersed 2D surface, parametrized by $(u, v)$) , stored as a 8-vector:

$$(\Gamma^1_{11}, \Gamma^1_{12}, \Gamma^1_{21}, \Gamma^1_{22}, \Gamma^2_{11}, \Gamma^2_{12}, \Gamma^2_{21}, \Gamma^2_{22})$$

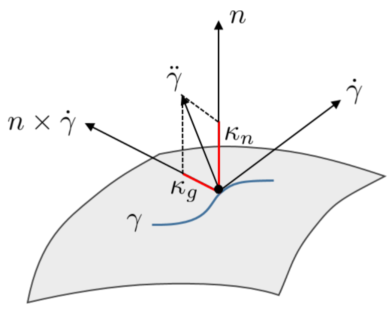
```
Matrix<real_t> jacobian(const Point& t, DiffOpType d=_id) const;          //jacobian matrix
Vector<real_t> metricTensor(const Point& t, DiffOpType d=_id) const;      //metric tensor
Vector<real_t> christoffel (const Point& t, DiffOpType d=_id) const;      //Christoffel symbols
```

When dealing with curve on immersed surface ($s \to \gamma(s) = \varphi(u(s), v(s))$), the *normal curvature* at $s$ is defined as

$$\begin{aligned}\kappa_n &= (\ddot\gamma(s)|n), \quad (n \text{ a normal to the surface})\\ &= \frac{L\dot u^2 + 2M\dot u\dot v + N\dot u^2}{E\dot u^2 + 2F\dot u\dot v + G\dot u^2}\end{aligned}$$

with $E, F, G$ the coefficients of the 1-form and $L, M, N$ the coefficients of the 2-form. Be careful, the sign of normal curvature depends on the choice of the surface normal. As the normal curvature depends only of the tangent $d = \dot\gamma(s)$ of the curve at $\gamma(s)$, a more general tools is provided computing the normal curvature at $\varphi(u, v)$ relatively to the direction $d$ ($\dot u = (d|d_v\varphi \times n),\ \dot v = (d|d_u\varphi \times n)$):

```
real_t normalCurvature(const Point& uv, const Vector<real_t>& d) const;      //normal curvature
     relatively to d
Vector<real_t> curvatures(const Point& uv, const Vector<real_t>& d) const;  //Gauss, mean and
     normal curvature
```



Up to now, the geodesic curvature $\kappa_g$ is not available. Note that the curve curvature $\kappa$ is related to the normal and geodesic curvatures by $\kappa^2 = \kappa_g^2 + \kappa_n^2$.

Finally, the `Parametrization` provides some printing tools:

```
void print(std::ostream&) const;
void print(PrintStream& os) const;
friend ostream& operator<< (std::ostream&, const Parametrization&);
```

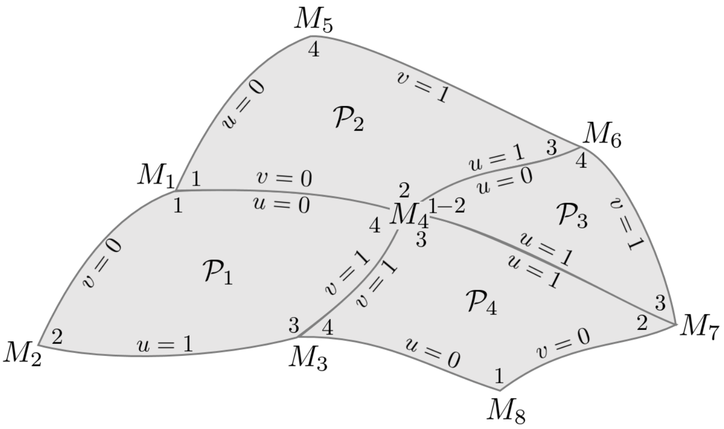
### 4.8.2 Parametrization of a piecewise geometry

A piecewise geometry is a `Geometry` object that have several geometry components. As a consequence, a parametrization of such object consists in the collection of parametrizations of each geometry component. To deal with, a `PiecewiseParametrization`, inheriting of `Parametrization`, is provided. It handles 1D case (collection of arcs) , 2D case (collection of surface patches) but not yet the 3D case (collection of volume patches)!

```
class PiecewiseParametrization : public Parametrization
{ public:
  vector<Point> vertices;
  map<Parametrization*,std::vector<number_t> > vertexIndexes;
  map<Parametrization*, std::vector<std::pair<Parametrization*,number_t> > > neighborParsMap;
...};
```

with

- the vector `vertices` collecting all the vertices (global numbering)
- the map `vertexIndexes` collecting for each parametrization the local vertex numbers (relatively to global numbering)
- the map `neighborParsMap` collecting for each parametrization and each of its sides, the neigbor parametrization (if exists) and it relative side number (the side numbering being the following : side 1 → $v = 0$, side 2 → $u = 1$, side 3 → $v = 1$, side 4 → $u = 0$).



On the example made of surface patches :

| | |
|---|---|
| `vertices :` | $(M_1, M_2, M_3, M_4, M_5, M_6, M_7, M_8)$ |
| `vertexIndexes :` | $[(1,2,3,4),(1,4,6,5),(4,4,7,6),(8,7,4,3)]$ |
| `neighborParsMap :` | $[(<0,0>,<0,0>,<\mathscr{P}_4,3>,<\mathscr{P}_2,1>),(<\mathscr{P}_1,4>,<\mathscr{P}_3,4>),<0,0>,<0,0>),$<br>$(<0,0>,<\mathscr{P}_4,2>,,<0,0>,<\mathscr{P}_2,2>),(<0,0>,<\mathscr{P}_3,2>,<\mathscr{P}_1,3>,<0,0>)]$ |

The `neighborParsMap` map allows to travel the piecewise parametrization by crossing patch interfaces. In 2D case, the piecewise parametrization is based on "quadrangular" patches but they can be degenerated (triangular

patches) ; but not fully degenerated (line).
Note that this piecewise parametrization is not global $C^0$. It is quite easy to produce a global $C^0$ parametrization in 1D case but it is an other story in 2D case!

In addition to the `Parametrization` member functions, the `PiecewiseParametrization` class provides some tools to build the structure `vertices` , `vertexIndexes` and `neighborParsMap` from the sides map (for each side $s$ of a domain, the list of all geometries connected to the side $s$ ):

```
void buildNeighborParsMap(map<set<number_t>, list<std::pair<Geometry*, number_t> > >& sidemap);
void buildVertices();
```

some tools to locate the parametrization patch and computes various quantities

```
Parametrization* locateParametrization(const Point& p, const Point& dp, Parametrization* par0,
                                       Point& q, real_t& d) const;
Vector<real_t> funParametrization(const Point& pt, Parameters& pars, DiffComputation dc,
                                  DiffOpType d=_id) const;
Vector<real_t> invParametrization(const Point& pt, Parameters& pars, DiffOpType d=_id) const;
Point toParameter(const Point& p) const;
virtual Vector<real_t> lengths(const Point& P, DiffOpType d=_id) const ;
virtual Vector<real_t> curvatures(const Point& P, DiffOpType d =_id) const ;
```

and finally to print informations related to

```
void print(std::ostream&) const;
void print(PrintStream& os) const ;
```

| | |
|---:|---|
| library : | **geometry** |
| header : | **Parametrization.hpp** |
| implementation : | **Parametrization.cpp** |
| unitary tests : | **test_Parametrization.cpp** |
| header dependences : | **config.h, utils.h** |

# 5 The *finiteElements* library

The *finiteElements* library concerns all the stuff related to the the elementary objects of a finite elements discretization. When these objects are provided by a mesh tool, they are `GeomElement` (for geometric element) and when they also carry interpolation information, they are `Element`. In few words, a `Mesh` is a collection of `GeomElement` and a finite element `Space` is a collection of `Element`. In the framework of the finite elements, it is common (and useful) to link any element to a reference element, named in this library: `GeomRefElement` and `RefElement`. `GeomRefElement` is a class whom inherit fundamental geometric elements `GeomSegment`, `GeomTriangle`, ... and `RefElement` is a class whom inherit all the finite element types `LagrangeSegment, LagrangeTriangle, LagrangeTetrahedron, ...`. The `Interpolation` class carries some general informations on the finite element such that the finite element type and its conforming space. Besides, this library provides integration method stuff (`IntegrationMethod, Quadrature, QuadratureRule`).

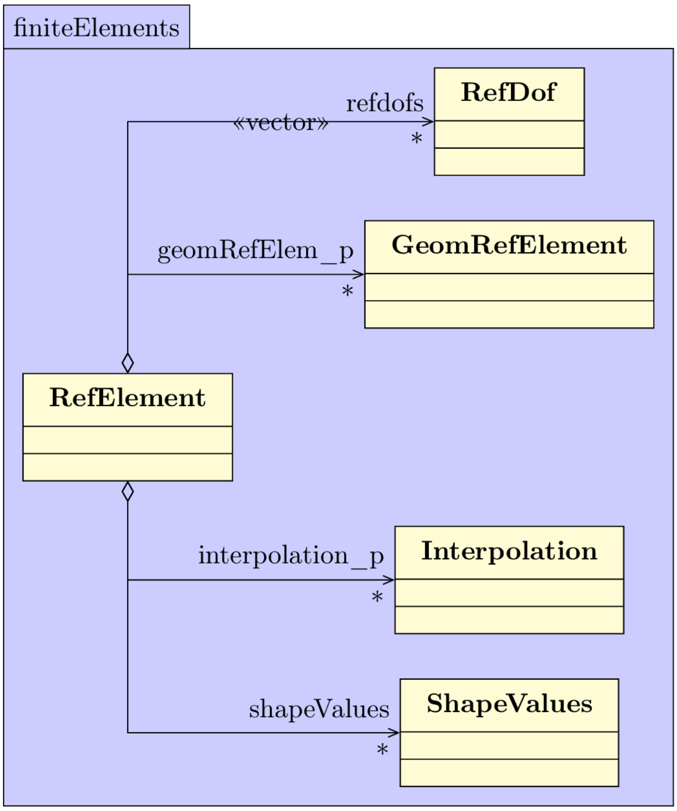


Figure 5.1: The *finiteElements* library main class diagram

## 5.1 The `Interpolation` class

The purpose of the `Interpolation` class is to store data related to finite element interpolation. It concerns only general description of an interpolation: type of the finite element interpolation (Lagrange, Hermite, ...), a subtype among standard, Gauss-Lobatto (only for Lagrange) and first or second family (only for Nedelec), the "order" of the interpolation for Lagrange family and the space conformity (L2,H1,Hdiv,...). For instance, a Lagrange standard P1 with H1 conforming is the classic P1 Lagrange interpolation but a Lagrange standard P1 with L2 conforming means a discontinuous interpolation (like Galerkin discontinuous approximation) where the vertices of an element are not shared. For the moment, this class is only intended to support the following choices:

| type | subtype | order |
|---|---|---|
| Lagrange | standard, Gauss-Lobatto | any order |
| Hermite | standard | |
| Morley | standard | order 2 |
| Argyris | standard | order 5 |
| Crouzet-Raviart | standard | order 1 |
| Raviart-Thomas | standard | any order |
| Nedelec | first or second family | any order |
| Nedelec face | first or second family | any order |
| Nedelec edge | first or second family | any order |

Nedelec face and Nedelec edge are specific to 3D. Nedelec face corresponds to the 2D Raviart-Thomas family and Nedelec edge corresponds to the 2D Nedelec family.

The Interpolation class is intended to support a lot of finite element family but all are not available. See child classes of RefElement class to know which families are actually available.

This class is mainly used with the GeomElement class (definition of the geometric transformation) and the Space class (definition of the finite element approximation related to the discretized space).

The class Interpolation has the following attributes:

```
class Interpolation
{private:
   const FEType type_;          //interpolation type
   const FESubType subtype_;    //interpolation subtype
   const number_t numtype_;     //additionnal number type (degree for Lagrange)
   SobolevType conformSpace_;   //conforming space
   bool isoparametric_;         //isoparametric flag
   String name_;                //name of the interpolation type
   String subname_;             //interpolation sub_name
...
};
```

**FEType**, **FESubType** and **SpaceType** are enumerations defined in the *config.hpp* file as follow:

```
enum SobolevType{L2=0,H1,Hdiv,Hcurl,Hrot=Hcurl,H2,Hinf};
enum FEType {Lagrange,Hermite,CrouzeixRaviart,Nedelec,RaviartThomas,NedelecFace,
     NedelecEdge,BuffaChristiansen, BuffaChristiansen,_Morley,_Argyris};
enum FESubType  {standard=0,gaussLobatto,firstFamily,secondFamily};
```

In addition, there are a static attribute to manage a unique list of instanciated Interpolation objects.

```
static std::vector<Interpolation*> theInterpolations;
```

This class proposes some access member functions and functions returning some interpolation properties:

```
FEType type() const;
FESubType subtype() const;
number_t numtype() const;
SobolevType conformSpace() const;
String name() const;
String subName() const;
String conformSpaceName();
bool isIsoparametric() const;
void isIsoparametric(bool is) ;
bool isContinuous();
bool areDofsAllScalar();
number_t maximumDegree();
```

some error member functions:

```
void badType() const;
void badSubType() const;
void badSpace() const;
void badType(const number_t) const;
void badSubType(const number_t) const;
void badDegree(const number_t) const;
```

There is only one explicit constructor (no copy constructor):

```
Interpolation(FEType, FESubType, number_t, SobolevType);
```

that initializes the attributes and add the created object in the static list **theInterpolations**.

The process creating a `Interpolation` object is governed by other classes (in particular the `Space` class) using the function:

```
Interpolation* findInterpolation(FEType, FESubType, number_t, SpaceType);
Interpolation& interpolation(FEType, FESubType, number_t, SobolevType);
```

These functions try to find an existing `Interpolation` object corresponding to the given parameters, if it does not exist one, a new object is created by calling the constructor.

It is possible to work with a collection of `Interpolation` objects that are handles as a vector by the `Interpolations` class (see the definition of `PCollection`). It may be used as following:

```
Interpolations ints(3);
for(Number i=1;i<=3;i++) ints(i)=interpolation(Lagrange,_standard,i,H1);
```

| | |
|---:|:---|
| library : | **finiteElements** |
| header : | **Interpolation.hpp** |
| implementation : | **Interpolation.cpp** |
| unitary tests : | **test_Interpolation.cpp** |
| header dependences : | **config.h, utils.h** |

## 5.2 The `RefDof` class

The `RefDof` class is a class representing a generalized degree of freedom in a reference element.
It is defined by:

- A support that can be a point, a side, a side of side or the whole element. When it is a point, we also have its coordinates.
- A dimension, that means the number of components of shape functions of the DoF.

- Projections data (type and direction) when the DoF is a projection DoF. The projection type is 0 for a general projection, 1 for a $u\dot{n}$ DoF, 2 for a $u \times n$ DoF.
- Derivative data (order and direction) when the DoF is a derivative DoF. The order is 0 when the DoF is defined by an 'integral' over its support, or $n$ for a Hermite DoF derivative of order $n > 0$ or a moment DoF of order $n > 0$.
- A shareable property: A DoF is shareable when it is shared between adjacent elements according to space conformity. Such a DoF can be shared or not according to interpolation. For example, every DoF of a Lagrange H1-confirming element on a side is shared, while DoF in discontinuous interpolation are not.

```
class RefDof
{
 private:
 bool sharable_;                   //D.o.F is shared according to space conformity
 DofLocalization where_;           //hierarchic localization of dof
 number_t supportNum_;             //support localization
 number_t index_;                  //rank of the dof in its localization
 dimen_t supportDim_;              //dimension of the D.o.F geometric support
 number_t nodeNum_;                //node number when a point dof
 dimen_t dim_;                     //number of components of shape functions of D.o.F
 std::vector<real_t> coords_;      //coordinates of D.o.F support if supportDim_=0
 number_t order_;                  //order of a derivative D.o.F or a moment D.o.F
 std::vector<real_t> derivativeVector_;  //direction vector(s) of a derivative
 ProjectionType projectionType_;         //type of projection
 std::vector<real_t> projectionVector_;  //direction vector(s) of a projection
 DiffOpType diffop_;                     //dof differential operator (_id,_dx,_dy, ...)
 string_t name_;                         //D.o.F-type name for documentation
```

This class proposes mainly a full constructor and accessors to member data.

For non nodal dofs (`supportDim_=0`), virtual coordinates are also defined. They are useful when dealing with essential conditions.

Up to now, derivative vectors are not used and the normal vector involved in $n.\nabla$ dofs is stored in the projection vector.

In order to sort dofs in an efficient way, the following class is offered:

```
class DofKey
{
 public:
 DofLocalization where;
 number_t v1, v2;               //used for vertex, edge, element dofs
 std::vector<number_t> vs;      //used for face dofs
 number_t locIndex;             //local dof index
 }
```

assiciated to the comparison operator:

```
bool operator<(const DofKey& k1, const DofKey& k2);
```

| | |
|---|---|
| library : | **finiteElements** |
| header : | **RefDof.hpp** |
| implementation : | **RefDof.cpp** |
| unitary tests : | **test_segment.cpp, test_triangle.cpp, test_quadrangle.cpp, test_tetrahedron.cpp, test_hexahedron.cpp, test_prism.cpp** |
| header dependences : | **config.h, utils.h** |

## 5.3 Geometric data of a reference element

### 5.3.1 The GeomRefElement class

The GeomRefElement object carries geometric data of a reference element: type, dimension, number of vertices, sides and side of sides, measure, and coordinates of vertices. Furthermore, to help finding geometric data on sides, it also carries type, vertex numbers of each side on the first hand, and vertex numbers and relative number to parent side of each side of side on the second hand.

```
class GeomRefElement
{
protected:
  ShapeType shapeType_;      //element shape
  const Dimen dim_;          //element dimension
  const Number nbVertices_, nbSides_, nbSideOfSides_; //number of vertices, ...
  const Real measure_;                         //length or area or volume
  vector<Real> centroid_;                      //coordinates of centroid
  vector<Real> vertices_;                      //coordinates of vertices
  vector<ShapeType> sideShapeTypes_;           //shape type of each side
  vector<vector<Number> > sideVertexNumbers_;
  vector<vector<Number> > sideOfSideVertexNumbers_;
  vector<vector<Number> > sideOfSideNumbers_;

public:
  static vector<GeomRefElement*> theGeomRefElements; //vector carrying all GeomReferenceElements
};
```

It offers:

- few constructors (the default one, a general one with dimension, measure, centroid, and number of vertices, edges and faces and one more specific for each dimension):

```
GeomRefElement(); //default constructor
GeomRefElement(ShapeType, const Dimen d, const Real m, const Real c,
               const Number v, const Number e, const Number f);        //general
GeomRefElement(ShapeType, const Real m = 1.0, const Real c = 0.5);      //1D
GeomRefElement(ShapeType, const Real m, const Real c, const Number v); //2D
GeomRefElement(ShapeType, const Real m, const Real c, const Number v,
               const Number e);                                        //3D
```

- a private copy constructor and a private assign operator,
- some public access functions to data:

```
Dimen dim() const;
Number nbSides() const;
Number nbSideOfSides() const;
Real measure() const;
vector<Real>::const_iterator centroid() const;
vector<Real>::const_iterator vertices() const;
```

```
vector<ShapeType> sideShapeTypes() const;
const std::vector<std::vector<Number> >& sideVertexNumbers() const;
const std::vector<std::vector<Number> >& sideOfSideVertexNumbers() const;
```

- some public methods to get data on sides and side of sides:

```
String shape(const Number sideNum = 0) const; //element (side) shape as a string
ShapeType shapeType(const Number sideNum = 0) const; /element (side) shape as a ShapeType
bool isSimplex() const;                        //true if a simplex
Number nbVertices(const Number sideNum = 0) const;   //number of element (side) vertices
Number sideVertex(const Number id, const Number sideNum = 0) const;//number of element (side)
std::vector<Real>::const_iterator vertex(const Number vNum) const; //coordinates of n-th vertex
Number sideVertexNumber(const Number vNum, const Number sideNum) const;
Number sideOfSideVertexNumber(const Number vNum, const Number sideOfSideNum) const;
Number sideOfSideNumber(const Number i, const Number sideNum) const; //local number of i-th edge
void rotateVertices(const number_t newFirst,vector<number_t>&) const;// circular permutation
vector<real_t> sideToElt(number_t,vector<real_t>::const_iterator) const;
virtual Real measure(const Dimen dim, const Number sideNum = 0) const = 0;
// projection of a point onto ref element
virtual std::vector<real_t> projection(const vector<real_t>&, real_t&) const;
// test if a point belongs to current element
virtual bool contains(std::vector<real_t>& p, real_t tol= theTolerance) const;
```

- some protected append methods for vertices:

```
//build vertex 1d/2d/3d coordinates
void vertex(vector<Real>::iterator& it, const Real x1);
void vertex(vector<Real>::iterator& it, const Real x1, const Real x2);
void vertex(vector<Real>::iterator& it, const Real x1, const Real x2, const Real x3);
```

- some public error handlers:

```
void noSuchSideOfSide(const Number) const;
void noSuchSide(const Number) const;
void noSuchSide(const Number, const Number, const Number = 0, const Number = 0) const;
void noSuchFunction(const String& s) const;
```

- an external search function in the static run-time list of `GeomRefElement`:

```
GeomRefElement* findGeomRefElement(ShapeType);
```

| | |
|---|---|
| library : | **finiteElements** |
| header : | **GeomRefElement.hpp** |
| implementation : | **GeomRefElement.cpp** |
| unitary tests : | **test_segment.cpp, test_triangle.cpp, test_quadrangle.cpp, test_tetrahedron.cpp, test_hexahedron.cpp, test_prism.cpp** |
| header dependences : | **config.h, GeomRefSegment.hpp, GeomRefTriangle.hpp, GeomRefQuadrangle.hpp, GeomRefTetrahedron.hpp, GeomRefHexahedron.hpp, GeomRefPrism.hpp** |

### 5.3.2 Child classes of `GeomRefElement`

The child classes of `GeomRefElement` are `GeomRefSegment` in 1D, `GeomRefTriangle` and `GeomRefQuadrangle` in 2D and `GeomRefHexahedron`, `GeomRefTetrahedron`, `GeomRefPrism` and `GeomRefPyramid` in 3D.
Except implementation of virtual functions, these child classes provide 2 new member functions used in class constructors:

```
void sideNumbering();       //local numbers of vertices on sides
void sideOfSideNumbering(); //local numbers of vertices on side of sides
```

The last one is not defined for `GeomRefSegment`.

| | |
|---|---|
| library : | **finiteElements** |
| header : | **GeomRefSegment.hpp** |
| implementation : | **GeomRefSegment.cpp** |
| unitary tests : | **test_segment.cpp** |
| header dependences : | **config.h, GeomRefElement.hpp** |

| | |
|---|---|
| library : | **finiteElements** |
| header : | **GeomRefTriangle.hpp** |
| implementation : | **GeomRefTriangle.cpp** |
| unitary tests : | **test_triangle.cpp** |
| header dependences : | **config.h, GeomRefElement.hpp** |

| | |
|---|---|
| library : | **finiteElements** |
| header : | **GeomRefQuadrangle.hpp** |
| implementation : | **GeomRefQuadrangle.cpp** |
| unitary tests : | **test_quadrangle.cpp** |
| header dependences : | **config.h, GeomRefElement.hpp** |

| | |
|---|---|
| library : | **finiteElements** |
| header : | **GeomRefTetrahedron.hpp** |
| implementation : | **GeomRefTetrahedron.cpp** |
| unitary tests : | **test_tetrahedron.cpp** |
| header dependences : | **config.h, GeomRefElement.hpp** |

| | |
|---|---|
| library : | **finiteElements** |
| header : | **GeomRefHexahedron.hpp** |
| implementation : | **GeomRefHexahedron.cpp** |
| unitary tests : | **test_hexahedron.cpp** |
| header dependences : | **config.h, GeomRefElement.hpp** |

| | |
|---|---|
| library : | **finiteElements** |
| header : | **GeomRefPrism.hpp** |
| implementation : | **GeomRefPrism.cpp** |
| unitary tests : | **test_prism.cpp** |
| header dependences : | **config.h, GeomRefElement.hpp** |

| | |
|---|---|
| library : | **finiteElements** |
| header : | **GeomRefPyramid.hpp** |
| implementation : | **GeomRefPyramid.cpp** |
| unitary tests : | **test_pyramid.cpp** |
| header dependences : | **config.h, GeomRefElement.hpp** |

## 5.4 Reference elements

### 5.4.1 The ShapeValues class

A ShapeValues object stores the evaluation of a shape function at a given point. Thus, it carries 2 real vectors of:

```
class ShapeValues
{
public:
  vector<Real> w;           //shape functions at a  point
  vector<vector<Real>> dw;  //first derivatives (dx,dy,[dz])
  vector<vector<Real>> d2w; //2nd derivatives   (dxx,dyy,dxy,[dzz,dxz, dyz])

};
```

It offers:

- basic constructors:

```
ShapeValues();   //!< default constructor
ShapeValues(const ShapeValues&);                          //copy constructor
ShapeValues& operator=(const ShapeValues&);  // assignment operator=
ShapeValues(const RefElement&);              //constructor with associated RefElement
ShapeValues(const RefElement&, const Dimen); //constructor with associated RefElement
```

- two public size accessors and empty query :

```
Dimen dim() const;
Number nbDofs() const;
bool isEmpty() const;
```

- some functions addressing the data:

```
void resize(const RefElement&, const Dimen); // resize
void set(const real_t);              // set shape functions to const value
void assign(const ShapeValues&);     // fast assign of shapevalues into current
```

- some mapping functions

```
void extendToVector(dimen_t d);   //extend scalar shape function to vector
void map(const ShapeValues&, const GeomMapData&, bool der1, bool der2);   //standard mapping
void contravariantPiolaMap(const ShapeValues&, const GeomMapData&, bool der1, bool der2);
void covariantPiolaMap(const ShapeValues&, const GeomMapData&, bool der1, bool der2);
void Morley2dMap(const ShapeValues&, const GeomMapData&, bool der1, bool der2);
void Argyris2dMap(const ShapeValues& rsv, const GeomMapData& gd, bool der1, bool der2);
void changeSign(const std::vector<real_t>&, dimen_t);   //change sign of shape functions according
    to a sign vector
```

The contravariant and covariant Piola maps are respectively used for Hdiv and Hcurl finite element families. They preserve respectively the normal and tangential traces.If $J$ denotes the jacobian of the mapping from the reference element to any element, the covariant map is $J^{-t}\hat{\mathbf{u}}$ and the contravariant map $J/|J|\hat{\mathbf{u}}$ where $\hat{\mathbf{u}}$ is a vector fiels in the reference space. The Morley and Argyris map are specific to these elements, they preserve first and second derivatives involved in such elements.

| | |
|---:|---|
| library : | **finiteElements** |
| header : | **ShapeValues.hpp** |
| implementation : | **ShapeValues.cpp** |
| unitary tests : | |
| header dependences : | **config.h, RefElement.hpp, utils.h** |

### 5.4.2 The `RefElement` class

The `RefElement` is the main class of the *finiteElement* library. First, it has an object of each type previously seen in this chapter, namely `Interpolation`, GeomRefElement, `ShapeValues` and `RefDof`. Next, It is the mother class of the wide range of true reference elements, identified by shape and interpolation type. That is why it is a complex class collecting a lot of information and providing many numbering functions such as the number of DoFs, the same number on vertices, on sides, on side of sides, . . .

To define completely a reference element, we also need data on sides and on side of sides, such as DoF numbers and reference elements. Side and side of side reference elements will be built only when they are needed, equivalent to say only they have meaning. It is the case for H1 finite elements, but not for Hcurl and Hdiv finite elements.

So, the `RefElement` attributes are:

```
class RefElement
{
public:
  GeomRefElement* geomRefElem_p;          //pointer to geometric reference element
  const Interpolation* interpolation_p; //interpolation parameters
  vector<RefDof*> refDofs;              //local reference Degrees of Freedom
  FEMapType mapType;                    //type of map applied to shape functions of reference element
  DofCompatibility dofCompatibility;//compatibility rule to applied to side dofs
  dimen_t dimShapeFunction;             //dimension of shape function
  bool rotateDof;                       //if true, apply rotation (given by childs) to shape values
  number_t maxDegree;                   //maximum degree of shape functions

protected:
  String name_;    //reference element name (for documentation)
  Number nbDofs_;  //number of Degrees Of Freedom
  Number nbPts_;   //number of Points (for local coordinates of points)
  Number nbDofsOnVertices_;    //nb of sharable D.o.F on vertices (first D.o.F)
  Number nbDofsInSideOfSides_;//nb of sharable D.o.F on side of sides (edges)
  Number nbDofsInSides_;       //nb of sharable D.o.F on sides (faces or edges)
  Number nbInternalDofs_;      //nb of non-sharable D.o.F's
  vector<RefElement*> sideRefElems_;        //pointers to side reference elements
  vector<RefElement*> sideOfSideRefElems_; //pointers to side of side reference elements

public:
  vector<vector<Number>> sideDofNumbers_;        //dof numbers for each side
  vector<vector<Number>> sideOfSideDofNumbers_; //dof numbers for each side of side
  PolynomialsBasis Wk;                        //shape functions basis as polynomials
  vector<PolynomialsBasis> dWk;               //derivatives of shape functions basis as polynomials
  bool hasShapeValues;                        //ref element has shapevalues, generally true
  map<Quadrature*,vector<ShapeValues>> qshvs_;    //temporary structure to store shape values
  map<Quadrature*,vector<ShapeValues>> qshvs_aux;//other temporary structure to store shape values

  static vector<RefElement*> theRefElements; //to store run-time RefElement pointers
  static const bool isSharable_ = true;
```

The folllowing enumeration collects the types of affine mapping from reference element to any element. It depends on finite element type :

```
enum FEMapType {_standardMap,_contravariantPiolaMap,_covariantPiolaMap,_MorleyMap,_ArgyrisMap};
```

It offers:

- some constructors, the default one and a constructor by shape type and interpolation:

```
RefElement(); //default constructor
RefElement(ShapeType, const Interpolation* ); //constructor by shape & interpolation
```

  Note that the copy constructor and the assignment operator are private.

- some public accessors:

```
const Interpolation& interpolation() const;
String name() const;
Number nbPts() const;
Number nbDofsOnVertices() const;     //nb of D.o.F supported by vertices
Number nbDofsInSides() const;        //nb of D.o.F strictly supported by side
Number nbDofsInSideOfSides() const;  //nb of D.o.F strictly supported by side of side
bool isSimplex() const ;             //true if shape is a simplex
dimen_t dim() const;                 //element dimension

const RefElement* refElement(Number sideNum = 0) const; //reference element of side
const GeomRefElement* geomRefElement(Number sideNum = 0) const; //GeomRefElement of side
Number nbDofs(const Number sideNum = 0, const Dimen sideDim = 0) const;//number of  D.o.F by side
Number nbInternalDofs(const Number sideNum = 0, const Dimen sideDim = 0) const;
ShapeType shapeType() const;    //shape of element
```

- some build functions of side and side of side reference elements:

```
void sideOfSideRefElement();       //reference element constructors on element edges
void sideRefElement();             //reference element constructors on element faces
```

- some functions related to shape function computation

```
void buildPolynomialTree();        //build tree representation of polynomial shape functions
number_t shapeValueSize() const;
virtual void computeShapeFunctions()   //compute shape functions
virtual void computeShapeValues(vector<Real>::const_iterator it_pt, bool der1 = true,
             bool der2=false)  const = 0; //compute shape functions at point
```

  Shape function of high order element are boring to find. So, XLiFE++ provides tools to get them in a formal way, using `Polynomials` class. The virtual function `computeShapeFunctions` computes them and the `buildPolynomialTree` function builds a tree representation of the formal representation of shape functions, in order to make faster their computations.

- some virtual functions to guarantee correct matching of dofs

```
virtual vector<number_t> dofsMap(const number_t& i, const number_t& j, const number_t& k=0) const;
virtual number_t sideDofsMap(const number_t& n, const number_t& i, const number_t& j,
                               const number_ & k=0) const;
virtual number_t sideofsideDofsMap(const number_t& n, const number_t& i, const number_t&
     j=0)const;
number_t sideOf(number_t) const;        //side number of a dof
number_t sideOfSideOf(number_t) const;  //return side of side number of a dof
```

- some general build functions for DoFs:

```
void LagrangeRefDofs(const int, const int, const int, const Dimen);
```

As the inheritance diagram is based on shape, these functions specify the interpolation type

- For output purpose, a `RefElement` may be split in first order elements, either simplices or of same shape, at every order :

```
virtual vector<vector<number_t>> splitP1() const;
virtual vector<pair<ShapeType,vector<number_t>>> splitO1() const;
```

- some external functions to find a reference element in the static list of `RefElement` and create it if not found:

```
RefElement* findRefElement(ShapeType, const Interpolation*);
RefElement* selectRefSegment(const Interpolation*);
RefElement* selectRefTriangle(const Interpolation*);
RefElement* selectRefQuadrangle(const Interpolation*);
RefElement* selectRefTetrahedron(const Interpolation*);
RefElement* selectRefPrism(const Interpolation*);
RefElement* selectRefHexahedron(const Interpolation*);
RefElement* selectRefPyramid(const Interpolation*);
```

| | |
|---|---|
| library : | **finiteElements** |
| header : | **RefElement.hpp** |
| implementation : | **RefElement.cpp** |
| unitary tests : | **test_segment.cpp, test_triangle.cpp, test_quadrangle.cpp, test_tetrahedron.cpp, test_hexahedron.cpp, test_prism.cpp, test_pyramid.cpp** |
| header dependences : | **config.h, utils.h, Interpolation.hpp, ShapeValues.hpp, GeomRefElement.hpp, RefDof.hpp** |

### 5.4.3 Child classes for segment

The `RefSegment` class has three main child classes :

- `LagrangeStdSegment` which implements standard Lagrange element at any order
- `LagrangeGLSegment` which implements Lagrange element based on Gauss-Lobatto points at any order
- `HermiteStdSegment` which implements standard Hermite element, currently only P3 Hermite

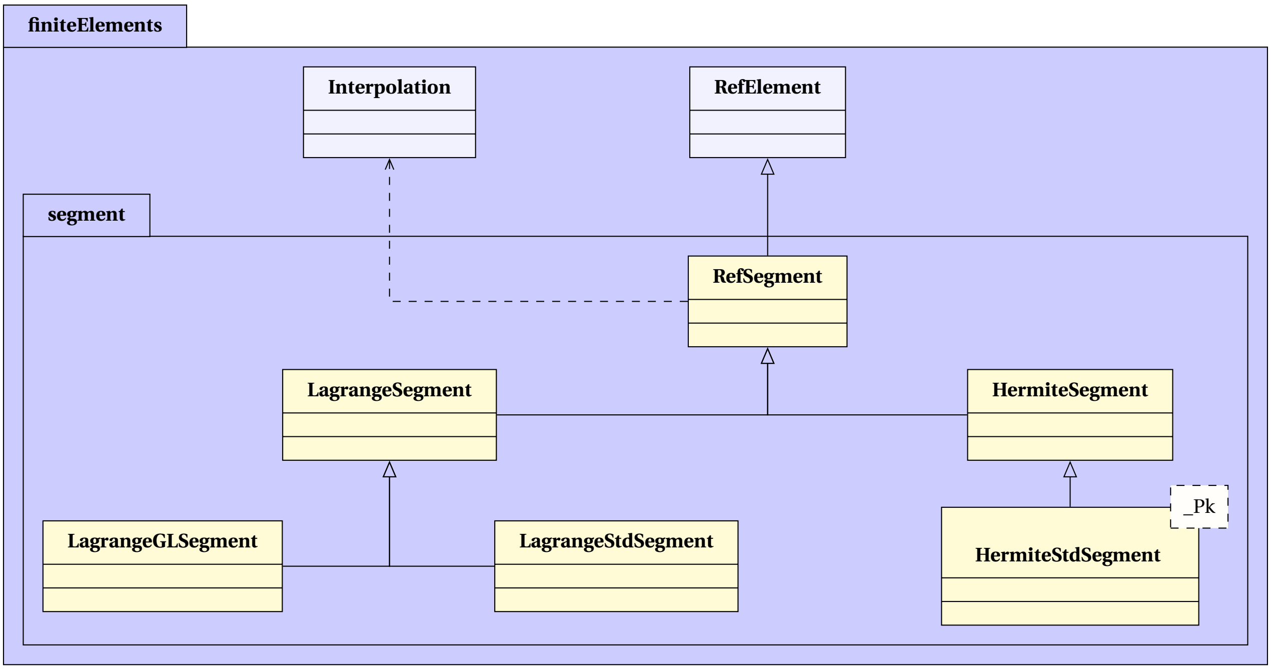


Figure 5.2: The RefSegment main class diagram.

### 5.4.4 Child classes for triangle

The RefTriangle class provides the following types of element:

- standard Lagrange element at any order LagrangeStdTriangle <_Pk> and LagrangeStdTrianglePk; the template LagrangeStdTriangle<_Pk> class is defined only for low order (up to 6) with best performance and LagrangeStdTrianglePk class is designed for any order. It uses a general representation of shape functions on xy-monoms basis get from the solving of a linear system. This method is not stable for very high order.

- HermiteStdTriangle which implements standard Hermite element, currently only P3 Hermite (not H2 comforming)

- CrouzeixRaviartStdTriangle which implements the Crouzet-Raviart element, currently only P1 (not H1 comforming)

- RaviartThomasTriangle which implements the Raviart-Thomas elements (Hdiv comforming) : RaviartThomasSt for Raviart-Thomas standard P1 element and RaviartThomasStdTrianglePk for Raviart-Thomas at any order.

- NedelecTriangle which implements the Nedelec elements (Hcurl comforming) : NedelecFirstTriangleP1 for Nedelec first family of order 1 element, NedelecFirstTrianglePk for Nedelec first family of any order and NedelecSecondTrianglePk for Nedelec second family of any order.

- MorleyTriangle and ArgyrisTriangle elements designed for H2-approximation (non H2 conforming and H2 conforming).

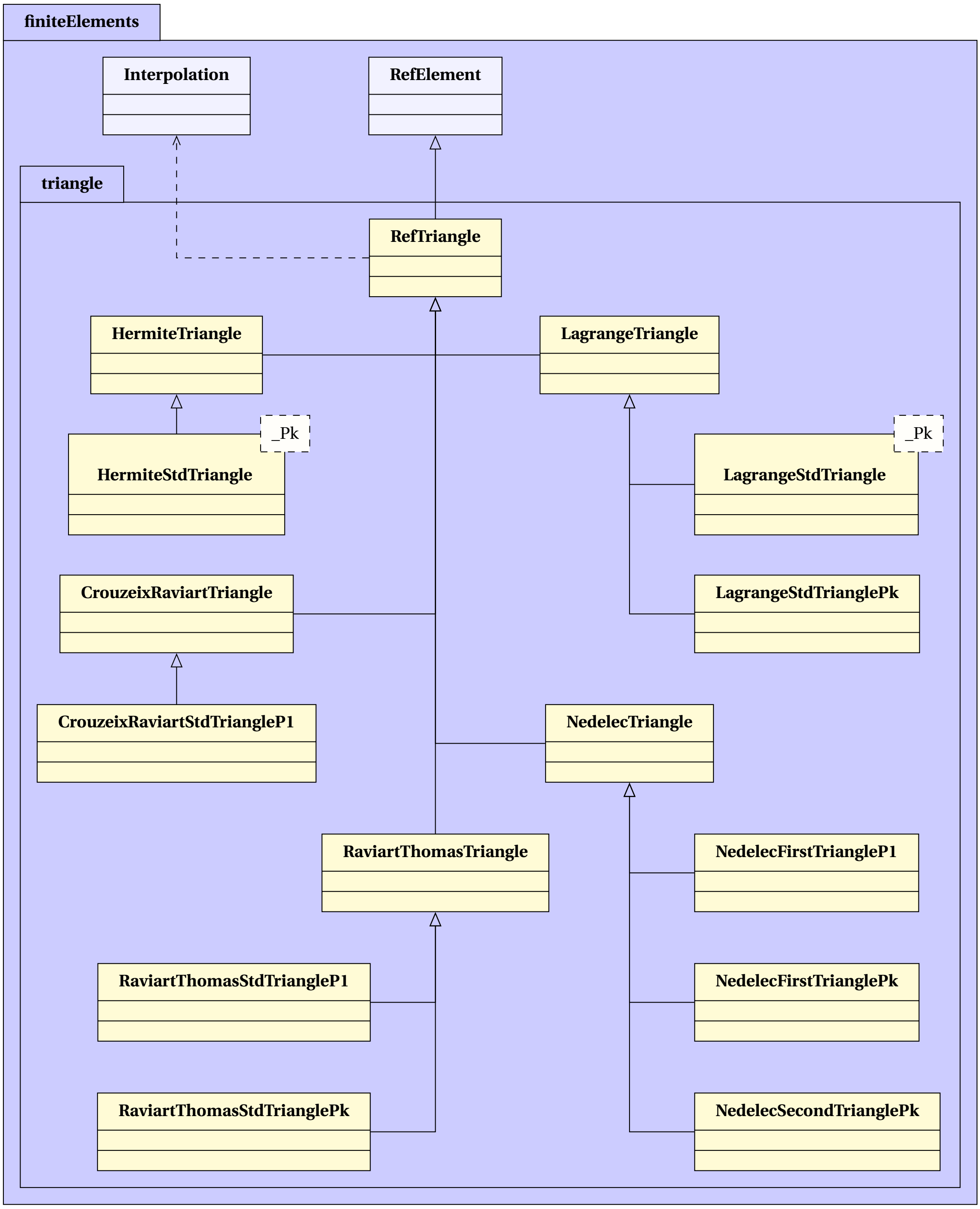


Figure 5.3: The `RefTriangle` main class diagram.

### 5.4.5 Child classes for quadrangle

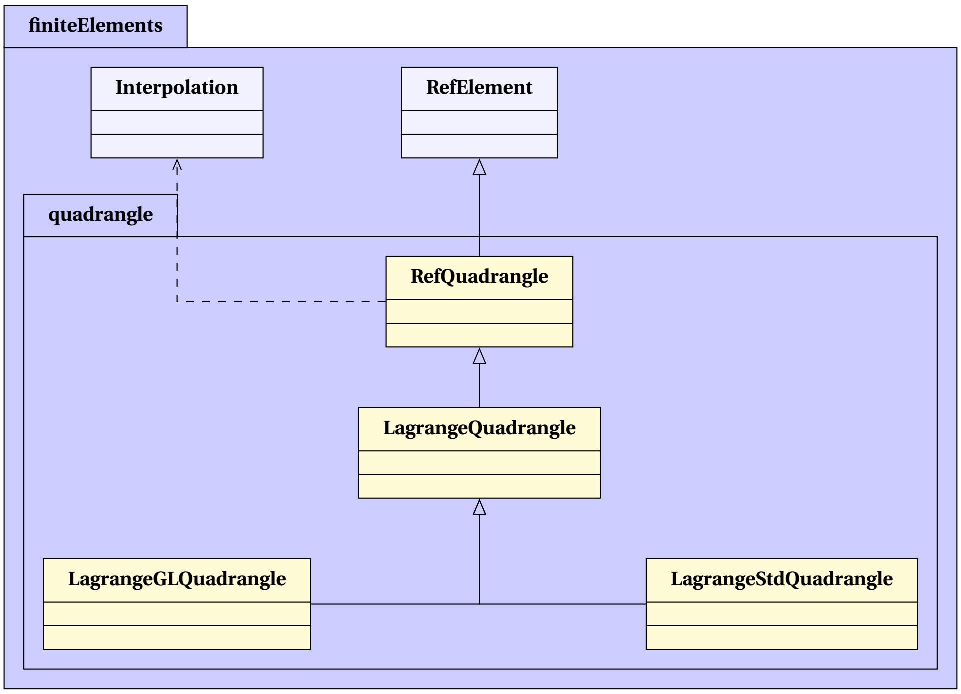


Figure 5.4: The `RefQuadrangle` main class diagram.

### 5.4.6 Child classes for tetrahedron

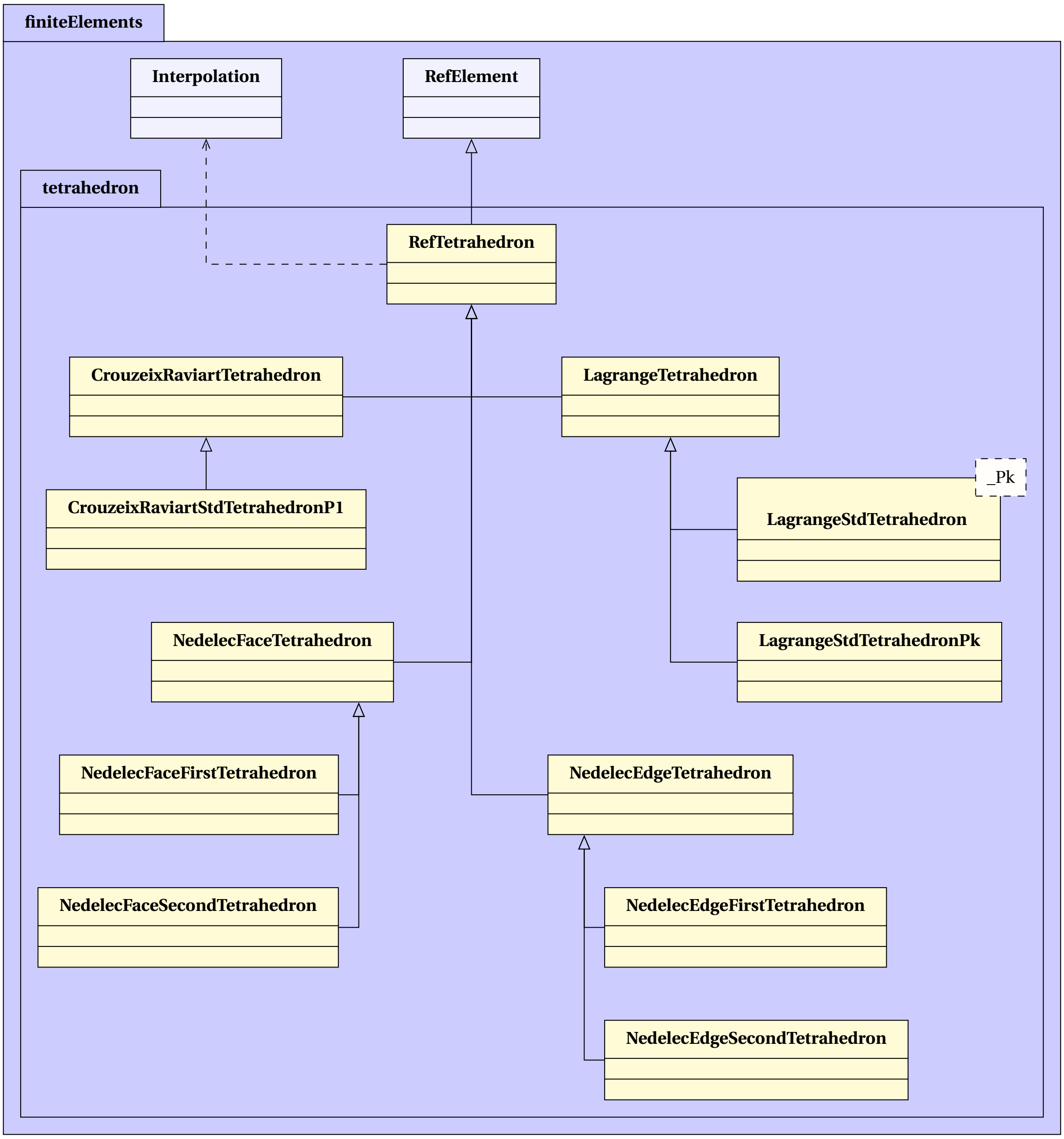


Figure 5.5: The RefTetrahedron main class diagram.

The RefTetrahedron class provides the following types of element:

- LagrangeStdTetrahedron<_Pk> class is defined only for low order (up to 6) with best performance and LagrangeStdTetrahedronPk class is designed for any order. It uses a general representation of shape functions on xyz-monoms basis get from the solving of a linear system. This method is not stable for very high order.

- CrouzeixRaviartTetrahedron which implements the Crouzet-Raviart element, currently only P1 (not H1 comforming)

- NedelecFaceTetrahedron which implements the Nedelec elements Hdiv comforming: NedelecFaceFirstTetrahe for Nedelec first family of any order and NedelecFaceSecondTetrahedronPk for Nedelec second family of any order. The second family is not yet available.

- NedelecEdgeTetrahedron which implements the Nedelec elements Hrot comforming : NedelecEdgeFirstTetrahe for Nedelec first family of any order and NedelecEdgeSecondTetrahedronPk for Nedelec second family of any order. The second family is not yet available.

Short identifiers of face/edge elements are defined in the following enumerations:

```
enum FeFaceType
{
  _RT_1 = 1, RT_1 = _RT_1, _NF1_1 = _RT_1, NF1_1 = _RT_1,
  _RT_2 ,    RT_2 = _RT_2, _NF1_2 = _RT_2, NF1_2 = _RT_2,
  _RT_3 ,    RT_3 = _RT_3, _NF1_3 = _RT_3, NF1_3 = _RT_3,
  _RT_4 ,    RT_4 = _RT_4, _NF1_4 = _RT_4, NF1_4 = _RT_4,
  _RT_5 ,    RT_5 = _RT_5, _NF1_5 = _RT_5, NF1_5 = _RT_5,
  _BDM_1 ,    BDM_1 = _BDM_1, _NF2_1 = _BDM_1, NF2_1 = _BDM_1,
  _BDM_2 ,    BDM_2 = _BDM_2, _NF2_2 = _BDM_2, NF2_2 = _BDM_2,
  _BDM_3 ,    BDM_3 = _BDM_3, _NF2_3 = _BDM_3, NF2_3 = _BDM_3,
  _BDM_4 ,    BDM_4 = _BDM_4, _NF2_4 = _BDM_4, NF2_4 = _BDM_4,
  _BDM_5 ,    BDM_5 = _BDM_5, _NF2_5 = _BDM_5, NF2_5 = _BDM_5
};

enum FeEdgeType
{
  _N1_1 = 1, N1_1 = _N1_1, _NE1_1 = _N1_1, NE1_1 = _N1_1,
  _N1_2 ,    N1_2 = _N1_2, _NE1_2 = _N1_2, NE1_2 = _N1_2,
  _N1_3 ,    N1_3 = _N1_3, _NE1_3 = _N1_3, NE1_3 = _N1_3,
  _N1_4 ,    N1_4 = _N1_4, _NE1_4 = _N1_4, NE1_4 = _N1_4,
  _N1_5 ,    N1_5 = _N1_5, _NE1_5 = _N1_5, NE1_5 = _N1_5,
  _N2_1 ,    N2_1 = _N2_1, _NE2_1 = _N2_1, NE2_1 = _N2_1,
  _N2_2 ,    N2_2 = _N2_2, _NE2_2 = _N2_2, NE2_2 = _N2_2,
  _N2_3 ,    N2_3 = _N2_3, _NE2_3 = _N2_3, NE2_3 = _N2_3,
  _N2_4 ,    N2_4 = _N2_4, _NE2_4 = _N2_4, NE2_4 = _N2_4,
  _N2_5 ,    N2_5 = _N2_5, _NE2_5 = _N2_5, NE2_5 = _N2_5
};
```

The naming convention is based on the FE periodic table. Note that there is an equivalence between NF1_k and RT_k (Raviart Thomas), NF2_k BDM_k (Brezzi Douglas Marini), N1_k and NE1_k and, N2_k and NE2_k.

NedelecEdgeTetrahedron and NedelecFaceTetrahedron classes use a general process to build shape functions as polynomials related to moment dofs. To match dofs on shared edge or shared face, the ascending numbering of vertices is implicitely used even if it is not in fact. This method is particular touchy in case of face dofs of Nedelec Edge element. Indeed, such dofs depend on the choice of two tangent vectors, generally two edges of faces of the reference terahedron that are mapped to some edges of physical element in a non trivial way. To ensure a correct matching of such dofs on a shared face, a rotation has to be applied to shape values to guarantee that they corresponds to the same tangent vectors. This is the role of the member function NedelecEdgeFirstTetrahedronPk::rotateDofs. Note that if the element vertex numbering and face vertex numbering are ascending, *rotateDofs* does nothing. This trick is commonly used to overcome this difficulty but as XLIFE++ makes no assumption on geometry, this dofs rotation is mandatory. More details on edge/face elements are provided in a specific paper.

### 5.4.7 Child classes for hexahedron

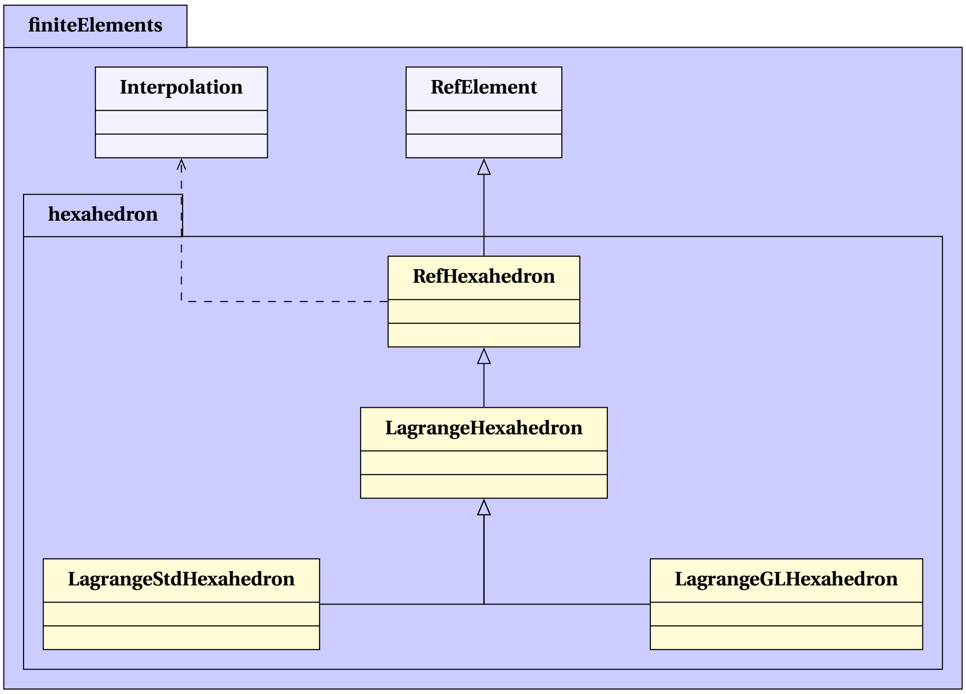


Figure 5.6: The `RefHexahedron` main class diagram.

### 5.4.8 Child classes for prism

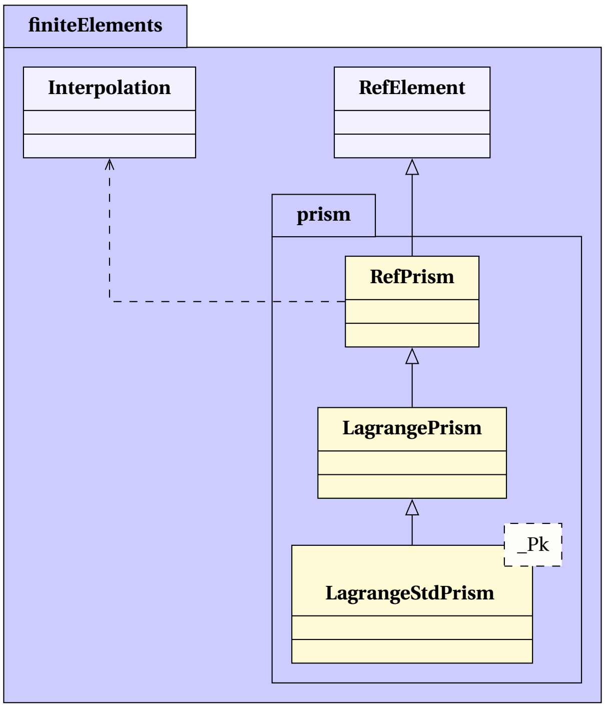


Figure 5.7: The `RefPrism` main class diagram.

### 5.4.9 Child classes for pyramid

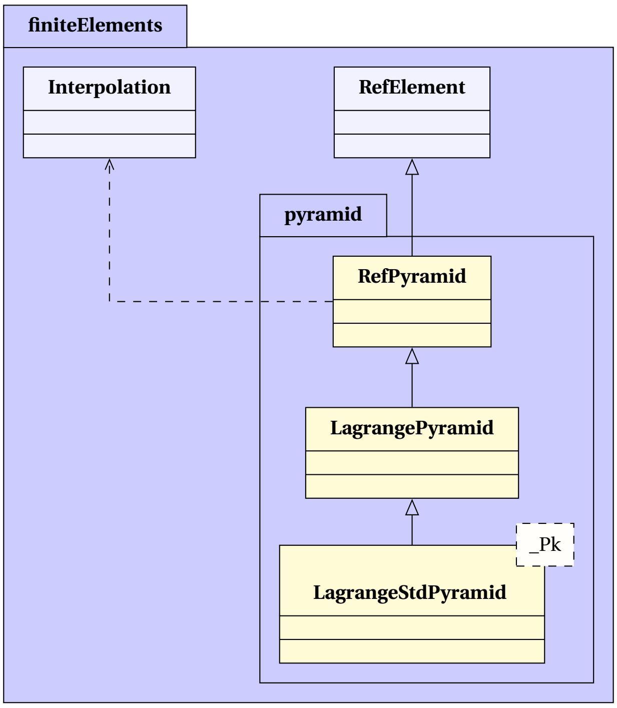
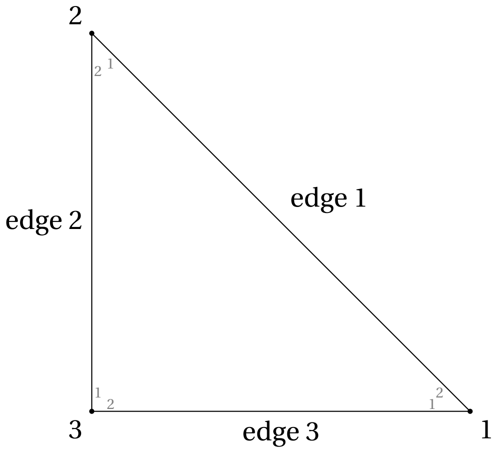
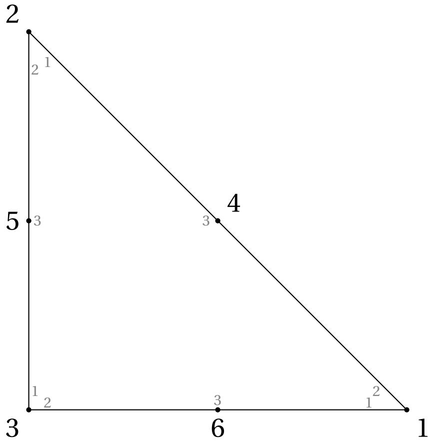


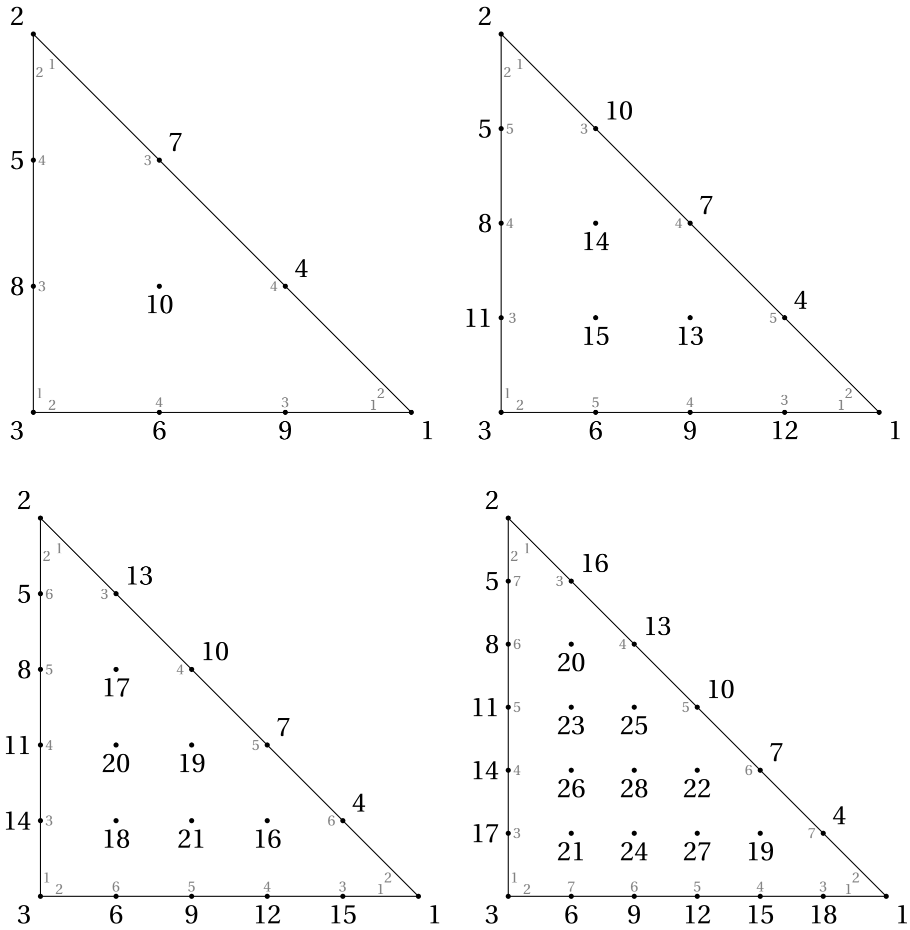
Figure 5.8: The `RefPyramid` main class diagram.

## 5.5 Examples of elements

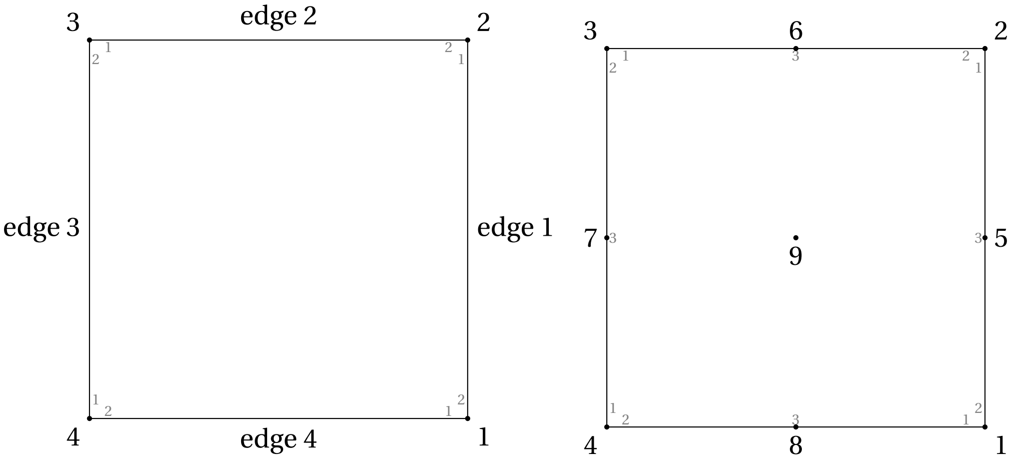
### 5.5.1 Examples of triangles

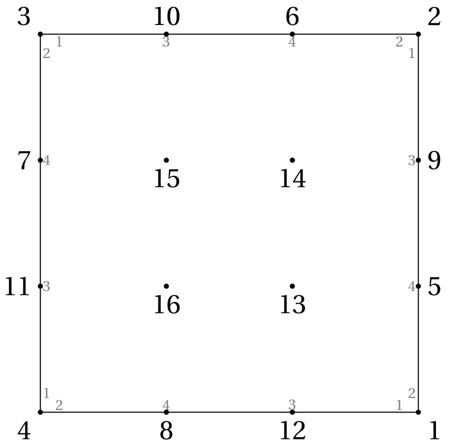


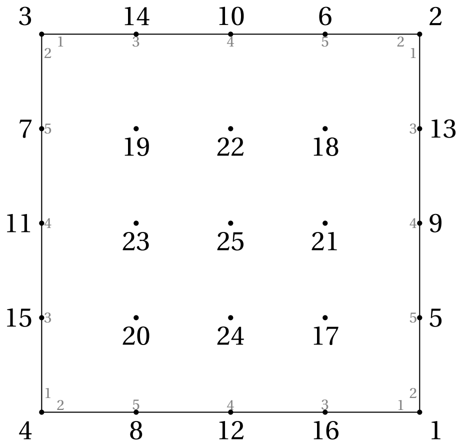


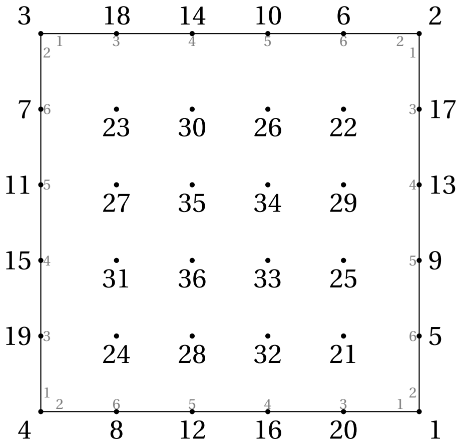


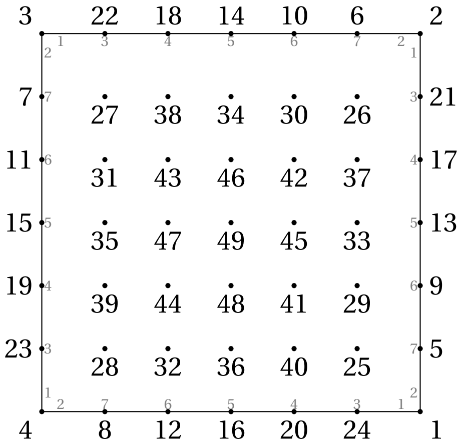
### 5.5.2 Examples of quadrangles



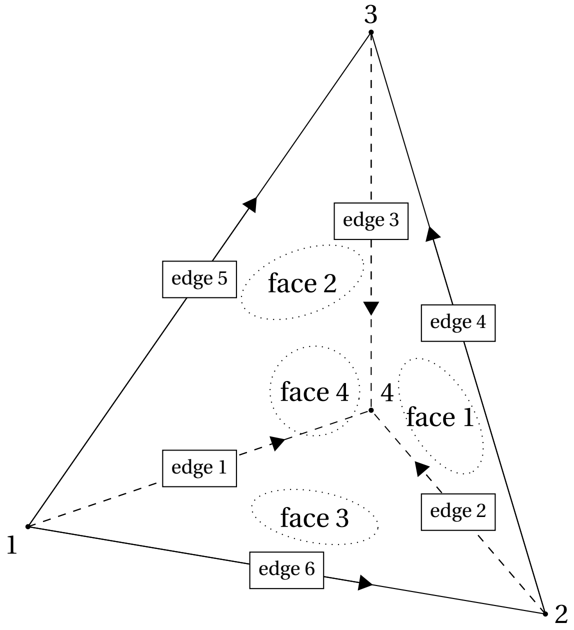


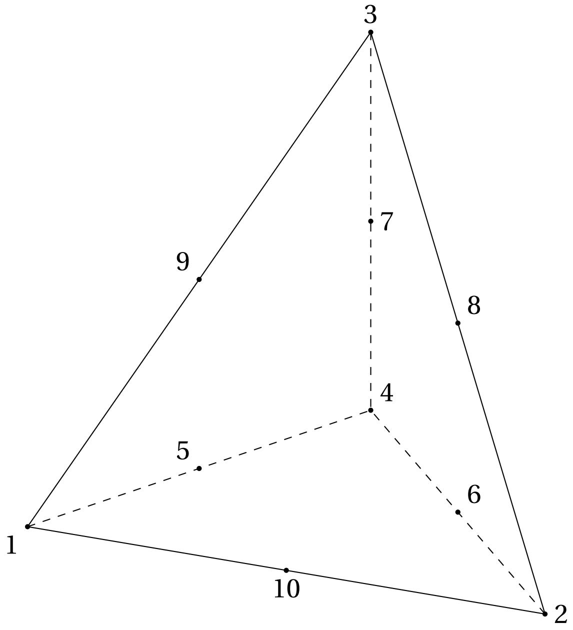


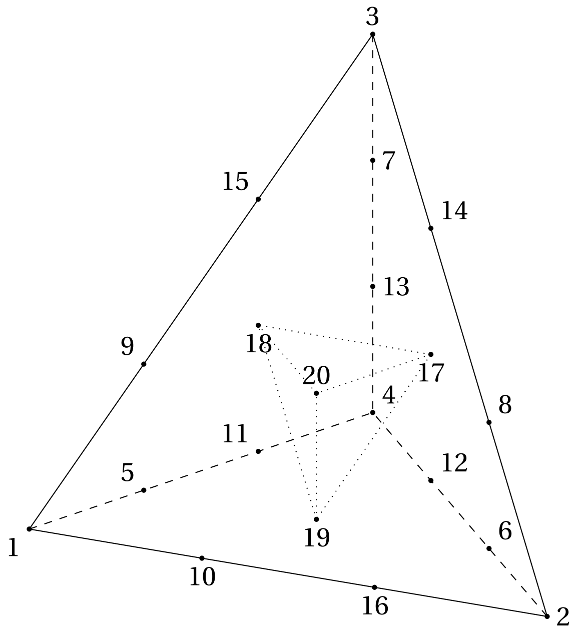


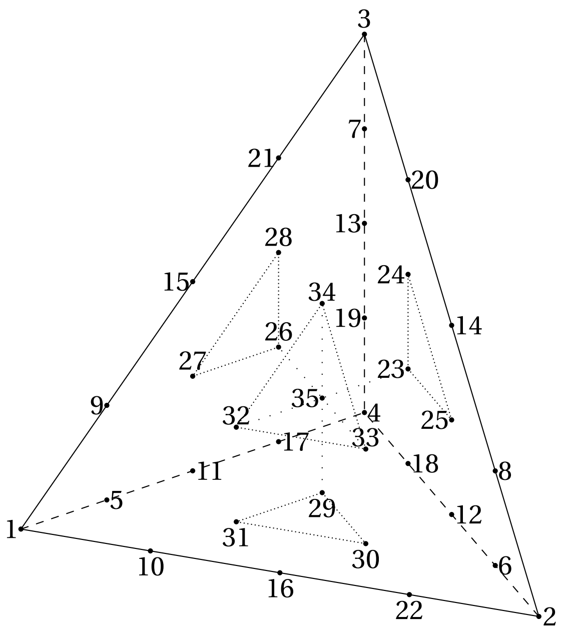


### 5.5.3 Examples of tetrahedra

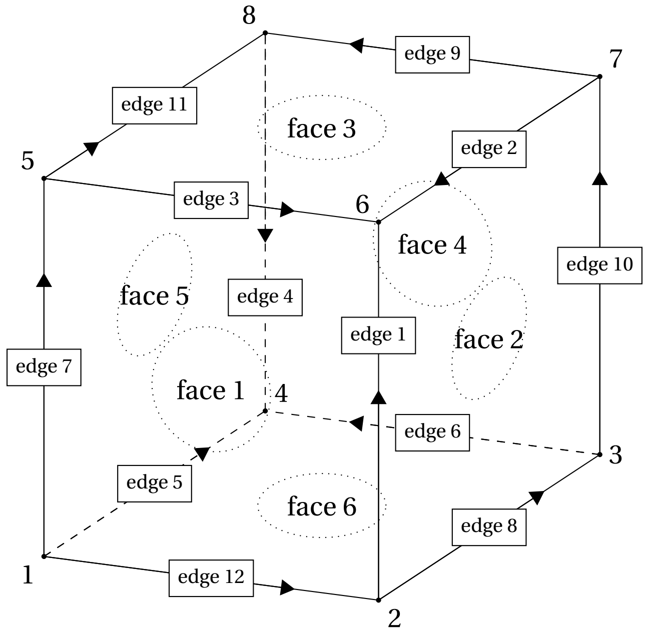


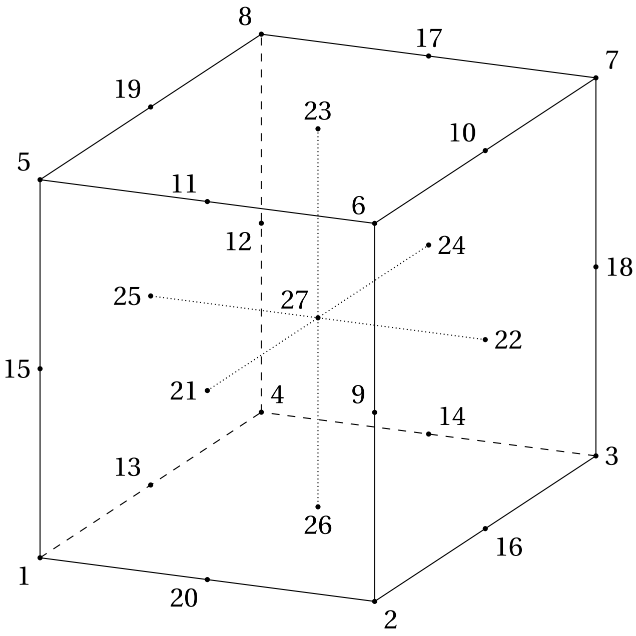


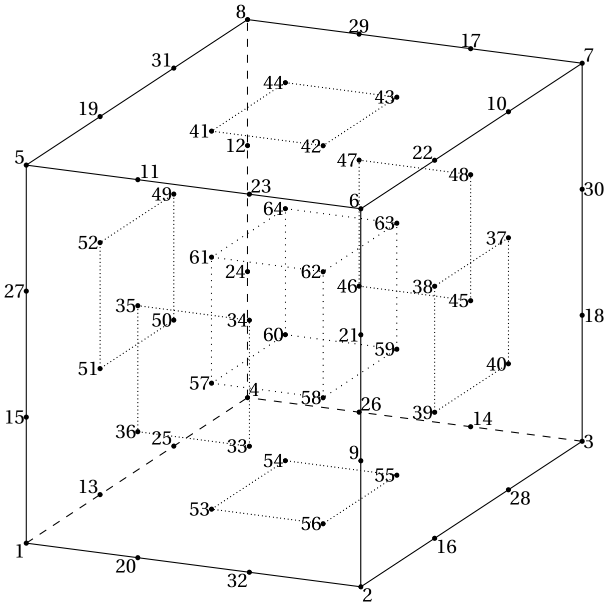




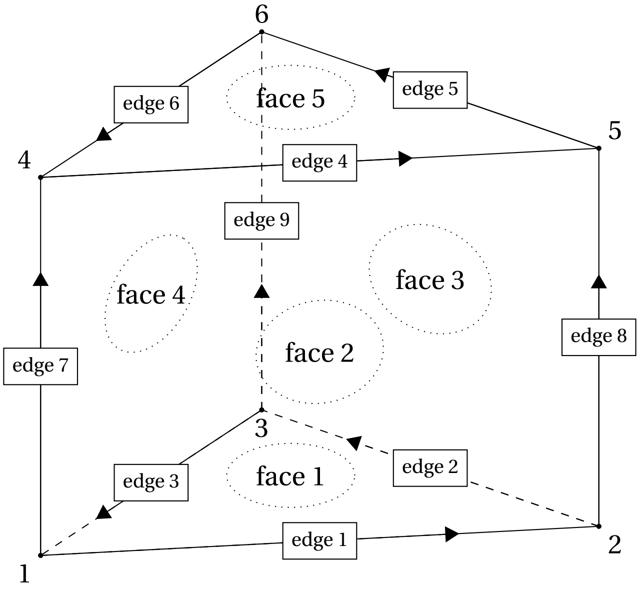
### 5.5.4 Examples of hexahedra

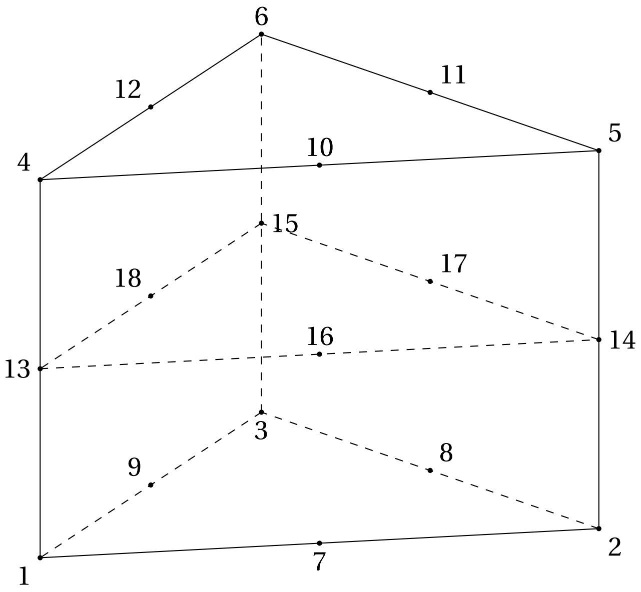




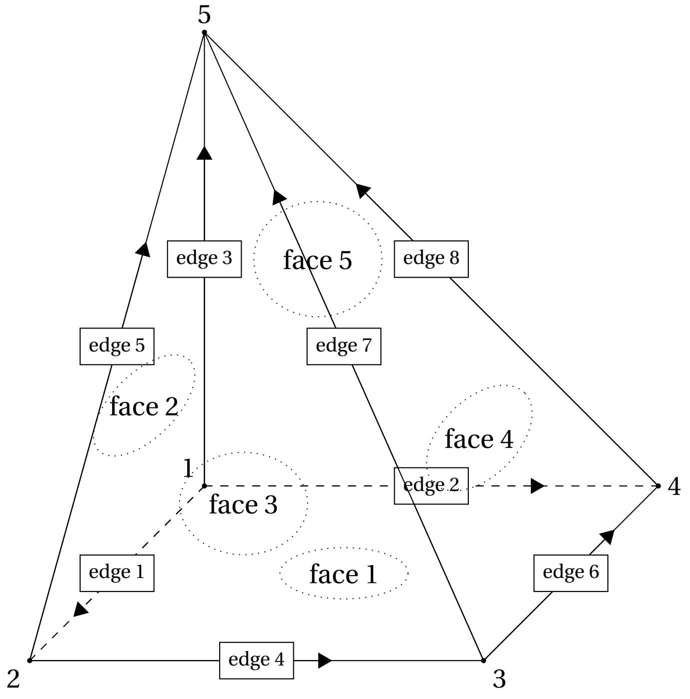


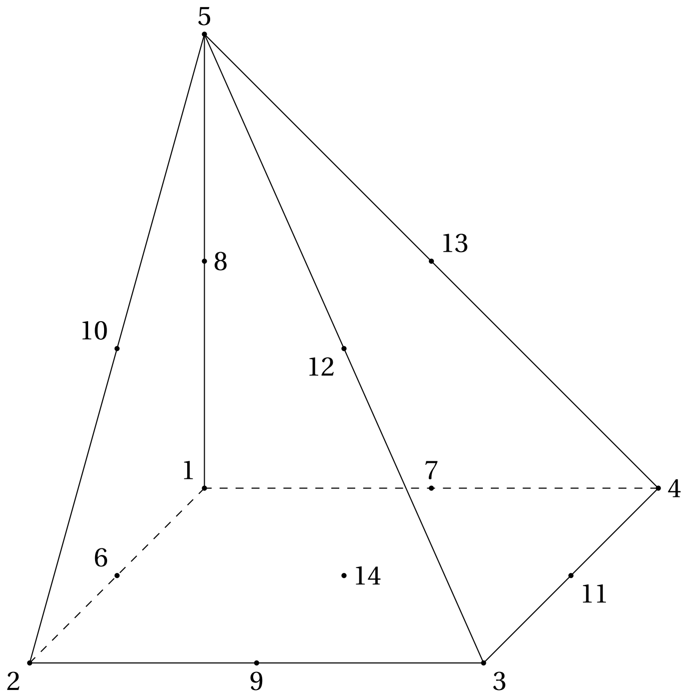
### 5.5.5 Examples of prisms





### 5.5.6 Examples of pyramids





## 5.6 Integration methods

To perform computation of integrals over elements, the library provides IntegrationMethod class which is an abstract class. Two abstract classes inherit from it : the SingleIM class to deal with single integral and the DoubleIM class to deal with double integral. All the classes have to inherit from these two classes.
Among integration methods, quadrature methods are general and well adapted to regular functions to be integrated. XLiFE++ provides the QuadratureIM class, inherited fom SingleIM class, which encapsulates the usual quadrature formulae defined in QuadratureIM class. Besides, the ProductIM class, inherited from doubleIM class, manages a pair of SingleIM object and may be used to take into double quadrature method (adapted to compute double integral with regular kernel).

The inheritance diagram looks like

```
IntegrationMethod ---> | SingleIM  ---> | QuadratureIM (based on Quadrature class)
    (abstract)         |(abstract)      | PolynomialIM (exact intg. of polynoms)
                       |                | LenoirSalles2dIR (analytic method for IR, Laplace P0, P1)
                       |                | LenoirSalles3dIR (analytic method for IR, Laplace triangle P0, P1)
                       |                | FilonIM (1D oscillatory integrals intg_0_T f(t)exp(-iat))
                       |
                       | DoubleIM  ---> | ProductIM         (product of single intg methods)
                        (abstract)      | LenoirSalles2DIM  (analytic method for BEM Laplace P0 and P1)
                                        | LenoirSalles3DIM  (analytic method for BEM Laplace triangle P0, P1)
                                        | SauterSchwabIM    (quadrature for BEM Laplace, Helmholtz triangle)
                                        | SauterSchwabSymIM (Sauter-Schwab method for symmetrical kernels)
                                        | DuffyIM           (quadrature for BEM Laplace, Helmholtz segment)
                                        | CollinoIM         (semi-analytic method for BEM Maxwell RT0)
```

As some computations, in particular BEM computations, require more than one integration method, XLiFE++ provides the IntegrationMethods class that collects IntegrationMethod objects with additional parameters (IntgMeth class).

### 5.6.1 The IntegrationMethod, SingleIM, DoubleIM classes

#### The IntegrationMethod class

The IntegrationMethod class, basis class of all integration methods, manages a name, a type of integral and two booleans:

```
class IntegrationMethod
{public :
  String name;
  IntegrationMethodType imType;
  bool requireRefElement;
  bool requirePhyElement;
};
```

Up to now, the types of integral defined in enumeration are:

```
enum IntegrationMethodType
  {_undefIM, _quadratureIM, _polynomialIM, _productIM,
   _LenoirSalles2dIM, Lenoir_Salles_2d =_LenoirSalles2dIM, _LenoirSalles3dIM, Lenoir_Salles_3d=
        _LenoirSalles3dIM, _LenoirSalles2dIR, _LenoirSalles3dIR,
   _SauterSchwabIM, Sauter_Schwab=_SauterSchwabIM, _SauterSchwabSymIM,
        Sauter_Schwab_sym=_SauterSchwabSymIM,
   _DuffyIM, Duffy = _DuffyIM, _DuffySymIM, Duffy_sym = _DuffySymIM,
   _HMatrixIM, H_Matrix= _HMatrixIM, _CollinoIM, _FilonIM
   };
```

The _HMatrixIM type is a very particular case because it is used to choose the HMatrix representation and compression methods which can be seen in some way as an integration method!

This class provides few general functions, most of them being virtual ones

```
IntegrationMethod(IntegrationMethodType imt=_undefIM, bool ref=false, bool phy=false, const
     String& na="")
virtual ~IntegrationMethod() {};
virtual bool isSingleIM() const =0;
virtual bool isDoubleIM() const =0;
virtual void print(std::ostream& os) const;
IntegrationMethodType type() const;
virtual bool useQuadraturePoints() const;

std::ostream& operator<<(std::ostream&, const IntegrationMethod&);
```

#### The SingleIM, DoubleIM classes

The SingleIM, DoubleIM derived classes provides only simple member functions :

```
class SingleIM : public IntegrationMethod
{public :
 bool isSingleIM() const {return true;}
 bool isDoubleIM() const {return false;}
 SingleIM(IntegrationMethodType imt=_undefIM);
 virtual void print(std::ostream& os) const;
}
```

```
class DoubleIM : public IntegrationMethod
{public :
 bool isSingleIM() const {return false;}
 bool isDoubleIM() const {return true;}
 DoubleIM(IntegrationMethodType imt=_undefIM);
 virtual void print(std::ostream& os) const;
}
```

### 5.6.2 The QuadratureIM class

The QuadratureIM class handles a list of QuadratureIM pointers indexed by ShapeType to deal with multiple quadrature rule in case of domain having more than one shape type. As theq uadrature rule are often involved in context of FE computation, the QuadratureIM class may store shape values (pointer):

```
class QuadratureIM : public SingleIM
{protected :
 std::map<ShapeType, Quadrature *> quadratures_;
 std::map<ShapeType, std::vector<ShapeValues>* > shapevalues_;
```

It provides two basic constructors, accessors and print facilities (all are public):

```
QuadratureIM( ShapeType, QuadRule =_defaultRule, Number =0);
QuadratureIM(const std::set<ShapeType>&, QuadRule =_defaultRule, Number =0);
virtual bool useQuadraturePoints() const;
Quadrature* getQuadrature(ShapeType) const;
void setShapeValues(ShapeType, std::vector<ShapeValues>*);
std::vector<ShapeValues>* getShapeValues(ShapeType);
virtual void print(std::ostream& os) const;
std::ostream& operator<<(std::ostream&, const QuadratureIM&);
```

### 5.6.3 The ProductIM class

In order to represent a product of integration method over a product of geometric domain, the ProductIM class carries two SingleIM pointers:

```
class ProductIM : public DoubleIM
{protected :
 SingleIM* im_x;     //!< integration method along x
 SingleIM* im_y;     //!< integration method along y
}
```

and provides simple member functions:

```

    ProductIM(SingleIM* imx=0, SingleIM* imy=0);
    SingleIM* getxIM();
    SingleIM* getyIM();
    virtual bool useQuadraturePoints() const;
    virtual void print(std::ostream& os) const;  //!< print on stream
};
```

### 5.6.4 The Quadrature, QuadratureRule classes

The quadrature formulae have the following form :

$$\int_{\hat{E}} f(\hat{x})d\hat{x} \approx \sum_{i=1,q} \omega_i f(\hat{x}_i)$$

where $(\hat{x}_i)_{i=1,q}$ are quadrature points belonging to reference element $\hat{E}$ and $(w_i)_{i=1,q}$ are quadrature weights. Up to now, there exist quadrature formulae for unit segment $]0,1[$, for unit triangle, for unit quadrangle (square), for unit tetrahedron, for unit hexahedron (cube) and for unit prism. The following tables give the list of quadrature formulae :

**General rules**

| | Gauss-Legendre | Gauss-Lobatto | Grundmann-Muller | symmetrical Gauss |
|---|---|---|---|---|
| segment | any odd degree | any odd degree | | |
| quadrangle | any odd degree | any odd degree | | odd degree up to 21 |
| triangle | any odd degree | | any odd degree | degree up to 10 |
| hexahedron | any odd degree | any odd degree | | odd degree up to 11 |
| tetrahedron | any odd degree | | any odd degree | degree up to 10 |
| prism | | | | degree up to 10 |
| pyramid | any odd degree | any odd degree | | degree up to 10 |

**Particular rules**

| | nodal | miscellaneous |
|---|---|---|
| segment | P1 to P4 | |
| quadrangle | Q1 to Q4 | |
| triangle | P1 to P3 | Hammer-Stroud 1 to 6 |
| hexahedron | Q1 to Q4 | |
| tetrahedron | P1, P3 | Stroud 1 to 5 |
| prism | P1 | centroid 1, tensor product 1,3,5 |
| pyramid | P1 | centroid 1, Stroud 7 |

More precisely, the rules that are implemented :

- 1D rules
  Gauss-Legendre rule, degree $2n+1$, $n$ points
  Gauss-Lobatto rule, degree $2n-1$, $n$ points
  trapezoidal rule, degree 1, 2 points
  Simpson rule, degree 3, 3 points
  Simpson 3 8 rule, degree 3, 4 points
  Booleb rule, degree 5, 5 points
  Wedge rule, degree 5, 6 points

- Rules over the unit simplex (less quadrature points BUT with negative weights)
  TN Grundmann-Moller rule, degree $2n+1$, $C^n_{n+d+1}$ points

- Rules over the unit triangle $\{x>0, y>0, x+y<1\}$
  T2P2 MidEdge rule
  T2P2 Hammer-Stroud rule
  T2P3 Albrecht-Collatz rule, degree 3, 6 points, Stroud (p.314)
  T2P3 Stroud rule, degree 3, 7 points, Stroud (p.308)
  T2P5 Radon-Hammer-Marlowe-Stroud rule, degree 6, 7 points, Stroud (p.314)
  T2P6 Hammer rule, degree 6, 12 points, G.Dhatt, G.Touzot (p.298)
  symmetrical Gauss up to degree 10

- Rules over the unit tetrahedron $\{x>0, y>0, z>0, x+y+z<1\}$
  T3P2 Hammer-Stroud rule, degree 2, 4 points, Stroud (p.307)
  T3P3 Stroud rule, degree 3, 8 points, Stroud (p.308)
  T3P5 Stroud rule, degree 5, 15 points, Stroud (p.315)
  symmetrical Gauss up to degree 10

- Rules over the unit prism $\{0 < x, y < 1, x + y < 1, 0 < z < 1\}$
  P1 nodal rule
  tensor product of 2-points Gauss-Legendre rule on [0,1] and Stroud 7 points formula on the unit triangle (degree 3)
  tensor product of 3-points Gauss-Legendre rule on [0,1] and Radon-Hammmer-Marlowe-Stroud 7 points formula on the unit triangle (degree 5)
  symmetrical Gauss up to degree 10

- Rules over the unit pyramid $\{0 < x, y < 1 - z, 0 < z < 1\}$
  P1 nodal rule
  symmetrical Gauss up to degree 10

- Rules built from lower dimension rules
  tensor product of quadrature rules (quadrangle and hexahedron)
  conical product of quadrature rules (triangle and pyramid)
  rule built from 1D nodal rule which are quadrangle nodal rule
  rule built from 1D nodal rule which are hexahedron nodal rule

References :

- A.H.Stroud, Approximate calculation of multiple integrals, Prentice Hall, 1971.

- G.Dhatt & G Touzot, The finite element method displayed, John Wiley & Sons, Chichester, 1984

- A. Grundmann & H.M. Moller, Invariant Integration Formulas for the N-Simplex by Combinatorial Methods, SIAM Journal on Numerical Analysis, Vol 15, No 2, Apr. 1978, pages 282-290.

- F.D. Witherden & P.E. Vincent, On the identification of symmetric quadrature rules for finite element methods, Computers & Mathematics with Applications, Volume 69, Issue 10, May 2015, Pages 1232-1241.

These quadrature formulae are provided by using two classes : the `Quadrature` class which handles the main quadrature objects and the `QuadratureRule` class carrying the quadrature points and weights.

### The `Quadrature` class

The `Quadrature` class manages all informations related to quadrature :

```
class Quadrature
{public:
 GeomRefElement* geomRefElt_p;   // geometric element bearing quadrature rule
 QuadratureRule quadratureRule; // embedded QuadratureRule object
 protected:
 QuadRule rule_;            // type of quadrature rule
 Number degree_;            // degree of quadrature rule
 bool hasPointsOnBoundary_; // as it reads
 String name_;              // name of quadrature formula
 public:
 static std::vector<Quadrature*> theQuadratureRules;
 ...
```

`QuadRule` is a enumeration of all types of quadrature supported:

```
enum QuadRule
{_defaultRule = 0, _GaussLegendreRule, _symmetricalGaussRule, _GaussLobattoRule, Gauss_Lobatto =
    _GaussLobattoRule,
  _nodalRule, _miscRule,_GrundmannMollerRule, _doubleQuadrature };
```

degree_ is either the degree of the quadrature rule or the degree of the polynomial interpolation in case of nodal quadrature rules. A Quadrature object has to be instanced only once and the static vector theQuadratureRules collects all the pointers to Quadrature object. Note that the shape bearing the quadrature is given through the GeomRefElement pointer.

The class proposes only a default constructor, a full basic constructor and a destructor :

```
Quadrature();
Quadrature(ShapeType , QuadRule, Number, const String&, bool pob = false);
```

Note that the basic constructor initializes member attributes but does not load the quadrature points and quadrature weights (QuadratureRule)! The practical "construction" is done by the external function findQuadrature. The copy constructor and assignment operator are defined as private member function to avoid duplicated Quadrature object

The following accessors (read only) are provided:

```
String name() const;
QuadRule rule() const;
Number degree() const;
bool hasPointsOnBoundary() const;
Dimen dim() const;
Number numberOfPoints() const;
ShapeType shapeType() const;
std::vector<Real>::const_iterator point(Number i = 0) const;
std::vector<Real>::const_iterator weight(Number i = 0) const;
```

To construct a Quadrature object, the external function findQuadrature has to be used :

```
friend Quadrature* findQuadrature(ShapeType shape, QuadRule rule, Number degree, bool hpob=
    false);
```

It searches in the static vector theQuadratureRules the quadrature rule defined by a shape, a quadrature rule and a degree. If it is not found, a new Quadrature object is created on the heap. In any case a pointer to the Quadrature object is returned.

There are few functions depending on the shape that are called during the creation process :

```
Quadrature* segmentQuadrature(QuadRule, Number);
Quadrature* triangleQuadrature(QuadRule, Number);
Quadrature* quadrangleQuadrature(QuadRule, Number);
Quadrature* tetrahedronQuadrature(QuadRule, Number);
Quadrature* hexahedronQuadrature(QuadRule, Number);
Quadrature* prismQuadrature(QuadRule, Number);
Quadrature* pyramidQuadrature(QuadRule, Number);
static void clear();
```

These functions loads quadrature points and quadrature weights in a QuadratureRule object using member functions of QuadratureRule class. The clear static function deletes quadrature objects stored in the theQuadratureRules static vector.

To choose quadrature rules, the class provides the static function bestQuadRule returning the 'best' quadrature rule for a given shape $S$ and a given polynomial degree $d$.

```
static QuadRule bestQuadRule(ShapeType, Number);
```

Best rule has to be understood as the rule on shape $S$ with the minimum of quadrature points integrating exactly polynomials of degree $d$. The following table gives the current best rules :

| shape | degree | quadrature rule | number of points |
|---|---|---|---|
| segment | 1 | Gauss-Legendre 1 | 1 |
| segment | $2,3$ | Gauss-Legendre 3 | 2 |
| segment | $4,5$ | Gauss-Legendre 5 | 3 |
| segment | $2n-1$ | Gauss-Legendre $2n-1$ | $n$ |

| shape | degree | quadrature rule | number of points |
|---|---|---|---|
| quadrangle | 1 | Gauss-Legendre 1 | 1 |
| quadrangle | $2,3$ | Gauss-Legendre 3 | 4 |
| quadrangle | $4,5$ | symmetrical Gauss 5 | 8 |
| quadrangle | $6,7$ | symmetrical Gauss 7 | 12 |
| quadrangle | $7,9$ | symmetrical Gauss 9 | 20 |
| quadrangle | $10,11$ | symmetrical Gauss 11 | 28 |
| quadrangle | $12,13$ | symmetrical Gauss 13 | 37 |
| quadrangle | $14,15$ | symmetrical Gauss 15 | 48 |
| quadrangle | $16,17$ | symmetrical Gauss 17 | 60 |
| quadrangle | $18,19$ | symmetrical Gauss 19 | 72 |
| quadrangle | $20,21$ | symmetrical Gauss 21 | 85 |
| quadrangle | $2n-1>21$ | Gauss-Legendre $2n-1$ | $n^2$ |

| shape | degree | quadrature rule | number of points |
|---|---|---|---|
| triangle | 1 | centroid rule (misc,1) | 1 |
| triangle | 2 | P2 Hammer-Stroud (misc,2) | 2 |
| triangle | 3 | Grundmann-Moller 3 | 3 |
| triangle | 4 | symmetrical Gauss 4 | 6 |
| triangle | 5 | symmetrical Gauss 5 | 7 |
| triangle | 6 | symmetrical Gauss 6 | 12 |
| triangle | 7 | symmetrical Gauss 7 | 15 |
| triangle | 8 | symmetrical Gauss 8 | 16 |
| triangle | 9 | symmetrical Gauss 9 | 19 |
| triangle | 10 | symmetrical Gauss 10 | 25 |
| triangle | 11 | symmetrical Gauss 11 | 28 |
| triangle | 12 | symmetrical Gauss 12 | 33 |
| triangle | 13 | symmetrical Gauss 13 | 37 |
| triangle | 14 | symmetrical Gauss 14 | 42 |
| triangle | 15 | symmetrical Gauss 15 | 49 |
| triangle | 16 | symmetrical Gauss 16 | 55 |
| triangle | 17 | symmetrical Gauss 17 | 60 |
| triangle | 18 | symmetrical Gauss 18 | 67 |
| triangle | 19 | symmetrical Gauss 19 | 73 |
| triangle | 20 | symmetrical Gauss 20 | 79 |
| triangle | $2n-1>20$ | Gauss-Legendre $2n-1$ | ? |

| shape | degree | quadrature rule | number of points |
|---|---|---|---|
| hexahedron | 1 | Gauss-Legendre 1 | 1 |
| hexahedron | $2,3$ | symmetrical Gauss 3 | 6 |
| hexahedron | $4,5$ | symmetrical Gauss 5 | 14 |
| hexahedron | $6,7$ | symmetrical Gauss 7 | 34 |
| hexahedron | $8,9$ | symmetrical Gauss 9 | 58 |
| hexahedron | $10,11$ | symmetrical Gauss 11 | 90 |
| hexahedron | $2n-1\geq 12$ | Gauss-Legendre $2n-1$ | $n^3$ |

| shape | degree | quadrature rule | number of points |
|---|---|---|---|
| tetrahedron | 1 | centroid rule (misc,1) | 1 |
| tetrahedron | 2 | P2 Hammer-Stroud (misc,2) | 4 |
| tetrahedron | 3 | Grundmann-Moller 3 | 5 |
| tetrahedron | $4,5$ | symmetrical Gauss 5 | 14 |
| tetrahedron | 6 | symmetrical Gauss 6 | 24 |
| tetrahedron | 7 | symmetrical Gauss 7 | 35 |
| tetrahedron | 8 | symmetrical Gauss 8 | 46 |
| tetrahedron | 9 | symmetrical Gauss 9 | 59 |
| tetrahedron | 10 | symmetrical Gauss 10 | 81 |
| tetrahedron | $2n-1\geq 11$ | Grundmann-Moller $2n-1$ | ? |

| shape | degree | quadrature rule | number of points |
|---|---|---|---|
| prism | 1 | centroid rule (misc,1) | 1 |
| prism | 2 | symmetrical Gauss 2 | 5 |
| prism | 3 | symmetrical Gauss 3 | 8 |
| prism | 4 | symmetrical Gauss 4 | 11 |
| prism | 5 | symmetrical Gauss 5 | 16 |
| prism | 6 | symmetrical Gauss 6 | 28 |
| prism | 7 | symmetrical Gauss 7 | 35 |
| prism | 8 | symmetrical Gauss 8 | 46 |
| prism | 9 | symmetrical Gauss 9 | 60 |
| prism | 10 | symmetrical Gauss 10 | 85 |

| shape | degree | quadrature rule | number of points |
|---|---|---|---|
| pyramid | 1 | centroid rule (misc,1) | 1 |
| pyramid | 2 | symmetrical Gauss 2 | 5 |
| pyramid | 3 | symmetrical Gauss 3 | 6 |
| pyramid | 4 | symmetrical Gauss 4 | 10 |
| pyramid | 5 | symmetrical Gauss 5 | 15 |
| pyramid | 6 | symmetrical Gauss 6 | 24 |
| pyramid | 7 | symmetrical Gauss 7 | 31 |
| pyramid | 8 | symmetrical Gauss 8 | 47 |
| pyramid | 9 | symmetrical Gauss 9 | 62 |
| pyramid | 10 | symmetrical Gauss 10 | 83 |

Finally, `Quadrature` class provides some print and error utilities:

```
void badNodeRule(int n_nodes);
void badDegreeRule();
void noEvenDegreeRule();
void upperDegreeRule();
friend std::ostream& operator<<(std::ostream&, const Quadrature&);
friend void alternateRule(QuadRule, ShapeType, const String&);
```

### The QuadratureRule class

The QuadratureRule class stores quadrature points and quadrature weights and provides member functions to load them :

```
class QuadratureRule
{private:
 std::vector<Real> coords_;     // point coordinates of quadrature rule
 std::vector<Real> weights_;    // weights of quadrature rule
 Dimen dim_;                    // dimension of points
...
```

the following constructors are proposed:

```
QuadratureRule(const std::vector<Real>&, Real);
QuadratureRule(const std::vector<Real>&, const std::vector<Real>&);
QuadratureRule(Dimen , Number s);
```

and the following accessors are provided :

```
Dimen dim() const;
Number size() const;
std::vector<Real> coords() const;
std::vector<Real>::const_iterator point(Number i = 0) const;
std::vector<Real>::iterator point(Number i = 0);
std::vector<Real>::const_iterator weight(Number i = 0) const;
std::vector<Real>::iterator weight(const Number i = 0);
```

Some utilities are also helpful:

```
void point(std::vector<Real>::iterator&, Real, std::vector<Real>::iterator&, Real);
void point(std::vector<Real>::iterator&, Real, Real, std::vector<Real>::iterator&, Real);
void point(std::vector<Real>::iterator&, Real, Real, Real,std::vector<Real>::iterator&, Real);
void coords(std::vector<Real>::iterator&, Dimen, std::vector<Real>::const_iterator&);
void coords(std::vector<Real>::const_iterator);
void coords(const std::vector<Real>&);
void coords(Real);
void weights(const std::vector<Real>&);
void weights(Real);
friend std::ostream& operator<<(std::ostream&, const QuadratureRule&);
```

The main task of this class is to load quadrature points and weights. Thus, there are a lot of member functions to load these values. Some of them have a general purpose (for instance to build quadrature rules from tensor or conical products of 1D rules) and others are specific to one quadrature rule:

```
//tensor and conical product
  QuadratureRule& tensorRule(const QuadratureRule&, const QuadratureRule&);
  QuadratureRule& tensorRule(const QuadratureRule&, const QuadratureRule&, const QuadratureRule&);
  QuadratureRule& conicalRule(const QuadratureRule&, const QuadratureRule&);
  QuadratureRule& conicalRule(const QuadratureRule&, const QuadratureRule&, const
      QuadratureRule&);
//nodal tensor product rules for quadrangle and hexahedron
  QuadratureRule& quadrangleNodalRule(const QuadratureRule&);
  QuadratureRule& hexahedronNodalRule(const QuadratureRule&);
//1D Gauss rules
  QuadratureRule& gaussLegendreRules(Number);
  QuadratureRule& gaussLobattoRules(Number);
  QuadratureRule& ruleOn01(Number);
//1D Newton-Cotes closed rules (P_k node rules on [0,1])
  QuadratureRule& trapezoidalRule();
  QuadratureRule& simpsonRule();
  QuadratureRule& simpson38Rule();
  QuadratureRule& booleRule();
//Grundmann-Moller rules for n dimensional simplex
  QuadratureRule& tNGrundmannMollerRule(int, Dimen);
  void TNGrundmannMollerSet(int);    //utility for Grundmann-Moller
//special (Misc) rules for unit Triangle { x + y < 1 , 0 < x,y < 1}
  QuadratureRule& t2P2MidEdgeRule();
  QuadratureRule& t2P2HammerStroudRule();
  QuadratureRule& t2P3AlbrechtCollatzRule();
  QuadratureRule& t2P3StroudRule();
  QuadratureRule& t2P5RadonHammerMarloweStroudRule();
  QuadratureRule& t2P6HammerRule();
//special (Misc) rules for unit Tetrahedron { x + y + z < 1 , 0 < x,y,z < 1 }
  QuadratureRule& t3P2HammerStroudRule();
  QuadratureRule& t3P3StroudRule();
  QuadratureRule& t3P5StroudRule();
//special (Misc) rules for unit pyramid { 0 < x,y < 1 - z , 0 < z < 1 }
  QuadratureRule& pyramidRule(const QuadratureRule&); //conical product
  QuadratureRule& pyramidStroudRule();                //degree 7, 48 points
//symmetrical Gauss rules for any shape
  QuadratureRule& symmetricalGaussTriangleRule(number_t);     //degree up <= 20
  QuadratureRule& symmetricalGaussQuadrangleRule(number_t);   //odd degree <= 21
  QuadratureRule& symmetricalGaussTetrahedronRule(number_t);  //degree <= 10
  QuadratureRule& symmetricalGaussHexahedronRule(number_t);   //odd degree <= 11
  QuadratureRule& symmetricalGaussPrismRule(number_t);        //degre <= 10
  QuadratureRule& symmetricalGaussPyramidRule(number_t);      //degree <= 10
```

Here is a simple example of how to use quadrature objects :

```
Quadrature* q=findQuadrature(_triangle,_GaussLegendreRule, 3);
Real S=0, x,y;
Number k=0;
for(Number i =0;i<q->quadratureRule.size();i++,k+=2)
   {
    x=q->quadratureRule.coords()[k];
    y=q->quadratureRule.coords()[k+1];
    S+=q->quadratureRule.weights()[i]*std::sin(x*y);
   }
std::cout<<"S="<<S;
```

### 5.6.5 How to add a new quadrature formula ?

When you want to add a new quadrature formula on a unit element, say *geomelt*,

- you have to modify the member function :
  `Quadrature::`*geomelt*`Quadrature(QuadRule rule, Number deg)`
  by adding in the right *case* statement the properties of your quadrature formula

- to add in `QuadratureRule` class the member function defining the quadrature points and weights.

Be care with the type and the number (degree) defining your quadrature formula, because they can be used by an other formula. To avoid this difficulty, it is possible to create new type of quadrature. In that case the enumeration `QuadRule` has to be modified, implying to update the dictionnaries and may be, the `Quadrature::bestQuadRule` static function.

### 5.6.6 Integration methods for singular kernels

To deal with single or double integral involving a kernel with a singularity, XLiFE++ provides some additional classes.

### DuffyIM class

This class deals with double integral over segments involving 2d kernel $K$ with $\log|x-y|$ singularity, in other words:

$$\int_{S_1}\int_{S_2} p_1(x)\,K(x,y)\,p_2(y)\,dy\,dx$$

```
class DuffyIM : public DoubleIM
{
 public:
 Quadrature* quadSelf; //quadrature for self influence
 Quadrature* quadAdjt; //quadrature for adjacent elements
 number_t ordSelf;     //order of quadrature for self influence
 number_t ordAdjt;     //order of quadrature for adjacent elements

 DuffyIM(IntegrationMethodType);
 DuffyIM(number_t =6);          //full constructor from quadrature order
 DuffyIM(const Quadrature&); //full constructor from a quadrature
```

### SauterSchwabIM class

This class deals with double integral over triangles involving 3d kernel $K$ with $|x-y|^{-1}$ singularity, say

$$\int_{T_1}\int_{T_2} p_1(x)\,K(x,y)\,p_2(y)\,dy\,dx$$

```
class SauterSchwabIM : public DoubleIM
{
 public:
 Quadrature* quadSelf;     //quadrature for self influence
 Quadrature* quadEdge;     //quadrature for elements adjacent by edge
 Quadrature* quadVertex;   //quadrature for elements adjacent by vertex
 number_t ordSelf;         //order of quadrature for self influence
 number_t ordEdge;         //order of quadrature for edge adjacence
 number_t ordVertex;       //order of quadrature for vertex adjacence

 SauterSchwabIM(number_t =3); //basic constructor (order 3)
 SauterSchwabIM(Quadrature&); //full constructor from quadrature object
```

### LenoirSalles2dIM and LenoirSalles3dIM classes

The LenoirSalles2dIM class can compute analytically

$$-\frac{1}{2\pi}\int_{S_1}\int_{S_2} p_1(x)\,\log|x-y|\,p_2(y)\,dy\,dx \quad \text{(single layer)}$$

$$\frac{1}{2\pi}\int_{S_1}\int_{S_2} p_1(x)\,\frac{(x-y).n_y}{|x-y|^2}\,p_2(y)\,dy\,dx \quad \text{(double layer)}$$

where $p_1$ and $p_2$ are either the P0 or P1 shape functions on segments $S_1$ and $S_2$ and the LenoirSalles3dIM class computes analytically

$$\frac{1}{4\pi}\int_{T_1}\int_{T_2} p_1(x)\,\frac{1}{|x-y|}\,p_2(y)\,dy\,dx \quad \text{(single layer)}$$

$$-\frac{1}{4\pi}\int_{T_1}\int_{T_2} p_1(x)\,\frac{(x-y).n_y}{|x-y|^3}\,p_2(y)\,dy\,dx \quad \text{(double layer)}$$

where $p_1$ and $p_2$ are the P0 shape functions (say 1) on triangles $T_1$ and $T_2$.
These two classes have no member data and only one basic constructor.

### LenoirSalles2dIR and LenoirSalles3dIR classes

The LenoirSalles2dIR class can compute analytically

$$-\frac{1}{2\pi}\int_S \log|x-y|\,p(y)\,dy\,dx \quad \text{(single layer)}$$

$$\frac{1}{2\pi}\int_S \frac{(x-y).n_y}{|x-y|^2}\,p(y)\,dy\,dx \quad \text{(double layer)}$$

where $p$ is either the P0 or P1 shape functions on segment $S$ and the LenoirSalles3dIR classe that computes analytically

$$\frac{1}{4\pi}\int_T \frac{1}{|x-y|}\,p(y)\,dy\,dx \quad \text{(single layer)}$$

$$-\frac{1}{4\pi}\int_{TS} \frac{(x-y).n_y}{|x-y|^3}\,p(y)\,dy\,dx \quad \text{(double layer)}$$

where $p$ is the P0 or P1 shape functions on triangle $T$.
These two classes have no member data and only one basic constructor.

All the previous classes provides, a clone method, an access to the list of quadratures if there are ones and an interface to the computation functions:

```
virtual LenoirSalles2dIM* clone() const;   //covariant
virtual std::list<Quadrature*> quadratures() const; //list of quadratures
template<typename K>
void computeIE(const Element* S, const Element* T, AdjacenceInfo& adj,
               const KernelOperatorOnUnknowns& kuv, Matrix<K>& res,
               IEcomputationParameters& iep,
               Vector<K>& vopu, Vector<K>& vopv, Vector<K>& vopk) const;
```

### CollinoIM class

The CollinoIM class is a wrapper to an integration method developped by F. Collino to deal with some integrals involved in 3D Maxwell BEM when using Raviart-Thomas elements of order 1 (triangle). More precisely, it can compute the integrals:

$$\int_\Gamma\int_\Gamma\left(k\,H(k;x,y)\,w\,j(y).w_i(x)-\frac{1}{k}H(k;x,y)\,\mathrm{div}\,w_j(y)\,\mathrm{div}\,w_i(x)\right)$$

and

$$\int_\Gamma\int_\Gamma\left(\nabla_y H(k;x,y)\times w_j(y)\right).w_i(x),$$

where $(w_i)_{i=1,n}$ denote the Raviart-Thomas shape functions and $H(k;x,y)$ the Green function of the Helmholtz equation (wave number k) in the 3D free space. The class looks like

```
enum ComputeIntgFlag {_computeI1=1, _computeI2,_computeBoth};

class CollinoIM : public DoubleIM
{
 private:
 myquad_t* quads_;
 public:
 number_t ordSNear;  //default 12
 number_t ordTNear;  //default 64
 number_t ordTFar;   //default 3
 real_t eta;         //default 3.
 ComputeIntgFlag computeFlag;
```

```
CollinoIM();
CollinoIM(ComputeIntgFlag cf, number_t otf, number_t otn, number_t osn, real_t e);
CollinoIM(const CollinoIM&);
~CollinoIM();
virtual CollinoIM* clone() const;
CollinoIM& operator=(const CollinoIM&);

virtual std::list<Quadrature*> quadratures() const;
virtual void print(std::ostream& os) const;
template<typename K>
void computeIE(const Element*, const Element*, AdjacenceInfo&,
               const KernelOperatorOnUnknowns&, Matrix<K>&,
               IEcomputationParameters&,Vector<K>&,Vector<K>&,Vector<K>&) const;
```

quads_ is a pointer to a quadrature structure provided by the Collino package, ordSNear, ordTNear, ordTFar are order of quadrature rules used, eta is a relative distance used to separate far and near triangle interactions and computeFlag allows to choose the the integrals that have to be computed. computeIE is the main computation function calling the real computation function (ElemTools_weakstrong_c) provided by the Collino package (see files *Collino.hpp* and *Collino.cpp*).

### 5.6.7 The IntegrationMethods class

The IntegrationMethods class collects some IntgMeth objects that handle an integration method pointer with some additional parameters:

```
class IntgMeth
{ public:
  const IntegrationMethod* intgMeth;
  FunctionPart functionPart; //_allFunction, _regularPart, _singularPart
  real_t bound;              //bound value
}
```

The bound value may be used to select an integration method regarding a criteria. For instance, in BEM computation the criteria is the relative distance between the centroids of elements. Besides, using functionPart member, different integration method may be called on different part of the kernel, see Kernel class. This class has only some constructors and print stuff:

```
IntgMeth(const IntegrationMethod& im, FunctionPart fp=_allFunction, real_t b=0);
IntgMeth(const IntgMeth&);
~IntgMeth();
IntgMeth& operator=(const IntgMeth&);
void print(std::ostream&) const;
void print(PrintStream&) const;
friend ostream& operator<<(ostream&, const IntgMeth&)
```

For safe multithreading behaviour, copy constructor and assign operator do a full copy of IntegrationMethod object.

The IntegrationMethods class is simply a vector of IntMeth object:

```
class IntegrationMethods
{public:
 vector<IntgMeth> intgMethods;
 typedef vector<IntgMeth>::const_iterator const_iterator;
 typedef vector<IntgMeth>::iterator iterator;
 ...}
```

This class provides many constructors depending to the number of integration methods given (up to 3 at this time), to some shortcuts :

```
IntegrationMethods() {};
IntegrationMethods(const IntegrationMethod&,FunctionPart=_allFunction, real_t=0);
...
void add(const IntegrationMethod&, FunctionPart=_allFunction, real_t=0);
void push_back(const IntgMeth&);
```

To handle more than 3 integration methods, use the `add` member function.

Besides, the class offers some accessors and print stuff:

```
const IntgMeth& operator[](number_t) cons ;
vector<IntgMeth>::const_iterator begin() const;
vector<IntgMeth>::const_iterator end() const;
vector<IntgMeth>::iterator begin();
vector<IntgMeth>::iterator end();
bool empty() const {return intgMethods.empty();}
void print(ostream&) const;
void print(PrintStream&) const;
friend ostream& operator<<(ostream&, const IntegrationMethods&);
```

In BEM computation, the following relative distance between two elements $(E_i, E_j)$ is used:

$$dr(E_i,E_j) = \frac{||C_i - C_j||}{\max(diam(E_i), diam(E_j))} \text{ where } C_i \text{ is the centroid of } E_i.$$

So defining for instance

```
IntegrationMethods ims(SauterSchwabIM(4), 0., symmetrical_Gauss, 5, 1.,
                       symmetrical_Gauss, 3);
```

the BEM computation algorithm will perform on function (all part):

| | |
|---|---|
| Sauter-Schwab with quadrature of order 4 on segment | if $dr(E_i,E_j) = 0$ |
| Symmetrical gauss quadrature of order 5 on triangle | if $0 < dr(E_i,E_j) <= 1$ |
| Symmetrical gauss quadrature of order 3 on triangle | if $dr(E_i,E_j) > 1$ |

### 5.6.8 Standard integration method

For various integration purpose, XLiFE++ provides the uniform rectangle, trapeze and Simpson method ($h = \frac{b-a}{n}$):

$$\begin{aligned}
\text{rectangle} \quad &: \int_a^b f(t)\,dt \sim h \sum_{i=0,n-1} f(a+ih) \\
\text{trapeze} \quad &: \int_a^b f(t)\,dt \sim \frac{h}{2}\left(f(a) + 4\sum_{i=1,n/2} f(a+(2i-1)h) + 2\sum_{i=1,n/2-1} f(a+2ih) + f(b)\right) \quad (n \text{ even}) \\
\text{Simpson} \quad &: \int_a^b f(t)\,dt \sim \frac{h}{3}\left(f(a) + 2\sum_{i=1,n-1} f(a+ih) + f(b)\right)
\end{aligned}$$

with $f$ a real or complex function. The rectangle method integrates exactly P0 polynomials, the trapeze method integrates exactly P1 polynomials whereas the Simpson method integrates exactly P3 polynomials. They respectively approximate the integral with order 1, 2 and 3.

For each of them, four template functions (with names `rectangle`, `trapz`, `simpson`) are provided according to the user gives the values of $f$ on a uniform set of points, the function $f$ or a function $f$ with some parameters (e.g trapeze method):

```
template<typename T, typename Iterator>
 T trapz(number_t n, real_t h, Iterator itb, T& intg);
template<typename T>
 T trapz(const std::vector<T>& f, real_t h);
 T trapz(T(*f)(real_t), real_t a, real_t b, number_t n);
 T trapz(T(*f)(real_t, Parameters&), Parameters& pars, real_t a, real_t b, number_t n);
```

XLiFE++ provides also an adaptive trapeze method using the improved trapeze method $(0.25(b-a)(f(a)+2f((a+b)/2)+f(b)))$ to get an estimator. The user has to give its function (with parameters if required), the integral bounds an a tolerance factor ($10^{-6}$ if not given):

```
template<typename T>
 T adaptiveTrapz(T(*f)(real_t), real_t a, real_t b, real_t eps=1E-6);
 T adaptiveTrapz(T(*f)(real_t,Parameters&), Parameters& pars, real_t a, real_t b, real_t eps=1E-6)
```

Because at the first step, the adaptive method uses 5 points uniformly distributed, the result may be surprising if unfortunately the function takes the same value at these points!

### 5.6.9 Discrete Fast Fourier Transform (FFT)

XLiFE++ provides the standard 1D discrete fast Fourier transform with $2^n$ values:

$$g_k = \sum_{j=0,n-1} f_j e^{-2i\pi\frac{jk}{n}}.$$

FFT and inverse FFT are computed using some functions addressing iterators on a collection of real or complex values:

```
template<class Iterator>
void  fft(Iterator ita, Iterator itb, number_t log2n);
void ifft(Iterator ita, Iterator itb, number_t log2n);
```

Computations from real or complex vectors is also available, but the results are always some complex vectors:

```
template<typename T>
vector<complex_t>&  fft(vector<T>& f, vector<complex_t>& g);
vector<complex_t>& ifft(vector<T>& f, vector<complex_t>& g);
```

The following example shows how to use them:

```
Number ln=6, n=64;
Vector<Complex> f(n),g(n),f2(n);
for(number_t i=0; i<n; i++) f[i]=std::sin(2*i*pi_/(n-1));
fft(f.begin(),g.begin(),ln);
ifft(g.begin(),f2.begin(),ln); //f2 should be very close to f
// or
fft(f,g); ifft(g,f2);
```

### 5.6.10 Integration methods for oscillatory integrals

Up to now, only one method is provided to compute 1D oscillatory integrals based on the Filon's method.

### FilonIM class

The Filon's method XLIFE++ proposes is designed to compute an approximation of the following oscillatory integral:

$$I(x)=\int_0^T f(t)\,e^{-ixt}$$

where $f$ is a slowly varying function with real or complex values (template type).

Considering a uniform grid $t_n = n\,dt,\ \forall n = 0, N$ and an interpolation space on this grid, say vect $(w_n)_{n=0,N}$ where $w_n$ are polynomial on each segment $[t_{n-1}, t_n]$; the Filon's method consists in interpolating the function $f$:

$$f(t)=\sum_{n=1,N} a_n w_n(t).$$

Substituting $f$ by its interpolation in integral and collecting terms in a particular way, the integral $I(x)$ is thus approximated as follows:

$$I_N(x)=dt\sum_{j=1,p} C_j(x)\sum_{n=1,N} f(t_n^j)exp^{-ixt_{n-1}}+dt^2\sum_{j=1,p} C'_j(x)\sum_{n=1,N} f'(t_n^j)exp^{-ixt_{n-1}}$$

where $Cj(x)$ and $C'_j$ are coefficients of the form $\int_0^1 \tau_j(s)exp^{-ixsdt}ds$ with $\tau_j$ some shape functions on the the segment $[0,1]$ ant $t_n^j$ the support of the $j^{th}$ dof on the segment $[t_{n-1}, t_n]$. The second sum in $I_N$ appears only when using Hermite interpolation; for Lagrange interpolation, $C'_j(x) = 0$.

If the values $f(t_n^j)_{n=0,N}$ and $f'(t_n^j)_{n=0,N}$ (if Hermite interpolation) are pre-computed, the computation of $I_N(x)$ for many values of $x$ may be very efficient!

The FilonIMT is a template class, FilonIM being its complex specialization:

```
template <typename T = complex_t>
class FilonIMT : public SingleIM
{typedef T(*funT)(real_t);  // T function pointer alias
protected:
number_t ord_;          //interpolation order of (0,1 or 2)
real_t tf_;             //upper bound of integral (lower bound is 0)
real_t dt_;             //grid step if uniform
number_t ns_;           //number of segments
Vector<T> fn_;          //values of f (and df if required) on the grid
Vector<real_t> tn_;     //grid points
...
}
```

ord_ corresponds to the interpolation used : 0 for Lagrange P0, 1 for Lagrange P1 and 2 for Hermite P3. The values $f(t_n^j)_{n=0,N}$ and $f'(t_n^j)_{n=0,N}$ are collected (only one copy) in the same vector with the following storage:

- Lagrange P0 : $f(dt/2)f(3dt/2),\dots f((N-1/2)dt)$ ($N$ values)
- Lagrange P1 : $f(0)f(dt),\dots f(Ndt)$ ($N+1$ values)
- Hermite P3 : $f(0)f'(0)f(dt)f'(dt),\dots f(Ndt)f'(Ndt)$ ($2(N+1)$ values)

The FilonIMT class provides several constructors that pre-compute the values of $f$ and $f'$ from user's functions of the real variable with real or complex values. More precisely, the following types are available:

```
Real f(Real t) {...}
Complex f(Real t) {...}
Real f(Real t, Parameters& pars) {...}
Complex f(Real t, Parameters& pars) {...}
```

It is also possible to construct a `FilonIMT` object passing the values of $f$ at uniformly distributed points on$[0, t_f]$. In that case, Filon of order 1 is selected. So the class looks like

```
typedef T(*funT)(real_t);
typedef T(*funTP)(real_t, Parameters& pa);
FilonIMT();
FilonIMT(number_t o,number_t N,real_t tf,funT f);
FilonIMT(number_t o,number_t N,real_t tf,funT f,funT df);
FilonIMT(number_t o,number_t N,real_t tf,funTP f,Parameters& pars);
FilonIMT(number_t o,number_t N,real_t tf,funTP f,funTP df, Parameters& pars);
FilonIMT(const Vector<T>& vf, real_t tf);
void init(number_t N,funT f,funT df);
void init(number_t N,funTP f,funTP df,Parameters& pars);
number_t size() const {return tn_.size();}      //grid size
template <typename S>
complex_t coef(const S& x, number_t j) const;   //Filon's coefficients
complex_t compute(const S& x) const;            //compute I(x)
complex_t operator()(const S& x) const          //compute I(x)
virtual void print(std::ostream& os) const;     //print FilonIMT on stream
};
```

This class is quite easy to use, for instance to compute the integral

$$I(x) = \int_0^{10} e^{-t}\, e^{-ixt}$$

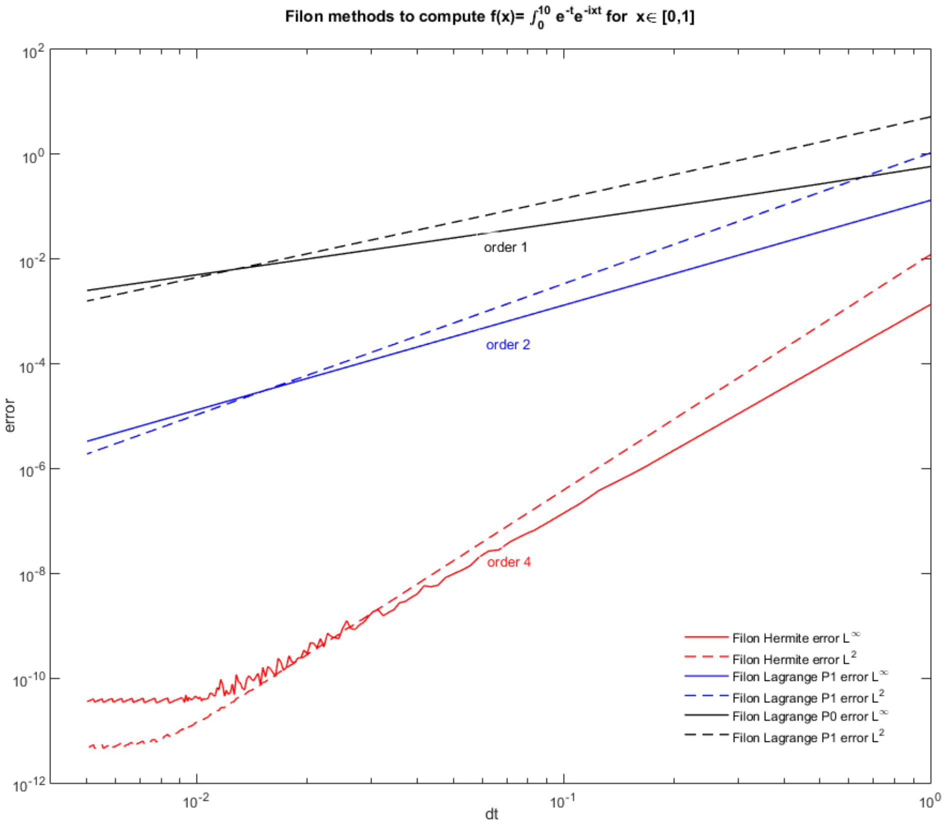
by the P1-Filon method:

```
Complex f(Real x) {return Complex(std::exp(-x),0.);}
...
FilonIM fim(1, 100, 10, f);
Complex y = fim(0.5);
// or in a more compact syntax if only one evaluation
Complex y = FilonIM(1, 100, 10, f) (0.5);
```

To invoke Hermite P3 Filon method, define also the derivative of $f$:

```
Complex f(Real x)  {return Complex(exp(-x),0.);}
Complex df(Real x) {return Complex(-exp(-x),0.);}
...
FilonIM fim(2, 100, 10, f, df);
Complex y = fim(0.5);
```

The P0 Filon method is of order 1, the P1 Filon is of order 2 while the Hermite P3 Filon is of order 4. The Hermite P3 Filon is less stable than the Lagrange Filon methods!



| | |
|---:|---|
| library : | **finiteElements** |
| header : | **Quadrature.hpp QuadratureRule.hpp IntegrationMethod.hpp** |
| implementation : | **Quadrature.cpp QuadratureRule.cpp IntegrationMethod.cpp** |
| unitary tests : | **test_Quadtrature.cpp** |
| header dependences : | **config.h, utils.h, LagrangeQuadrangle.hpp, LagrangeHexahedron.hpp, mathsResources.h** |

# 6 The *space* library

The *space* library collects all the classes and functionalities related to functions spaces. In the framework of the code, a space is a finite dimension vector space of functions defined on a geometrical domain (see GeomDomain), in other words, the space spanned by a finite number of independent functions (global basis functions). This collection of functions may be given either explicitly (say spectral basis) or using local definition of functions on geometric elements (say finite element basis). Besides, a space may be also a subspace of a space (in the meaning of a function subspace or the trace of a space on a geometric subdomain) or a tensor product of spaces. The space we used is no more than the finite dimension space involved in discrete variational formulations except the essential boundary conditions. Then the Space class is an essential concept of the code, in particular for users who have to deal with. A finite element space is essentially a list of Elements which supports finite element. A spectral space is essentially a list of GlobalFunction defined by the user either in an analytical form or an interpolate form. Finally, there are two related classes: the Unknown class to deal with an abstract element of a space and Dof which represents an generalized index of an unknown.

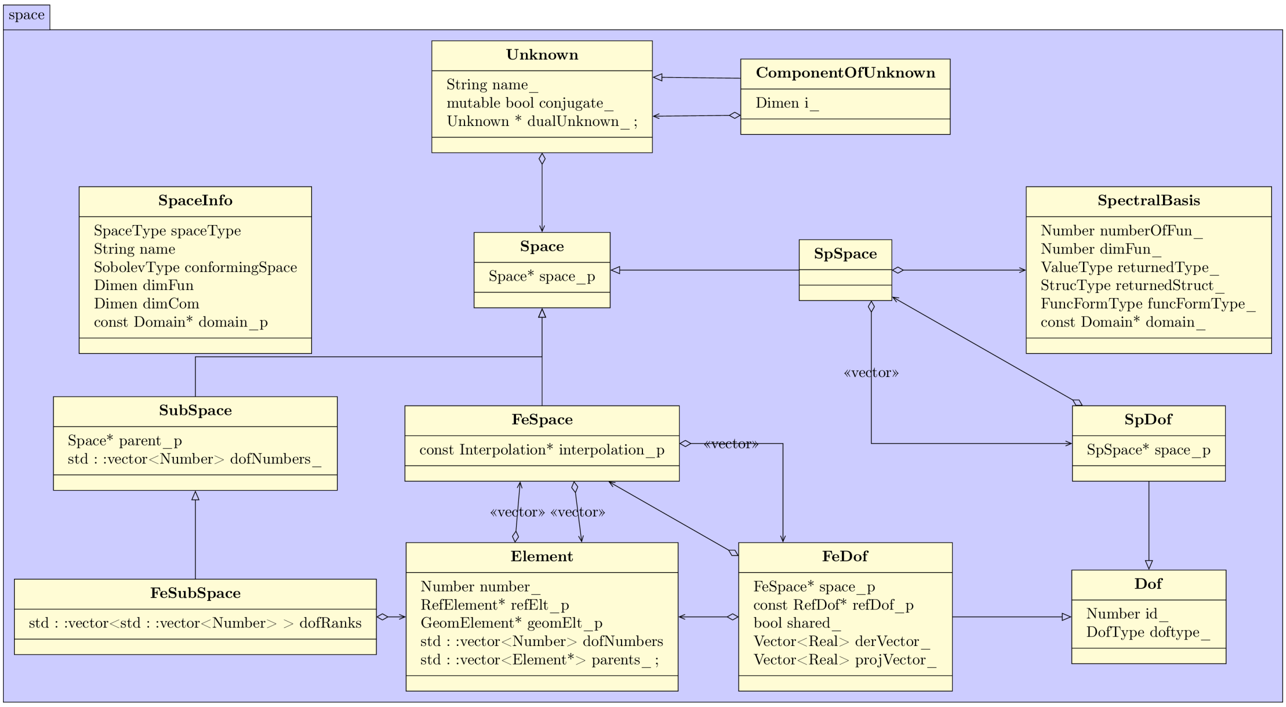


Figure 6.1: *space* library organisation

## 6.1 Space management

### 6.1.1 The Space and SpaceInfo classes

The Space class manages different kind of spaces using inherited classes: finite element space (FeSpace), spectral space (SpSpace), sub space ((SubSpace) and product space (ProdSpace). To avoid the user to deal explicitly with this space hierarchy, we use the following programming paradigm: Space class has a pointer to a Space as attribute, which contains either its own address or the address of a child. In a sense, the Space class is not an abstract class but has a the behaviour of an abstract one. When an end user declares a Space object, he induces the construction of a child Space. With this trick, an end user instantiates only `Space` object, never the child spaces. As a consequence, it requires a little more memory because member attributes are duplicated. In order to limit this effect, the common characteristics of a space are collected in the SpaceInfo class:

```
class SpaceInfo
 {public :
  String name_;                 // name of space
  Domain * domain_p;            // geometric domain supporting the space
  SobolevType spaceConforming_; // conforming space (L2,H1,Hdiv,Hcurl,H2,Hinf)
  dimen_t dimFun_;              // number of components of the basis functions
  Dimen dimCom;                 // number of components of the unknowns
  SpaceType spaceType_;         // space type (FESpace,SPSpace,SubSpace,ProductSpace)
  SpaceInfo() {};
  SpaceInfo(const String &,SobolevType,Domain *,dimen_t , SpaceType)
 };
```

The general characteristics of a space are the geometric domain supporting the basis functions, the space conformity which "tells" the regularity of the basis functions and the dimension of the basis functions. The space conformity property is a way to distinguish discontinuous finite element approximation from continuous one. The space conformity is given by the SobolevType enumeration declared in the *config.hpp* header file:

```
enum SobolevType {L2=0, L2=_L2,H1, H1=_H1,_Hdiv, Hdiv=_Hdiv,_Hcurl, Hcurl=_Hcurl,
                  _Hrot=_Hcurl, Hrot=_Hrot,_H2, H2=_H2,_Hinf, Hinf=_Hinf}
```

To be user friendly, several names are available for the same space.

The parent class `Space` has only two pointers and a static vector managing the list of all defined spaces:

```
class Space
{protected :
  Space * space_p;                      //pointer to the "true" space (child)
  SpaceInfo * spaceInfo_p;              //pointer to the space information structure
public :
  static std::vector<Space*> theSpaces; //unique list of defined spaces
```

Regarding the type of spaces, the `Space` provides several constructors to construct child spaces:

```
//constructors of trivial space of dim n, say Rn
Space(number_t, const string_t& ="Rn");
Space(number_t, const GeomDomain&, const string_t& ="Rn");

// internal constructors addressing spectral space
Space(const SpectralBasis&, const string_t&);  //from spectral basis

// internal constructors addressing FeSpace type from Interpolation or FE types
Space(const GeomDomain&, const Interpolation&, const string_t&, bool opt = true);

// constructors addressing SubSpace type
Space(const GeomDomain&, Space&, const string_t& na = "");
Space(const GeomDomain&, const vector<number_t>&, Space&, const string_t& na = "");
Space(const std::vector<number_t>&, Space&, const string_t& na = "");

// tools related to construtors
void buildSpFun(const GeomDomain&, const Function&, number_t,
                dimen_t, const string_t&);
SubSpace* createSubSpace(const GeomDomain&, Space&, const string_t& na);
void createSubSpaces(const vector<const GeomDomain*>&,vector<Space*>&);
Space* buildSubspaces(const vector<const GeomDomain*>&, vector<Space*>&);
```

These constructors work as follows (*(child)Space* denotes any inherited space class):

```
(child)Space* csp_p=new (child)Space(...); //create the (child)Space
space_p=static_cast<Space *>(csp_p);       //cast (child)Space* to Space*
spaceInfo_p=csp_p->spaceInfo_p;            //copy the SpaceInfo pointer
theSpaces.push_back(this);                 //store space in list of spaces
```

Note that it is the child constructors that set all the attributes (general ones and specific ones).

### 6.1.2 The key-value system

Most of the Space constructors use a key-value system, so there are Space constructors taking from 1 to 13 inputs of type Parameter:

| key(s) | authorized types / possible values | involved kind of space |
|---|---|---|
| **_domain** | Domain | Finite element space |
| **_FE_type** | Lagrange, Hermite, CrouzeixRaviart, Nedelec, NedelecFace, NedelecEdge or Morley | Finite element space |
| **_FE_subtype** | standard, GaussLobattoPoints, firstFamily or secondFamily | Finite element space |
| **_Sobolev_type** | L2, H1, Hdiv, Hcurl, Hrot, H2, Hinf or Linf | Finite element space |
| **_order** | single unsigned integer | Finite element space |
| **_interpolation** | P0 to P10, P1BubbleP3, Q0 to Q10, RT_1 to RT_5, NF1_1 to NF1_5, BDM_1 to BDM_5, NF2_1 to NF2_5, N1_1 to N1_5, N2_1 to N2_5 | Finite element space |
| **_name** | String | every kind of space |
| **_optimizeNumbering**, **_notOptimizeNumbering** | no value | Finite element space |
| **_withLocateData**, **_withoutLocateData** | no value | Finite element space |
| **_basis** | Function, TermVector | spectral space |
| **_dim** | single unsigned integer | spectral space |
| **_basis_dim** | single unsigned integer | spectral space |

These constructors transfer the building work to the following routines:

```
void buildSpace(const std::vector<Parameter>& ps);
```

This routine works in the same way as the internal constructors described in the previous subsection.

### 6.1.3 Space member functions

The Space class provides some accessors, some being virtual:

```
string_t name() const;                 //space name
SobolevType conformingSpace() const;   //space conformity
const GeomDomain* domain();            //related domain
dimen_t dimDomain() const;             //dimension of related domain
dimen_t dimPoint() const ;             //dimension of points
dimen_t dimFun() const;                //dimension of basis functions
SpaceType typeOfSpace() const;         //type of space
SpaceType typeOfSubSpace() const;      //type of sub-space
virtual bool isSpectral() const;       //true if spectral space
virtual bool isFE() const;             //true if FE space or FeSubspace
const Space* space() const;            //pointer to true space object
```

```
virtual number_t dimSpace() const;     //space dimension
virtual number_t nbDofs()const;        //number of dofs
virtual const FeSpace* feSpace() const;       //pointer to child fespace
virtual FeSpace* feSpace();                   //pointer to child fespace
virtual const FeSubSpace* feSubSpace() const; //pointer to child fesubspace
virtual const SpSpace* spSpace() const;       //pointer to child fesubspace
virtual const SubSpace* subSpace() const;     //pointer to child subspace
virtual SubSpace* subSpace();                 //pointer to child subspace
virtual const Space* rootSpace() const;       //pointer to root space
virtual Space* rootSpace();                   //pointer to root space
virtual ValueType valueType() const;          //value type of basis function
virtual StrucType strucType() const;          //structure type of basis function
virtual bool include(const Space*) const;     //inclusion test
virtual bool extensionRequired() const;       //rue if space has no trace space
```

To understand how works the non abstract/abstract class paradigm, here is the implementation of the access function *feSpace*:

```
FeSpace* Space::feSpace() const
{if(space_p!=this) return space_p->feSpace();     //call the true feSpace
 error("is_not_fespace",name());
 return 0;
}
FeSpace* FeSpace::feSpace() const {return *this;}
```

The test `space_p!=this` means that the current space is a user space (it has a child), the `fespace()` function is called by its child. By polymorphic behaviour, if `space_p` is a `FeSpace` the `FeSpace::fespace()` is called else `Space::fespace()` is again called, but with `space_p=this` and an error is thrown because the current space is not a `FeSpace`.

As you will see in section 6.2, the dof number is relative to the parent space. To get the global number of a dof or the dof itself and to manage dofs, Space provides the following functions :

```
virtual number_t dofId(number_t) const;         //n-th DoF id of space
virtual std::vector<number_t> dofIds() const;   //DoF ids on space
virtual const Dof& dof(number_t) const;         //n-th dof (n=1,...)
virtual std::pair<number_t, number_t> renumberDofs(); //optimize dofs numbering
virtual void shiftDofs(number_t n);      //shift dofs numbering from n (SpSpace)
```

When space is a FE space or a FE subspace, tools to access to finite element informations are provided:

```
virtual const Interpolation* interpolation() const;
virtual number_t nbOfElements() const;
virtual const Element* element_p(number_t k) const:
virtual const Element* element_p(GeomElement* gelt) const;
virtual number_t numElement(GeomElement* gelt) const;
virtual vector<number_t> elementDofs(number_t k) const;
virtual vector<number_t> elementParentDofs(number_t k) const;
virtual const set<RefElement*>& refElements() const;
virtual void buildgelt2elt() const;
virtual const vector<FeDof>& feDofs() const;
virtual const Point& feDofCoords(number_t k) const;
virtual void builddofid2rank() const;                      // built on fly
virtual const map<number_t, number_t>& dofid2rank() const; // built on fly
virtual Dof& locateDof(const Point&) const;
```

Finally, the `Space` provides some printing facilities:

```
void printSpaceInfo(std::ostream &) const;
virtual void print(std::ostream &) const;
```

```
friend std::ostream& operator<<(std::ostream&,const Space &);
```

Some functions managing subspaces (comparison, merging) are also available:

```
bool compareSpaceUsingSize(const Space*, const Space*);
vector<number_t> renumber(const Space*, const Space*);
Space& subSpace(Space&, const GeomDomain&);
inline Space& operator |(Space&, const GeomDomain&);
Space* mergeSubspaces(Space*&, Space*&, bool newSubspaces=false);
Space* mergeSubspaces(std::vector<Space*>&, bool newSubspaces=false);
Space* unionOf(std::vector<Space*>&);
vector<Point> dofCoords(Space&, const GeomDomain&);
```

Linked to the Space class, the DoF class stores characteristics of degree of freedom. Degree of freedom is like a key index of components of element of space. Generally, it handles a numeric index and carries some additionnal informations. From DoF class inherit the classes FeDoF and SpDoF (see section DoF).

| | |
|---:|---|
| library : | **space** |
| header : | **Space.hpp** |
| implementation : | **Space.cpp** |
| unitary tests : | **test_Space.cpp** |
| header dependences : | **config.h, geometry.h, Df.hpp** |

Now, let's have a look at the child space classes.

### 6.1.4 The FeSpace class

A finite elements space is defined from a finite set of functions given by an interpolation method on a mesh. The inherited FeSpace class is defined as follows :

```
class FeSpace : public Space
{protected :
  const Interpolation* interpolation_p;// pointer to finite element interpolation
  bool optimizedNumbering_;   // true if dof numbering is bandwidth optimized
 public:
  vector<Element> elements;   //list of finite elements
  vector<FeDof> dofs;         //list of global degrees of freedom
  set<RefElement *> refElts;  //set of RefElement pointers involved
  mutable map<GeomElement*, number_t> gelt2elt;  //map GeomElement->element number
  mutable map<number_t, number_t> dofid2rank_;   //map dof iD->rank in dofs vector
  static Number lastEltIndex;     //to manage a unique index for elements
};
```

Besides the two fundamental lists of elements and dofs, two useful maps gelt2elt and dofid2rank may be constructed on the fly. The first map is built when some interpolation operations are handled and the second one when some FE subspaces are involved. The set XXX collects the types of FE elements involved in the space, generally only one type. This class provides one constructor, using two member functions:

```
FeSpace(const Domain&, const Interpolation&, Dimen, const String&, bool opt=true, bool
    withLocateData=true);

void buildElements();     //construct the list of elements
void buildFeDofs();       //construct the list of FeDofs
void buildgelt2elt() const;    //construct the map gelt2elt
void builddofid2rank() const;  //construct the map dofid2rank
void buildBCRTSpace();    //construction of BuffaChristiansen-RT space
```

The buildElements() member functions create the list of elements (Element objects) from the list of geometric elements belonging to the domain supporting the space. The buildFeDofs() function is the most important one. It constructs from reference dofs the list of global dofs using a general algorithm based on the DofKey class that indexes dof regarding its localization in the mesh:

```
class DofKey
{public:
 DofLocalization where;
 number_t v1, v2;           //used for vertex, edge, element dofs
 std::vector<number_t> vs;  //used for face dofs
 number_t locIndex;
 friend bool operator<(const DofKey& k1, const DofKey& k2);
};
```

Using this indexing, the algorithm building the dofs set works as follows:

> - case of no shared dof (L2 conforming space), concatenate all local dofs and exit
> - case of shared dofs
>   - construct a DofKey map by traveling elements
>   - construct the list of global dofs from the DofKey map and update elements

To insure the right matching between shared dofs on edge or face, this algorithm uses the sideDofsMap and sideOfSideDofsMap member functions of finite element classes. These functions relate dof numbering to one edge/face to an other edge/face.

The FeSpace class provides also some specific accessors and properties:

```
virtual Number nbDofs() const; //number of dofs (a dof may be a vector dof)
Dimen dimElements() const;      //return the dimension of FE elements
number_t nbOfElements() const; //number of elements
const Interpolation* interpolation() const; //return pointer to interpolation
virtual Space* rootSpace();          //root space pointer
virtual number_t dimSpace()const;    //the space dimension
virtual number_t nbDofs()const;      //number of dofs (may be a vector dof)
virtual number_t dofId(number_t n) const;      //the DoF id of n-th space DoF
virtual vector<number_t> dofIds() const;       //the DoF ids on space
virtual const Dof& dof(number_t n) const;      //n-th FeDof as Dof (n=1,...)
virtual const FeDof& fedof(number_t n) const   //n-th FeDof (n=1,...)
virtual const std::vector<FeDof>& feDofs() const; //dofs vector
dimen_t dimElements() const;                   //the dimension of FE elements
const Interpolation* interpolation() const;    //pointer to interpolation
const set<RefElement*>& refElements() const;   //set of pointer to RefElement
number_t maxDegree() const;                    //max degree of shape functions involved
virtual bool include(const Space*) const;      //true if space is included in current space
virtual ValueType valueType() const;           //value type of basis function
virtual StrucType strucType() const;           //structure type of basis function
virtual bool isSpectral() const;               //true if spectral space
virtual bool isFE() const;                     //true if FE space or FeSubspace
virtual bool extensionRequired() const;        //true if space has no trace space
```

The FeSpace class has functions related to renumbering:

```
Graph graphOfDofs(); //create dof connection graph
const Element* element_p(Number k) const; //k-th (k>=0) element (pointer)
vector<Number> elementDofs(Number k) const; //dofs ranks (local numbering) of k-th (>=0) element
vector<Number> elementParentDofs(Number k) const; //dofs ranks (parent numbering, same as local)
     of k-th (>=0) element
const map<number_t, number_t>& dofid2rank() const; //map dof to rank, built on fly
void shiftDofs(number_t); //shift dofs numbering from n (see SpSpace)
```

and functions related to interpolation operations:

```
vector<number_t> dofsOn(const GeomDomain&) const; //set of dof numbers of dofs
Dof& locateDof(const Point &) const;               //dof nearest a given point
template <typename T, typename K>
T& interpolate(const Vector<K>&, const Point&, T&, DiffOpType =_id) const; //interpolation value
    at P
```

| | |
|---|---|
| library : | **space** |
| header : | **FeSpace.hpp** |
| implementation : | **FeSpace.cpp** |
| unitary tests : | **test_Space.cpp** |
| header dependences : | **config.h, Elements.hpp, Space.hpp, dof.hpp, finiteElement.h** |

### 6.1.5 The SpSpace class

A spectral space is defined by a finite set of functions given by analytic expression or by interpolated form. These global basis functions defined over a geometric domain are collected in the SpectralBasis class declared in the *SpectralBasis.hpp* header file (see the section SpectralBasis). The inherited SpSpace class is defined as follows:

```
class SpSpace : public Space
{
  protected :
    SpectralBasis* spectralBasis_; //! object function encapsulating the spectral functions
    //either defined in an analytical form or by interpolated functions (TermVector)
  public :
    std::vector<SpDof> dofs;       //! list of global degrees of freedom
};
```

This class provides one constructor, a destructor, several accessors and a printing function:

```
SpSpace(const String&, Domain&, number_t, dimen_t, SpectralBasis*);
~SpSpace();
SpectralBasis* spectralBasis() const;
virtual Number nbDofs() const;     //!< number of dofs (a dof may be a vector dof)
```

| | |
|---|---|
| library : | **space** |
| header : | **SpSpace.hpp** |
| implementation : | **SpSpace.cpp** |
| unitary tests : | **test_Space.cpp** |
| header dependences : | **config.h, Elements.hpp, Space.hpp, dof.hpp** |

### 6.1.6 The SubSpace and FeSubSpace classes

A subspace is part of a space. Its dofs are a subset of the parent dofs. The inherited SubSpace class is defined as follows:

```
class SubSpace : public Space
{
  protected :
    Space* parent_p;                  //!< the parent space
    std::vector<Number> dofNumbers_;  //!< global numbers of D.o.Fs in parent D.o.Fs numbering
};
```

This class provides two constructor, a destructor, and several specific accessors about the `dofNumbers_` attribute or about the type of subspace :

```
SubSpace()                                                    //!< default constructor
SubSpace(const Domain&, Space&, const String& na = ""); //!< constructor specifying geom domain,
    parent space and name
~SubSpace();                                                  //! destructor

std::vector<Number>& dofNumbers()                             //!< access to dofNumbers list
const std::vector<Number>& dofNumbers() const                 //!< access to dofNumbers list (const)
std::vector<Number> dofRootNumbers() const;                   //!< access to dofNumbers list in root
    space numbering
Number dofRootNumber(Number k) const;                         //!< access to dof number in root space
    numbering
virtual Number nbDofs() const                                 //! number of dofs (a dof may be a
    vector dof)
virtual bool isFeSubspace();
virtual const FeSubSpace* fesubspace() const;
```

It also provides functions for numbering management:

```
void createNumbering();    //!< create numbering of subspace DoFs
void dofsOfFeSubspace();   //!< build dofs numbering of Fe SubSpace
void dofsOfSpSubspace();   //!< build dofs numbering of Sp SubSpace
void dofsOfSubSubspace();  //!< build dofs numbering of Subspace of SubSpace
```

| | |
|---|---|
| library : | **space** |
| header : | **SubSpace.hpp** |
| implementation : | **SubSpace.cpp** |
| unitary tests : | **test_Space.cpp** |
| header dependences : | **config.h, Elements.hpp, Space.hpp, Dof.hpp** |

The `FeSubSpace` class concerns subspaces of finite element spaces. It is defined as follows:

```
class FeSubSpace : public SubSpace
{
  public :
    std::vector<Element*> elements;                    //!< list of finite elements (or subelements)
    std::vector<std::vector<Number> > dofRanks;        //!< numbering of D.o.Fs of domain elements in
        domain D.o.Fs
};
```

This class provides one constructor, a destructor, and several specific functions, also provided by the `FeSpace` class :

```
FeSubSpace(const Domain&, Space&, const String& na = ""); //!< constructor specifying geom
    domain, parent space and name
~FeSubSpace();                                          //!< destructor
Number nbOfElements() const;                            //!< number of elements
const Element* element_p(Number k) const;               //!< access to k-th (k>=0) element
    (pointer)
std::vector<Number> elementDofs(Number k) const;        //!< access to dofs ranks (local
    numbering) of k-th (>=0) element
std::vector<Number> elementParentDofs(Number k) const; //!< access to dofs ranks (parent
    numbering) of k-th (>=0) element
```

| | |
|---|---|
| library : | **space** |
| header : | **FeSubSpace.hpp** |
| implementation : | **FeSubSpace.cpp** |
| unitary tests : | **test_Space.cpp** |
| header dependences : | **config.h, Elements.hpp, SubSpace.hpp, dof.hpp** |

### 6.1.7 The `ProdSpace` class

The `ProdSpace` class manages product of spaces using a vector of space pointers :

```
class ProdSpace : public Space
{
  protected :
    std::vector<Space*> spaces_;
  public :
    virtual Number dimSpace() const;
    virtual Number nbdofs() const;
    virtual const Space* rootSpace() const
    {return static_cast<const Space*>(this);}
    virtual Space* rootSpace()
    {return static_cast<Space*>(this);}
    virtual Number dofId(Number n) const
    {error("no_dof_numbering", name());
     return 0;}
};
```

It is currently not used.

### 6.1.8 The `Spaces` class

`Spaces` is an alias of `PCollection<Space>` class that manages a collection of `Space` objects, in fact a `std::vector<Space*>`. Be cautious when using it because the Space pointers are shared; in particular when using temporary instance of Space! It is the reason why the `PCollectionItem` class is overloaded to protect pointer in assign syntax `sp(i)=Space(...)`:

```
template<> class PCollectionItem<Space>
{public:
 typename std::vector<Space*>::iterator itp;
 PCollectionItem(typename std::vector<Space*>::iterator it) : itp(it){}
 Space& operator = (const Space& sp); //protected assignment
 operator Space&(){return **itp;}      //autocast PCollectionItem->Space&
};
```

Main usages of this class are the following:

```
Space V1(omega,_P1,"V1"), V2(omega,_P2,"V2"), V3(omega,_P3,"V3");
Spaces Vs2(V1,V2);
Spaces Vs3(V1,V2,V3);
Spaces Vs4; Vs4<<V1<<V2<<V3<<V1;
Spaces Vs5(5);
for(Number i=1;i<=5;i++)
   Vs5(i)=Space(omega,interpolation(Lagrange,_standard,i,H1),"V_"+tostring(i));
```

If C++11 is available (the library has to be compiled in C++11), the following syntax is also working:

```
Spaces vs={V1,V2,V3};
```

Collection of spaces can also be set by the following functions from one or several domains and one or several interpolations:

```
Spaces spaces(const Domains&,const Interpolations&,bool=true);
Spaces spaces(const Domains&,const Interpolation&,bool=true);
Spaces spaces(const GeomDomain&,const Interpolations&,bool=true);
```

| | |
|---:|:---|
| library : | **space** |
| header : | **ProdSpace.hpp** |
| implementation : | **ProdSpace.cpp** |
| unitary tests : | **test_space.cpp** |
| header dependences : | **config.h, Space.hpp** |

## 6.2 DoF management

### 6.2.1 The Dof class

Linked to the Space class, the DoF class stores characteristics of degree of freedom. Degree of freedom is like a key index of components of element of space. Generally, it handles a numeric index and carries some additional informations. For instance, in case of Lagrange interpolation it carries the geometrical point associated to the basis function. From DoF class inherit the classes FeDoF and SpDoF.

```
class Dof
{protected :
    number_t id_;               //id of dof
    DofType doftype_;           //type of dof
 public :
    Dof(DofType t=_otherDof, number_t i=0);
    virtual~Dof() {};
    DofType dofType()const;
    number_t id() const;
    number_t& id();
    virtual void print(std::ostream&) const;
    friend std::ostream& operator<<(std::ostream&, const Dof &);
};
```

The type of DoF are enumerated by

```
enum DofType {_feDof,_spDof,_otherDof};
```

### 6.2.2 FeDof and SpDof classes

Inherited classes are very simple:

```
class FeDof: public Dof
{protected :
    FeSpace* space_p;          // pointer to FeSpace
    const RefDof*  refDof_p;    // pointer to a Reference D.o.F
    bool shared_;               // implies D.o.F is shared between elements
    Vector<Real> derVector_;  // direction vector(s) of a derivative D.o.F (specific
        interpolation)
    Vector<Real> projVector_; // direction vector(s) of a projection D.o.F (specific
        interpolation)
    std::vector<std::pair<Element*, Number> > inElements; // list of elements related to Dof and
        local number of dof in elements
 public :
    FeDof();
    FeDof(FeSpace& sp, number_t i=0)
    virtual void print(std::ostream&) const;
};
```

```
class SpDof : public Dof
{protected :
    SpSpace * space_p;          //pointer to SpSpace
public :
    SpDof()
    SpDof(SpSpace& sp, number_t i)
    virtual void print(std::ostream&) const;
};
```

| | |
|---|---|
| library : | **space** |
| header : | **DoF.hpp** |
| implementation : | **DoF.cpp** |
| unitary tests : | **test_Space.cpp** |
| header dependences : | **config.h, utils.h** |

### 6.2.3 The `DofComponent` class

This class defined an extended representation of dof, useful to adress components of a vector dof:

```
class DofComponent
{
public :
    const Unknown* u_p;     //unknown
    Number dofnum;          //dof number
    Dimen numc;             //component

    DofComponent(const Unknown* u=0, Number dn=0, Dimen nc=1);
    DofComponent dual() const;
    void print(std::ostream& os) const;
    friend std::ostream& operator<<(std::ostream&, const DofComponent&);
};
```

The `dual()` function returns the 'dual' dof component. Besides, this class provides some comparison operators (partial ordering) :

```
bool operator < (const DofComponent&, const DofComponent&);
bool operator ==(const DofComponent&, const DofComponent&);
bool operator !=(const DofComponent&, const DofComponent&);
```

and somefunctions manipulating list of component dofs :

```
vector<DofComponent> createCdofs(const Unknown* u, const vector<Number>& dofs);
vector<Number> renumber(const vector<DofComponent>&, const vector<DofComponent>&);
```

| | |
|---|---|
| library : | **space** |
| header : | **DoF.hpp** |
| implementation : | **DoF.cpp** |
| unitary tests : | **test_Space.cpp** |
| header dependences : | **config.h, utils.h** |

## 6.3 Unknown management

### 6.3.1 The `Unknown` class

The `Unknown` class manages element of a space (`Space`). It is mainly used as an abstract object in the description of a variational problem. It has the `ComponentOfUnknown` class as child which represents a component of a vector unknown. Do not confuse vector unknown on a scalar space and scalar unknown on a vector space. Vector unknown on a scalar space is a way to define an unknown on a product of scalar spaces (same space!), for instance the displacement field. Whereas on a vector space (say a space spanned by vector functions), unknown are generaly a scalar one; for instance Hrot or Hdiv comform spaces. Up to now, it is not possible to deal with general product spaces.

```
class Unknown
{protected:
   String name_;              // name of the unknown
   Space * space_p;           // pointer to the space where the unknown lives
   mutable bool conjugate_;   // temporary flag for conjugate operation
   Unknown * dualUnknown_;    // pointer to dual Unknown (test function)
   Number rank_;              // rank to order unknowns
  public:
   bool isUnknown;            // true if an unknown, false if a test function
   static std::vector<Unknown*> theUnknowns;  //list of all Unknowns
```

The temporary `conjugate_` flag is used to mark in a `OperatorOnUnknown` construction that an unknown is conjugate. The static attribute `theUnknowns` traces all defined unknowns. Besides, each unknown has a rank, by default its creation number (first unknown created has rank 1 and so on). This rank is used to order blocks in vector or matrix in case of multiple unknowns terms.
There is no class to deal with test function. There exists only an alias `TestFunction` of `Unknown`:

```
typedef Unknown TestFunction;
```

So, to distinguish, unknown from test function, the flag `isUnknown` is used. It is set to true when using the constructor from a Space and set to false when using the constructor from unknown, implicitely the test function constructor:

```
Unknown();
Unknown(const string_t&, Space&,
        dimen_t d=1, number_t r=0);// unknown constructor from space
Unknown(Unknown&,const string_t& na="",
        number_t r=0);             // test function constructor from unknown
~Unknown();
```

and the following accessors:

```
String name() const;               // return name
Space * space() const;             // return pointer to space
UnknownType type() const;          // return type of unknown
StrucType strucType() const;       // return the structure type of an unknown
number_t index() const;            // return index of unknown
bool conjugate() const;            // return the conjugate state flag
```

```
bool& conjugate();                    // return the conjugate state flag
void conjugate(bool v) const ;        // set the conjugate state flag
friend Unknown& conj(Unknown &);      // conjugate an unknown
Number rank() const;                  // return the unknown rank
```

The member function index() returns the rank of the unknown in the theUnknowns list. It may be useful to order the unknowns. The member function type() returns the type of unknown as an element of the UnknownType enumeration (defined in *config.hpp* header file):

```
enum UnknownType {_feUnknown,_spUnknown,_mixedUnknown};
```

There are particular virtual member functions linked to the ComponentOfUnknown child class:

```
virtual dimen_t nbOfComponents() const;   // dimension of unknown
virtual bool isComponent() const;         // true if a ComponentOfUnknown
virtual const Unknown* parent() const;    // return parent (or itself)
virtual Dimen componentIndex() const;     // return component index if a ComponentOfUnknown, 0 if
     not
virtual const ComponentOfUnknown* asComponent() const; // return Unknown as a ComponentOfUnknown
     if it is
Unknown& operator[](dimen_t);             // create the ComponentOfUnknown u_i
```

Unknown class provides printing facility also:

```
friend std::ostream& operator<<(std::ostream&, const Unknown&);

void setRanks(std::vector<Unknown*>&, const std::vector<Number>&);
void setRanks(Unknown&, Number r);
void setRanks(Unknown&, Number, Unknown&, Number);
void setRanks(Unknown&, Number, Unknown&, Number, ...);
```

The setRanks functions are useful to define the internal order of unknowns in multiple unknowns objects such as TermMatrix or TermVector. The unknown ranks have to be unique but it is not mandatory that they follow. By default, first created unknown has rank 1, the second created has rank 2, and so on.

### 6.3.2 The ComponentOfUnknown class

To access to a component of a vector unknown as an unknown, the ComponentOfUnknown child class is provided:

```
class ComponentOfUnknown: public Unknown
{protected :
   const Unknown * u_p;      //Unknown which this unknown is a component
   Dimen i_;                 //index of the component
 public :
   ComponentOfUnknown(const Unknown &,dimen_t);
   virtual Dimen nbOfComponents() const;
   virtual Dimen dimFun() const;
   virtual bool isComponent() const;
   virtual const Unknown* parent() const;
   virtual Dimen componentIndex() const;
   virtual const ComponentOfUnknown* asComponent() const;
};
```

Note that the operator Unknown::[](Dimen) creates a ComponentOnUnknown object returned as an Unknown object.

### 6.3.3 The Unknowns class

Unknowns is an alias of PCollection<Unknown> class that manages a collection of Unknown objects, in fact a std::vector<Unknown*>. Be cautious when using it because the Unknown pointers are shared; in particular when using temporary instance of Unknown! It is the reason why the PCollectionItem class is overloaded to protect pointer in assign syntax sp(i)=Unknown(...):

```
template<> class PCollectionItem<Unknown>
{public:
typename std::vector<Unknown*>::iterator itp;
PCollectionItem(typename std::vector<Unknown*>::iterator it) : itp(it){}
Unknown& operator = (const Unknown& sp); //protected assignment
operator Unknown&(){return **itp;}      //autocast PCollectionItem->Unknown&
};
```

Main usages of this class are the following:

```
Unknown u1(V1,"u1"), u2(V2,"u2"), u3(V3,"u3");
Unknowns us1(u1,u2,u3);
Unknowns us2; us2<<u1<<u2<<u3;
Unknowns us5(5);
for(Number i=1;i<=5;i++) us5(i)=Unknown(Vs5(i),"u_"+tostring(i));
```

If C++11 is available (the library has to be compiled in C++11), the following syntax is also working:

```
Unknowns us={u1,u2,u3};
```

In a same way, TestFunctions is an alias of PCollection<TestFunction*> class that manages a collection of TestFunction objects. It works as the Unknowns class. The following function allows to create a collection of testfunctions related to a collection of unknowns:

```
TestFunctions dualOf(const Unknowns& us);
```

| | |
|---|---|
| library : | **space** |
| header : | **Unknown.hpp** |
| implementation : | **Unknown.cpp** |
| unitary tests : | **test_Space.cpp** |
| header dependences : | **config.h, utils.h** |

## 6.4 The Element class

A finite element is mainly defined by its geometric support and its finite element interpolation. It carries also its dof numbering. The dedicated Element class is defined as follows:

```
class Element
{
  protected:
    FeSpace* feSpace_p;             //pointer to Finite Element parent space
    Number number_;                 //element number in FeSpace
  public:
    FeSubSpace* feSubSpace_p;       //pointer to Finite Element parent sub space
    RefElement* refElt_p;           //pointer to reference element object
    GeomElement* geomElt_p;         //pointer to Geometric Element support
    std::vector<Number> dofNumbers; //global numbering of element dofs
    std::vector<Element*> parents_; // parent elements when a side of element
};
```

The `Element` class provides:

- One constructor

```
Element(FeSpace*, Number, RefElement*, GeomElement*, FeSubspace*=0);
```

- Some accessors

```
Dimen dim() const;               //dimension of the element
Number number() const;           //return number_ attribute
ShapeType shapeType() const;     //shape of the element
FEType feType() const;           //FE type ( _Lagrange, _Hermite, ...)
Number feOrder() const;          //FE numtype (order for Lagrange)
Dimen dimFun() const;            //dimension of shape functions
```

- a dofs renumbering function and a tool to get index of dof

```
void dofsRenumbered(const std::vector<Number>&, std::vector<FeDof>&);
number_t refDofNumber(number_t) const;
```

- some utilities to compute normal vectors at a physical point and to access to:

```
ShapeValues computeShapeValues(const Point&, bool withderivative = false) const;
Vector<real_t> computeNormalVector(const Point&) const;
Vector<real_t> computeNormalVector() const;
const Vector<real_t>& normalVector() const;
Vector<real_t>& normalVector();
```

- some interpolation tools:

```
Point toReferenceSpace(const Point& p) const; // physical to reference space
template<typename T>
  T& interpolate(const Vector<T>&, const Point&, const std::vector<number_t>&,
                 T&, DiffOpType =_id) const;
template<typename T>
   Vector<T>& interpolate(const Vector<T>&, const Point&,
                          const std::vector<number_t>&, Vector<T>&,
                          DiffOpType =_id) const;
template<typename T>
  T& interpolate(const Vector<Vector<T> >&, const Point&,
                 const std::vector<number_t>&, T&,
                 DiffOpType = _id)const;
template<typename T>
  T& interpolate(const VectorEntry&, const Point&,
                 const std::vector<number_t>&, T&,
                 DiffOpType =_id)const;
```

> Interpolation tools are useful when evaluating an element of FE space at a given point, say $P$. It is an expansive process requiring to locate the element containing the point $P$, to get its location in reference space (inverse map) to apply local interpolation. The previous `interpolate` functions are not concerned by the localization of element containing $P$, they only compute local interpolation.

- a function dedicated to split a finite element in first order finite elements

```
std::vector<std::pair<ShapeType, std::vector<Number> > >
     splitO1(std::map<Number,Number>* renumbering) const;
```

- some print functions

```
void print(std::ostream&) const; //!< print utility
friend std::ostream& operator<<(std::ostream&, const Element&);
```

| | |
|---|---|
| library : | **space** |
| header : | **Element.hpp** |
| implementation : | **Element.cpp** |
| unitary tests : | **test_Space.cpp** |
| header dependences : | **config.h, utils.h, finiteElements.h, geometry.h, Dof.hpp, SpectralBasis.hpp** |

## 6.5 Spectral basis management

### 6.5.1 The SpectralBasis class

For spectral finite elements, the basis is defined by a finite set of functions globally defined over a geometric domain. The SpectralBasis class is devoted to this set of functions over a spectral space. This class is defined as follows:

```
class SpectralBasis
{
  protected :
    Number numberOfFun_;          //!< number of function in the basis
    Number dimFun_;               //!< dimension of the spectral functions
    const Domain* domain_;        //!< geometric domain support
    ValueType returnedType_;      //!< type of returned value (one among _real, _complex)
    StrucType returnedStruct_;    //!< structure of returned value (one among _scalar, _vector)
    FuncFormType funcFormType_;   //!< type of basis functions (_analytical,_interpolated)
};
```

The SpectralBasis class provides:

- One constructor

```
SpectralBasis(Number n, Number d, const Domain& g, ValueType r = _real, StrucType s = _scalar);
```

- Some accessors

```
Number numberOfFun() const;
Dimen dimFun() const;
Number dimSpace() const;
FuncFormType funcFormType() const;
```

- some functions about the basis functions :

```
virtual Function& functions(); //!< return basis function object (only for SpectralBasisFun)
template<typename T>
T& functions(Number, const Point&, T&); //!< compute n-th function
template<typename T>
Vector<T>& functions(const Point& P, Vector<T>& res); //!< compute all functions
```

- some print functions

```
virtual void print(std::ostream&) const = 0;
```

As you may have noticed, the SpectralBasis class is an abstract class. Indeed, a spectral basis can be defined with an analytical expression or by a set of interpolate functions. That is why the SpectralBasis class has 2 childs : SpectralBasisFun and SpectralBasisInt.

### 6.5.2 The SpectralBasisFun class

The SpectralBasisFun class is dedicated to a spectral basis defined with an analytical expression, namely a Function object.

```
class SpectralBasisFun : public SpectralBasis
{
  protected :
    Function functions_;
  public :
    SpectralBasisFun(Domain&, Function&, Number, Number); //!< constructor
};
```

### 6.5.3 The SpectralBasisInt class

The SpectralBasisInt class is dedicated to a spectral basis defined by a set of interpolate functions, namely a set of TermVector objects:

```
class SpectralBasisInt : public SpectralBasis
{
  protected :
    std::vector<TermVector*> functions_;
  public :
    SpectralBasisInt(Domain&, Number, Number);   //!< constructor
};
```

| | |
|---|---|
| library : | **space** |
| header : | **SpectralBasis.hpp** |
| implementation : | **SpectralBasis.cpp** |
| unitary tests : | **test_Space.cpp** |
| header dependences : | **config.h, utils.h, geometry.h** |

# 7 The *operator* library

The *operator* library collects the classes and functionalities related to the description of differential operators acting on unknown or test function in linear, bilinear form and essential condition expressions. As we wish to propose to end users, a C++ description of such operators as close as possible to the mathematical description, few operators are overloaded and a lot of possibilities are offered, for instance:

| mathematical expression | C++ translation | comment |
|---|---|---|
| $\nabla(u)$ | grad(u) | u unknown |
| $\nabla(u).\nabla(v)$ | grad(u)\|grad(v) | u unknown, v test function |
| $(A*\nabla(u)).\nabla(v)$ | (A*grad(u))\|grad(v) | u unknown, v test function, A a matrix |
| $(F(x)*\nabla(u)).\nabla(\overline{v})$ | (F*grad(u))\|grad(conj(v)) | u unknown, v test function, F a function |

As a consequence, this library is quite intricate. It is based on

- the class of differential operator: `DifferentialOperator` collecting all the differential operators that can be applied to an unknown or a test function,
- the class of operand: `Operand`, describing the operations performed at left and right of a differential operator acting on an unknown or a test function,
- the class of operator acting on unknown: `OperatorOnUnknown` which collects the differential operator acting on unknown and the left and right operands if exists.
- the `OperatorOnUnknowns` which relies two operators on unknown as they appear in a bilinear form.
- the class of linear combination of operators acting on unknown: `LcOperatorOnUnknown` which manages a list of pair of `OperatorOnUnknown` and complex coefficient. This class is also able to attach geometric domain to each pair.

A linear form will be defined from one `OperatorOnUnknown` object and a bilinear form from `OperatorOnUnknowns` objects; see the *form* library

Besides, this library provides additional classes to deal with expression involving `Kernel` functions:

- the `OperatorOnKernel` class which handles differential operator applied to a kernel.
- the `KernelOperatorOnUnknowns` class which relies two operators on unknown and a kernel.
- the `TensorKernel` class inherited from `Kernel` and implementing particular kernel.

## 7.1 The `DifferentialOperator` class

The `DifferentialOperator` class is intended to describe various operators that can be act on a scalar function or a vector function. They may be either differential operator (involving derivatives) or 0 order operators (not involving derivative). The attributes of this class are the following:

```
class DifferentialOperator
{
 private:
   DiffOpType type_;           //type of differential operator
   number_t order_;            //derivation order
   bool requiresExtension_;    //does operator involve non-tangential derivatives
   bool requiresNormal_;       //is normal vector required for this operator
   String name_;               //operator name
```

The differential operators supported are list in the *DiffOpType* enumeration:

```
enum DiffOpType
{
_id, _d0, _dt = _d0, _d1, _dx = _d1, _d2, _dy = _d2, _d3, _dz = _d3,
_grad, _nabla = _grad, _div, _curl, _rot = _curl,
_gradS, _nablaS = _gradS, _divS, _curlS, _rotS = _curlS,
_nx, _ndot, _ncross, _ncrossncross, _ndotgrad, _ndiv, _ncrosscurl,
_divG, _gradG, _nablaG = _gradG, _curlG, _rotG = _curlG, _epsilon,
_jump, _mean}
```

with the following meaning (u is either a scalar or vector unknown, x, y and z are the cartesian coordinates and n is the normal):

| enum value | mathematical | builtin functions | unknown |
|---|---|---|---|
| _id | identity | `id(u)` or `u` | scalar or vector |
| _d0=_dt | $\partial_t$ | `d0(u)` or `dt(u)` | scalar or vector |
| _d1=_dx | $\partial_x$ | `d1(u)` or `dx(u)` | scalar or vector |
| _d2=_dy | $\partial_y$ | `d2(u)` or `dy(u)` | scalar or vector |
| _d3=_dz | $\partial_z$ | `d3(u)` or `dz(u)` | scalar or vector |
| _grad=_nabla | $\nabla$ | `grad(u)` or `nabla(u)` | scalar or vector |
| _div | div | `div(u)` | vector |
| _curl=_rot | curl | `curl(u) or \verbrot(u)` | vector |
| _gradS=_nablaS | $\nabla_\tau$ (surfacic) | `gradS(u)` or `nablaS(u)` | scalar or vector |
| _divS | $\text{div}_\tau$ (surfacic) | `divS(u)` | vector |
| _curlS=_rotS | $\text{curl}_\tau$ (surfacic) | `curlS(u)` or `rotS(u)` | vector |
| _gradG=_nablaG | $\nabla_{abc} = (a\partial_x, b\partial_y, c\partial_z)$ | `gradG(u,a,b,c)` or `nablaG(u,a,b,c)` | scalar or vector |
| _divG | $\nabla_{abc}.$ | `divG(u,a,b,c)` | vector |
| _curlG=_rotG | $\nabla_{abc}\times$ | `curlG(u,a,b,c)` or `rotS(u,a,b,c)` | vector |
| _epsilon | elastic tensor | `epsilon(u)` | vector |
| _nx | $n*$ | `nx(u)` or `_n*u` | scalar |
| _ndot | $n.$ | `ndot(u)` or `_n.u` | vector |
| _ncross | $n\times$ | `ncross(u)` or `_n^u` | vector |
| _ncrossncross | $n\times n\times$ | `ncrossncross(u)` or `_n^_n^u` | vector |
| _ndotgrad | $n.\nabla$ | `ndotgrad(u)` or `_n.grad(u)` | scalar |
| _ndiv | $n\text{div}$ | `ndiv(u)` or `_n*div(u)` | vector |
| _ncrosscurl | $n\times\text{curl}$ | `ncrosscurl(u)` or `_n^curl(u)` | vector |
| _jump | [ ] (jump across) | `jump(u)` | scalar or vector |
| _mean | { } (mean across) | `mean(u)` | scalar or vector |

There is only one definition of differential operators stored (using their pointers) in the static variable:

```
static std::vector<DifferentialOperator*> theDifferentialOperators;
```

There is an explicit constructor of DifferentialOperator objects but they are also created using the find function:

```
DifferentialOperator* findDifferentialOperator(DiffOpType);
```

which creates the differential operator of a given type if it does not exist and returns a pointer to the differential operator if it exists or has just been created.
This class provides some useful accessors functions (only read):

```
String name() const {return name_;}
DiffOpType type() const {return type_;}
number_t order() const {return order_;}
bool normalRequired() const{return requiresNormal_;}
bool extensionRequired() const{ return requiresExtension_;}
```

and printing facilities:

```
std::ostream& operator<<(std::ostream&, const DifferentialOperator&);
void printListDiffOp(std::ostream&);
```

| | |
|---|---|
| library : | **operator** |
| header : | **DifferentialOperator.hpp** |
| implementation : | **DifferentialOperator.cpp** |
| unitary tests : | **test_operator.cpp** |
| header dependences : | **config.h, utils.h** |

## 7.2 The `Operand` class

The `Operand` class stores a `AlgebraicOperator`, a user data (either `Function` or `Value`) and conjugate, transpose flags. It is mainly used by the `OperatorOnUnknown` class as left or right-hand side of a generalized differential operator (see the next section). The only allowed algebraic operations defined in the `AlgebraicOperator` enumeration, are:

- the standard product, operator *
- the inner product (hermitian product), operator |
- the cross product, operator ^
- the contracted product, operator %

```
enum AlgebraicOperator {_product,_innerProduct,_crossProduct,_contractedProduct};
class Operand
{
protected :
   const Value* val_p;            // pointer to operand object (a Value)
   const Function * fun_p;        // pointer to Function object
   bool isFunction_;              // function flag
   bool conjugate_;               // true if the operand has to be conjugated
   bool transpose_;               // true if the operand has to be transposed
   AlgebraicOperator operation_; // operand operator
```

This class provides few public constructors:

```
Operand(const Function&,AlgebraicOperator); // from a Function
Operand(const Value&,AlgebraicOperator);    // from a Value  (Value is copied)
Operand(const Value*,AlgebraicOperator);    // from a Value* (Value is not copied)
template <typename T>
Operand(const T &,AlgebraicOperator);       // from a scalar, a Vector or a Matrix
```

The templated constructor avoids the user to give explicitly a Value object, "ordinary" objects such scalar, vector or matrix may be passed to the constructor.

The other member functions are some accessors functions:

```
bool isFunction() const;
bool conjugate() const;
bool& conjugate();
bool transpose() const;
bool& transpose();
AlgebraicOperator operation() const;
const Value& value() const;
const Function& function() const;
template<class T> T& valueT() const;
```

There are two printing facilities:

```
void Operand::print(std::ostream&) const;
std::ostream& operator<<(std::ostream&,const Operand &);
```

The Operand class is an internal class linked to the OperatorOnUnknown class. Normally, an end user does not use this class.

| | |
|---|---|
| library : | **operator** |
| header : | **Operand.hpp** |
| implementation : | **Operand.cpp** |
| unitary tests : | **test_operator.cpp** |
| header dependences : | **config.h, utils.h** |

## 7.3 The OperatorOnUnknown class

The OperatorOnUnknow class is intended to store the description of an expression involving a differential operator acting on an unknown (or a test function) with possibly operations at the left and the right. More precisely, the general form of the operator on unknown is:

**tr(data) op dif( tr(u) ) op tr(data)**

where

- **u** is an unknown,
- **dif** a differential operator,
- **data** is a user data (value or function),
- **op** an algebraic operation among * (product), | (inner product), ^ (cross product), : (contracted product),
- **tr** a transformation among conj (conjugate), tran (transpose) and adj (adjoint).

All is optional except the unknown u.

The simplest form is **u** and a more complex one is for instance, something like this ($f$ a matrix and $g$ a vector):

**adj**(**f**)* **grad**(**conj**(**u**[2])) | **conj**(**g**)

which mathematically reads:

$$f^* \nabla \overline{u}_2 . \overline{g}$$

The class has the following attributes:

```
class OperatorOnUnknown
{protected :
   const Unknown * u_p;              //unknown involved in operator
   bool conjugateUnknown_;           //true if the unknown has to be conjugated
   DifferentialOperator * difOp_p;  //differential operator involved in operator
   Operand * leftOperand_p;          //object before the diff operator
   Operand * rightOperand_p;         //object after the diff operator
   bool leftPriority_;               //priority order flag, true if left operand is prior
   Vector<complex_t> coefs_;         //coefficients for operator (gradG, divG, curlG)
   ValueType type_;                  //returned value (_real,_complex)
   StrucType struct_;                //returned structure (_scalar,_vector,_matrix)
```

Operand is a class storing a user data (value or function) and an algebraic operation (* | ^ %).

The class provides some basic constructors (from unknown and differential operator type), some useful constructors (from unknown and function or value), a copy constructor, the assignment operator and a destructor:

```
OperatorOnUnknown(const Unknown* un=0,DiffOpType=_id);
OperatorOnUnknown(const Unknown& un,DiffOpType=_id);
OperatorOnUnknown(const Unknown&,const Function&,AlgebraicOperator,bool);
OperatorOnUnknown(const Unknown&,const Value&,AlgebraicOperator,bool);
OperatorOnUnknown(const OperatorOnUnknown &);
~OperatorOnUnknown();
OperatorOnUnknown& operator=(const OperatorOnUnknown &);
```

Note that the DifferentialOperator object are created on the fly when creating OperatorOnUnknown from Unknown and DiffOpType.

The class provides some accessors (read or write):

```
DiffOpType difOpType() const ;
DifferentialOperator*& difOp() ;
ValueType& type();
Operand*& leftOperand();
Operand*& rightOperand();
Vector<complex_t>& coefs();
const Vector<complex_t>& coefs() const;
bool leftPriority() const;
bool& leftPriority();
```

and some utilities to update class attributes and print them:

```
void setReturnedType(const Unknown*,DiffOpType);
void updateReturnedType(AlgebraicOperator,ValueType,StrucType,bool);
void print(std::ostream&) const;
std::ostream& operator<<(std::ostream&,const OperatorOnUnknown &);  //extern
```

The two first one manage the returned types and check consistency of operations and the two last functions output on stream the OperatorOnUnknown characteristics.

To deal with the general syntax of OperatorOnUnknown, a lot of external functions are required, in particular some overloaded operators. The first family of functions concerns the creation of simple OperatorOfUnknown object from a differential operator and an unknown. Their names are the names of differential operator type (DiffOpType enumeration) without the leading underscore. We give only a few examples here (see OperatorOnUnknown.hpp header file for the complete list):

```
OperatorOnUnknown& id(const Unknown&);
OperatorOnUnknown& d0(const Unknown&);
...
OperatorOnUnknown& grad(const Unknown&);
OperatorOnUnknown& nabla(const Unknown&);
...
OperatorOnUnknown& nx(const Unknown&);
...
OperatorOnUnknown& gradG (const Unknown&,const complex_t&,const complex_t&,
                          const complex_t&,const complex_t&);
...
OperatorOnUnknown& mean(const Unknown&);
OperatorOnUnknown& jump(const Unknown&);
```

These functions constructs an `OperatorOnUnknown` in the heap memory and return a reference in order to be used in an chained expression. In this context, it may be occur a memory leak if nobody delete explicitly the `OperatorOnUnknown` object created on the fly.

To manage general syntax, the following c++ operators have been overloaded:

* : usual consistent product between scalars, vectors and matrices
| : inner product of vectors, for complex objects it is an hermitian product
^ : cross product of vectors
% : contracted product (the second term is transposed)

These operators are enumerated in the `AlgebraicOperator` enumeration.

They are overloaded for `Unknown` or `OperatorOnUnknown` and unitaryVector (`UnitaryVector` enumerates the normal vector _ n and the tangential vector _ t). When differential operators involve operation with normal, you can use the previous function (for instance *ndot*) or use their mathematical syntax (for instance *n*u*):

```
OperatorOnUnknown& operator*(UnitaryVector,const Unknown &);    // n*u
OperatorOnUnknown& operator*(const Unknown &,UnitaryVector);    // u*n
OperatorOnUnknown& operator|(UnitaryVector,const Unknown &);    // n|u
OperatorOnUnknown& operator^(UnitaryVector,const Unknown &);    // n^u
OperatorOnUnknown& operator|(const Unknown &,UnitaryVector);    // u|n
OperatorOnUnknown& operator|(UnitaryVector,OperatorOnUnknown&); // n|grad(u)
OperatorOnUnknown& operator^(UnitaryVector,OperatorOnUnknown&); // n^(n^u) or n^curl(u)
OperatorOnUnknown& operator*(UnitaryVector,OperatorOnUnknown&); // n*div
OperatorOnUnknown& operator|(OperatorOnUnknown&,UnitaryVector); // grad(u)|n
OperatorOnUnknown& operator*(OperatorOnUnknown&,UnitaryVector); // div*n
```

Note that all cases are not considered. It should be !?

To deal with left and right-hand side operations, these algebraic operators have been also overloaded for different types of objects (`Unknown`, `OperatorOnUnknown`, `Function`, `Value`, user c++ function or user value). The operator overloading with c++ function or user value avoids the user to explicitly encapsulate its own data (c++ function or scalar, vector, matrix) in Function object or Value object. There are shortcuts. In the following, only prototypes of * operator are presented.

### 7.3.1 Operations between `Unknown` and `Function`

```
OperatorOnUnknown&  operator*(const Unknown &,const Function&);    // u*F
OperatorOnUnknown&  operator*(const Function&,const Unknown &);    // F*u
template <typename T>
  OperatorOnUnknown& operator*(const Unknown &,T( )(const Point&,Parameters&));
  OperatorOnUnknown& operator*(T( )(const Point&,Parameters&),const Unknown &);
  OperatorOnUnknown& operator*(const Unknown &,
                              T( )(const Vector<Point>&,Parameters&));
  OperatorOnUnknown& operator*(T( )(const Vector<Point>&,Parameters&),
                              const Unknown &);
...
```

The two first one declarations concern Function object encapsulating c++ user functions whereas the templated forms concerns c++ user functions. As mentioned before, it avoids the user to encapsulate his c++ functions. Note that only c++ functions that can be encapsulated in Function object are working in templated forms. Other functions may be accepted in compilation process, but the result during execution may be hazardous!

⚠ Kernel type functions can not be use straightforward in operator. Contrary to the ordinary functions, they have to be encapsulated in `Function` objects!

### 7.3.2 Operations between `Unknown` and `Value`

```
OperatorOnUnknown&  operator*(const Unknown&,const Value&);        // u*V
OperatorOnUnknown&  operator*(const Value&,const Unknown&);        // V*u
template<typename T>
  OperatorOnUnknown&  operator*(const Unknown& ,const T& )         // u*T
  OperatorOnUnknown&  operator*(const T& ,const Unknown&)          // T*u
...
```

The two first one declarations concern Value object encapsulating c++ user data and the templated forms concerns c++ user data. Only c++ user data that can be encapsulated in Value object are working in templated forms.

### 7.3.3 Operations between `OperatorOnUnknown` and `Function`

The principle is the same as in previous cases.

```
OperatorOnUnknown& operator*(OperatorOnUnknown&,const Function &); // op(u)*F
OperatorOnUnknown& operator*(const Function &,OperatorOnUnknown&); // F*op(u)
template<typename T>
  OperatorOnUnknown& operator*(OperatorOnUnknown&, T( )(const Point&,Parameters&))
  OperatorOnUnknown& operator*(T( )(const Point&,Parameters&), OperatorOnUnknown&)
  OperatorOnUnknown& operator*(OperatorOnUnknown&,
                              T( )(const Vector<Point>&,Parameters&))
  OperatorOnUnknown& operator*(T( )(const Vector<Point>&,Parameters&),
                              OperatorOnUnknown&)
...
```

### 7.3.4 Operations between `OperatorOnUnknown` and `Value`

```
OperatorOnUnknown& operator*(OperatorOnUnknown&,const Value &);    // op(u)*V
OperatorOnUnknown& operator*(const Value &,OperatorOnUnknown&);    // V*op(u)
template<typename T>
  OperatorOnUnknown& operator*(OperatorOnUnknown&,const T&);       // op(u)*T
  OperatorOnUnknown& operator*(const T&,OperatorOnUnknown&);       // T*op(u)
...
```

Most of the previous overloaded operators use the following update functions:

```
OperatorOnUnknown& updateRight(OperatorOnUnknown&,const Function&,AlgebraicOperator);
OperatorOnUnknown& updateLeft (OperatorOnUnknown&,const Function&,AlgebraicOperator);
OperatorOnUnknown& updateRight(OperatorOnUnknown&,const Value&,AlgebraicOperator);
```

```
OperatorOnUnknown& updateLeft (OperatorOnUnknown&,const Value&,AlgebraicOperator);
template<typename T>
  OperatorOnUnknown& updateRight(OperatorOnUnknown&,const T&,AlgebraicOperator);
  OperatorOnUnknown& updateLeft(OperatorOnUnknown&,const T&,AlgebraicOperator);
```

Note that it is possible to use the transformations *conj*, *tran* and *adj* on Unknown, Value or Function. These functions are defined in the files related to these classes. For simplicity, it is not possible to apply such transformations to an `OperatorOnUnknown` object or a part of the expression. For instance, the syntax *conj(grad(u))* is not supported.

Finally, we give some examples to show how this machinery works:

```
//define some C++ functions
real_t F(const Point &P,Parameters& pa = defaultParameters) {...}
Vector<real_t> vecF(const Point &P,Parameters& pa = defaultParameters) {...}
Matrix<real_t> matF(const Point &P,Parameters& pa = defaultParameters) {...}
//define some constant values
real_t pi=3.14159; complex_t i(0,1);vector<real_t> v(3,1); matrix<complex_t> A(3,3,i);
//assume u is an Unknown (a vector of dimension 3)
OperatorOnUnknown opu=u;     //the simplest one
opu=grad(u);                 //involve only differential operator
opu=_n^curl(u);               //equivalent to ncrosscurl(u)
opu=v^u;                     //cross product with vector
opu=vecF^u;                  //cross product with vector function
opu=A*grad(u);               //left product with a matrix
opu=grad(u)*matF;            //right product with a matrix function
opu=(matF*grad(u))%A;        //product and contracted product
opu=curl(conj(u))|conj(v);   //use conj transformation
```

Be careful with operator priority. The C++ priority rules are applied and not the mathematical ones. In doubt, use parenthesis. The code performs some constancy checking on operand and operator but only on structure (scalar, vector, matrix) not on the dimension (see *upadateReturnedType* and *setReturnedType* functions).

| | |
|---:|:---|
| library : | **operator** |
| header : | **OperatorOnUnknown.hpp** |
| implementation : | **OperatorOnUnknown.cpp** |
| unitary tests : | **test_operator.cpp** |
| header dependences : | **config.h, utils.h** |

## 7.4 The `OperatorOnUnknowns` class

The `OperatorOnUnknowns` class deals with a pair of `OperatorOnUnknown` object related by an `AlgebraicOperator` (one of product, inner product, cross product or contracted product): It is useful to store syntax like *opu aop opv* occurring in bilinear forms.

```
class OperatorOnUnknowns
{
 protected :
 OperatorOnUnknown opu_;  //left operator on unknown
 OperatorOnUnknown opv_;  //right operator on unknown (test function)
 AlgebraicOperator aop_;  //algebraic operation (*,|,%,^)
}
```

The class provides basic constructor and accessors:

```
OperatorOnUnknowns() {};
OperatorOnUnknowns(const OperatorOnUnknown& operu, const OperatorOnUnknown& operv,
    AlgebraicOperator aop);
```

```
const OperatorOnUnknown& opu() const;
OperatorOnUnknown& opu();
OperatorOnUnknown& opv();
AlgebraicOperator algop();
ValueType valueType() const;
```

a function checking the consistancy of expression:

```
bool checkConsistancy();
```

The checkConsitancy function checks that the given OperatorOnUnknown objects are consistent (in structure not in dimension) with the given algebraic operation. If not an error is handled.
Some print facilities are provided:

```
void print(std::ostream&) const;
friend std::ostream& operator<<(std::ostream&, const OperatorOnUnknowns&);
```

Besides, some extern functions acts like constructors:

```
OperatorOnUnknowns operator*(OperatorOnUnknown&,OperatorOnUnknown&); //opu * opv
OperatorOnUnknowns operator|(OperatorOnUnknown&,OperatorOnUnknown&); //opu | opv
OperatorOnUnknowns operator^(OperatorOnUnknown&,OperatorOnUnknown&); //opu ^ opv
OperatorOnUnknowns operator%(OperatorOnUnknown&,OperatorOnUnknown&); //opu % opv
OperatorOnUnknowns operator*(OperatorOnUnknown&,Unknown&);           //opu * v
OperatorOnUnknowns operator|(OperatorOnUnknown&,Unknown&);           //opu | v
OperatorOnUnknowns operator^(OperatorOnUnknown&,Unknown&);           //opu ^ v
OperatorOnUnknowns operator%(OperatorOnUnknown&,Unknown&);           //opu % v
OperatorOnUnknowns operator*(Unknown&,OperatorOnUnknown&);           //u * opv
OperatorOnUnknowns operator|(Unknown&,OperatorOnUnknown&);           //u | opv
OperatorOnUnknowns operator^(Unknown&,OperatorOnUnknown&);           //u ^ opv
OperatorOnUnknowns operator%(Unknown&,OperatorOnUnknown&);           //u % opv
OperatorOnUnknowns operator*(Unknown&,Unknown&);                     //u * v
OperatorOnUnknowns operator|(Unknown&,Unknown&);                     //u | v
OperatorOnUnknowns operator^(Unknown&,Unknown&);                     //u ^ v
OperatorOnUnknowns operator%(Unknown&,Unknown&);                     //u % v
```

| | |
|---:|---|
| library : | **operator** |
| header : | **OperatorOnUnknowns.hpp** |
| implementation : | **OperatorOnUnknowns.cpp** |
| unitary tests : | **test_operator.cpp** |
| header dependences : | **OperatorOnUnknown.hpp, config.h, utils.h** |

## 7.5 The LcOperatorOnUnknown class

TheLcOperatorOnUnknown class deals with linear combination of OperatorOnUnknown objects :

$$\sum_{i=1,n} c_i\ op(u_i)|dom_i$$

where $c_i$ is a complex coefficient, $op(u_i)$ an operator on unknown $u_i$ (OperatorOnUnknown object) and possibly a geometrical domain $dom_i$ (Domain object). LcOperatorOnUnknown objects are useful to describe essential condition (see *essentialConditions* library):

$$\sum_{i=1,n} c_i\ op(u_i)|dom_i = g.$$

`LcOperatorOnUnknown` objects are also useful to create `LcOperatorOnUnknowns` in a condensed way:

$$\left(\sum_{i=1,n} c_i^u \; op(u_i)\right) \; O \; \left(\sum_{j=1,n} c_j^v \; op(u_j)\right) = \sum_{i,j=1,n} c_i^u c_j^v op(u_i) \; op(u_i) \; O \; op(v_j).$$

The`LcOperatorOnUnknown` class inherits from `std::vector` class :

```
typedef std::pair<OperatorOnUnknown*, Complex> OpuValPair;

class LcOperatorOnUnknown : public std::vector<OpuValPair>
{
public :
    std::vector<Domain*> domains_;
}
```

The class provides some basic constructors and related stuff (copy, clear)

```
LcOperatorOnUnknown() {};
LcOperatorOnUnknown(const OperatorOnUnknown&, const Real& = 1.);
LcOperatorOnUnknown(const OperatorOnUnknown&, const Complex&);
LcOperatorOnUnknown(const OperatorOnUnknown&, Domain&, const Real& = 1.);
LcOperatorOnUnknown(const OperatorOnUnknown&, Domain&, const Complex&);
LcOperatorOnUnknown(const Unknown&, const Real& = 1.);
LcOperatorOnUnknown(const Unknown&, const Complex&);
LcOperatorOnUnknown(const Unknown&, Domain&, const Real& = 1.);
LcOperatorOnUnknown(const Unknown&, Domain&, const Complex&);
LcOperatorOnUnknown(const LcOperatorOnUnknown&);
~LcOperatorOnUnknown();
LcOperatorOnUnknown& operator =(const LcOperatorOnUnknown&);
void clear();
void copy(const LcOperatorOnUnknown& lc);
```

To insert new item in the list, there are insertion member functions and overloaded operators:

```
void insert(const OperatorOnUnknown&, GeomDomain* =0);                // insert op(u)
void insert(const Real&, const OperatorOnUnknown&, GeomDomain* =0);   // insert a*op(u)
void insert(const Complex&, const OperatorOnUnknown&, GeomDomain* =0); // insert a*op(u)
void insert(const Unknown&, GeomDomain* =0);                          // insert u on D
void insert(const Real&, const Unknown&, GeomDomain* =0);             // insert a*u on D
void insert(const Complex&, const Unknown&, GeomDomain* =0);          // insert a*u on D
LcOperatorOnUnknown& operator+=(const OperatorOnUnknown&);           // lcop += opu
LcOperatorOnUnknown& operator+=(const Unknown&);             // lcop += u
LcOperatorOnUnknown& operator+=(const LcOperatorOnUnknown&); // lcop += lcop
LcOperatorOnUnknown& operator-=(const OperatorOnUnknown&);   // lcop -= opu
LcOperatorOnUnknown& operator-=(const Unknown&);             // lcop -= u
LcOperatorOnUnknown& operator-=(const LcOperatorOnUnknown&); // lcop -= lcop
LcOperatorOnUnknown& operator*=(const Real&);                // lcop *= r
LcOperatorOnUnknown& operator*=(const Complex&);             // lcop *= c
LcOperatorOnUnknown& operator/=(const Real&);                // lcop /= r
LcOperatorOnUnknown& operator/=(const Complex&);             // lcop /= c
```

Extern operators may also be used :

```
LcOperatorOnUnknown operator+(const LcOperatorOnUnknown&);
LcOperatorOnUnknown operator-(const LcOperatorOnUnknown&);
LcOperatorOnUnknown operator+(const LcOperatorOnUnknown&, const OperatorOnUnknown&);
LcOperatorOnUnknown operator-(const LcOperatorOnUnknown&, const OperatorOnUnknown&);
LcOperatorOnUnknown operator+(const OperatorOnUnknown&, const LcOperatorOnUnknown&);
LcOperatorOnUnknown operator-(const OperatorOnUnknown&, const LcOperatorOnUnknown&);
LcOperatorOnUnknown operator+(const LcOperatorOnUnknown&, const Unknown&);
LcOperatorOnUnknown operator-(const LcOperatorOnUnknown&, const Unknown&);
LcOperatorOnUnknown operator+(const Unknown&, const LcOperatorOnUnknown&);
LcOperatorOnUnknown operator-(const Unknown&, const LcOperatorOnUnknown&);
LcOperatorOnUnknown operator+(const LcOperatorOnUnknown&, const LcOperatorOnUnknown&);
LcOperatorOnUnknown operator-(const LcOperatorOnUnknown&, const LcOperatorOnUnknown&);
LcOperatorOnUnknown operator*(const LcOperatorOnUnknown&, const Real&);
LcOperatorOnUnknown operator*(const LcOperatorOnUnknown&, const Complex&);
LcOperatorOnUnknown operator*(const Real&, const LcOperatorOnUnknown&);
LcOperatorOnUnknown operator*(const Complex&, const LcOperatorOnUnknown&);
LcOperatorOnUnknown operator/(const LcOperatorOnUnknown&, const Real&);
LcOperatorOnUnknown operator/(const LcOperatorOnUnknown&, const Complex&);
LcOperatorOnUnknown operator+(const OperatorOnUnknown&, const OperatorOnUnknown&);
LcOperatorOnUnknown operator-(const OperatorOnUnknown&, const OperatorOnUnknown&);
LcOperatorOnUnknown operator+(const OperatorOnUnknown&, const Unknown&);
LcOperatorOnUnknown operator-(const OperatorOnUnknown&, const Unknown&);
LcOperatorOnUnknown operator+(const Unknown&, const OperatorOnUnknown&);
LcOperatorOnUnknown operator-(const Unknown&, const OperatorOnUnknown&);
LcOperatorOnUnknown operator+(const Unknown&, const Unknown&);
LcOperatorOnUnknown operator-(const Unknown&, const Unknown&);
```

`GeomDomain` may be affected using `SetDomain` or | operator :

```
void setDomain(GeomDomain&);
LcOperatorOnUnknown& operator|(GeomDomain&);
LcOperatorOnUnknown operator|(const Unknown&,GeomDomain&);
LcOperatorOnUnknown operator|(const OperatorOnUnknown&,GeomDomain&);
```

Note that when setting the domain, all previous domain definitions are overwritten.

It provides the following accessors and property accessors:

```
bool isSingleUnknown() const;
const Unknown* unknown() const;
std::set<const Unknown*> unknowns() const;
bool withDomains() const;
bool isSingleDomain() const;
Domain* domain() const;
std::set<Domain*> domains() const;
Complex coefficient() const;
std::vector<Complex> coefficients() const;
std::set<DiffOpType> diffOperators() const;
void print(std::ostream&, bool withdomain=true) const;
friend std::ostream& operator<<(std::ostream&, const LcOperatorOnUnknown&);
```

To create essential condition from `LcOperatorOnUnknown`, operator = is overloaded as following:

```
EssentialCondition operator=(const Real &);
EssentialCondition operator=(const Complex &);
EssentialCondition operator=(const Function &);
```

These functions are implemented in *EssentialCondition.cpp*!

| | |
|---|---|
| library : | **operator** |
| header : | **LcOperatorOnUnknowns.hpp** |
| implementation : | **LcOperatorOnUnknowns.cpp** |
| unitary tests : | **test_EssentialCondition.cpp** |
| header dependences : | **OperatorOnUnknown.hpp, config.h, utils.h** |

## 7.6 The LcOperatorOnUnknowns class

TheLcOperatorOnUnknowns class deals with linear combination of OperatorOnUnknowns objects :

$$\sum_{i=1,n} c_i \; op(u_i) \; O \; op(v_i)$$

where $c_i$ is a complex coefficient, $op(u_i)$ an operator on unknown $u_i$ (OperatorOnUnknown object), $O$ an algebraic operator and $op(v_i)$ an operator on test function $v_i$ (OperatorOnUnknown object). LcOperatorOnUnknowns objects are useful to describe linear and bilinear form (see *form* library):

$$\int_\Omega \sum_{i=1,n} c_i \; op(u_i) \; O \; op(v_i).$$

TheLcOperatorOnUnknowns class inherits from std::vector class :

```
typedef std::pair<OperatorOnUnknowns *, complex_t> OpusValPair;

class LcOperatorOnUnknowns : public std::vector<OpusValPair>
```

The class provides some basic constructors and related stuff (copy, clear)

```
    LcOperatorOnUnknowns() {}
    LcOperatorOnUnknowns(const OperatorOnUnknowns &, const real_t & = 1.);
    LcOperatorOnUnknowns(const OperatorOnUnknowns &, const complex_t &);
    LcOperatorOnUnknowns(const LcOperatorOnUnknowns &);
    ~LcOperatorOnUnknowns();
    LcOperatorOnUnknowns &operator=(const LcOperatorOnUnknowns &);
    void clear();
    void copy(const LcOperatorOnUnknowns &lc);
```

To insert new item in the list, there are insertion member functions and overloaded operators:

```
void insert(const OperatorOnUnknowns &);                    // insert opuv
void insert(const real_t &, const OperatorOnUnknowns &);     // insert a*opuv
void insert(const complex_t &, const OperatorOnUnknowns &); // insert
a*opuv
LcOperatorOnUnknowns &operator+=(const OperatorOnUnknowns &);    // lcopuv += opuv
LcOperatorOnUnknowns &operator+=(const LcOperatorOnUnknowns &); // lcopuv += lcopuv
LcOperatorOnUnknowns &operator-=(const OperatorOnUnknowns &);    // lcopuv -= opuv
LcOperatorOnUnknowns &operator-=(const LcOperatorOnUnknowns &); // lcopuv -= lcopuv
LcOperatorOnUnknowns &operator*=(const real_t &);                // lcopuv *= r
LcOperatorOnUnknowns &operator*=(const complex_t &);             // lcopuv *= c
LcOperatorOnUnknowns &operator/=(const real_t &);                // lcopuv /= r
LcOperatorOnUnknowns &operator/=(const complex_t &);             // lcopuv /= c
```

Extern operators may also be used :

```
// OperatoronUnknowns and OperatorOnUnknowns
LcOperatorOnUnknowns operator+(const OperatorOnUnknowns &, const OperatorOnUnknowns &);
LcOperatorOnUnknowns operator-(const OperatorOnUnknowns &, const OperatorOnUnknowns &);

// LcOperatorOnUnknowns and LcOperatorOnUnknowns
LcOperatorOnUnknowns operator+(const LcOperatorOnUnknowns &);
LcOperatorOnUnknowns operator-(const LcOperatorOnUnknowns &);
LcOperatorOnUnknowns operator+(const LcOperatorOnUnknowns &, const LcOperatorOnUnknowns &);
LcOperatorOnUnknowns operator-(const LcOperatorOnUnknowns &, const LcOperatorOnUnknowns &);

// LcOperatorOnUnknowns and OperatorOnUnknowns
LcOperatorOnUnknowns operator+(const LcOperatorOnUnknowns &, const OperatorOnUnknowns &);
LcOperatorOnUnknowns operator-(const LcOperatorOnUnknowns &, const OperatorOnUnknowns &);
LcOperatorOnUnknowns operator+(const OperatorOnUnknowns &, const LcOperatorOnUnknowns &);
LcOperatorOnUnknowns operator-(const OperatorOnUnknowns &, const LcOperatorOnUnknowns &);

// LcOperatorOnUnknowns and scalar
LcOperatorOnUnknowns operator*(const LcOperatorOnUnknowns &, const real_t &);
LcOperatorOnUnknowns operator*(const LcOperatorOnUnknowns &, const complex_t &);
LcOperatorOnUnknowns operator*(const real_t &, const LcOperatorOnUnknowns &);
LcOperatorOnUnknowns operator*(const complex_t &, const LcOperatorOnUnknowns &);
LcOperatorOnUnknowns operator/(const LcOperatorOnUnknowns &, const real_t &);
LcOperatorOnUnknowns operator/(const LcOperatorOnUnknowns &, const complex_t &);

// LcOperatorOnUnknown and OperatorOnUnkown
LcOperatorOnUnknowns operator*(const LcOperatorOnUnknown &, const OperatorOnUnknown &);
LcOperatorOnUnknowns operator*(const OperatorOnUnknown &, const LcOperatorOnUnknown &);
LcOperatorOnUnknowns operator%(const LcOperatorOnUnknown &, const OperatorOnUnknown &);
LcOperatorOnUnknowns operator%(const OperatorOnUnknown &, const LcOperatorOnUnknown &);
LcOperatorOnUnknowns operator|(const LcOperatorOnUnknown &, const OperatorOnUnknown &);
LcOperatorOnUnknowns operator|(const OperatorOnUnknown &, const LcOperatorOnUnknown &);

// LcOperatorOnUnknown and Unkown
LcOperatorOnUnknowns operator*(const LcOperatorOnUnknown &, const Unknown &);
LcOperatorOnUnknowns operator*(const Unknown &, const LcOperatorOnUnknown &);
LcOperatorOnUnknowns operator%(const LcOperatorOnUnknown &, const Unknown &);
LcOperatorOnUnknowns operator%(const Unknown &, const LcOperatorOnUnknown &);
LcOperatorOnUnknowns operator|(const LcOperatorOnUnknown &, const Unknown &);
LcOperatorOnUnknowns operator|(const Unknown &, const LcOperatorOnUnknown &);

// LcOperatorOnUnknown and LcOperatorOnUnkown
LcOperatorOnUnknowns operator*(const LcOperatorOnUnknown &, const LcOperatorOnUnknown &);
LcOperatorOnUnknowns operator%(const LcOperatorOnUnknown &, const LcOperatorOnUnknown &);
LcOperatorOnUnknowns operator|(const LcOperatorOnUnknown &, const LcOperatorOnUnknown &);
```

It provides the following accessors and property accessors:

```
  bool isSingleUVPair() const;                       // true if all terms involve the same
    unknown
  const OperatorOnUnknown *opu(number_t i = 1) const; // return ith left OperatorOnUnknown
    involved in LcOperator's
  const OperatorOnUnknown *opv(number_t i = 1) const; // return ith right OperatorOnUnknown
    involved in LcOperator's
  const Unknown *unknownu(number_t i = 1) const;      // return ith left Unknown involved in
    LcOperator
  const Unknown *unknownv(number_t i = 1) const;      // return ith right
  Unknown involved in LcOperator
  complex_t coefficient(number_t i = 1) const; // return ith coefficient
  std::vector<complex_t> coefficients() const; // return vector of coefficients involved in
    combination
 void print(std::ostream &) const;
 friend std::ostream &operator<<(std::ostream &, const LcOperatorOnUnknowns &);
```

| | |
|---|---|
| library : | **operator** |
| header : | **LcOperatorOnUnknowns.hpp** |
| implementation : | **LcOperatorOnUnknowns.cpp** |
| unitary tests : | **unit_LcOperatorOnUnknowns.cpp** |
| header dependences : | **LcOperatorOnUnknown.hpp, OperatorOnUnknown.hpp, config.h, utils.h** |

## 7.7 The OperatorOnKernel class

Kernel objects describes function of two points, say $K(x, y)$. The OperatorOnKernel class is intended to store the differential operators acting on Kernel, one for $x$ derivatives and one for $y$ derivatives :

```
class OperatorOnKernel
{
  protected :
    const Kernel* ker_p;            //Kernel involved in operator
    DifferentialOperator* xdifOp_p; //x differential operator involved in operator
    DifferentialOperator* ydifOp_p; //v differential operator involved in operator
    ValueType type_;                //type of returned value ( _real, _complex)
    StrucType struct_;              //structure of returned value (_scalar, _vector, _matrix)
        }
```

A null pointer *ker_p* means the kernel function $K(x, y) = 1$ and by default *xdifOp_p* and *ydifOp_p* point to identity differential operator.

OperatorOnKernel object are constructed either by constructor members or by external functions:

```
OperatorOnKernel();
OperatorOnKernel(const Kernel*, DiffOpType = _id, DiffOpType = _id, ValueType vt=_real, StrucType
     st=_scalar);
OperatorOnKernel(const Kernel&, DiffOpType = _id, DiffOpType = _id);
OperatorOnKernel(const OperatorOnKernel&);
OperatorOnKernel& operator=(const OperatorOnKernel&);

OperatorOnKernel& id(const Kernel&);                          //id(k)
OperatorOnKernel& grad_x(const Kernel&);                      //grad_x(k)
OperatorOnKernel& grad_y(const Kernel&);                      //grad_y(k)
...
OperatorOnKernel& id(OperatorOnKernel&);                      //id(opk)
OperatorOnKernel& grad_x(OperatorOnKernel&);                  //grad_x(opk)
OperatorOnKernel& grad_y(OperatorOnKernel&);                  //grad_y(opk)
...
OperatorOnKernel& operator*(UnitaryVector, const Kernel&);    //n*ker
OperatorOnKernel& operator*(const Kernel&, UnitaryVector);    //ker*n
OperatorOnKernel& operator|(UnitaryVector, const Kernel&);    //n|ker
OperatorOnKernel& operator|(const Kernel&, UnitaryVector);    //ker|n
OperatorOnKernel& operator^(UnitaryVector, const Kernel&);    //n^ker
OperatorOnKernel& operator*(UnitaryVector, OperatorOnKernel&); //n*opker
OperatorOnKernel& operator*(OperatorOnKernel&, UnitaryVector); //opker*n
OperatorOnKernel& operator|(UnitaryVector, OperatorOnKernel&); //n|opker
OperatorOnKernel& operator|(OperatorOnKernel&, UnitaryVector); //opker|n
OperatorOnKernel& operator^(UnitaryVector, OperatorOnKernel&); //n^opker
```

Note that operators return reference to object dynamically allocated.

The class provides some member accessors and property accessors

```
const Kernel* kernel() const;
DiffOpType xdifOpType() const;
DiffOpType ydifOpType() const;
DifferentialOperator*& xdifOp_();
DifferentialOperator& xdifOp() const;
DifferentialOperator*& ydifOp_();
DifferentialOperator& ydifOp() const;
ValueType& valueType();
ValueType valueType()const;
StrucType& strucType();
StrucType strucType() const;
Dimen xdiffOrder() const;
Dimen ydiffOrder() const;
bool voidKernel() const;
```

and print facilities

```
void print(std::ostream&) const;
friend std::ostream& operator<<(std::ostream& os, const OperatorOnKernel& opk);
```

Finally the class interfaces the computation of `OperatorOnKernel` at a couple of points or a list of couples of points using template functions:

```
template <typename T>
T& eval(const Point&,const Point&, T&) const;
template <typename T>
std::vector<T>& eval(const std::vector<Point>&,const std::vector<Point>&, std::vector<T>&) const;
```

| | |
|---|---|
| library : | **operator** |
| header : | **OperatorOnKernel.hpp** |
| implementation : | **OperatorOnKernbel.cpp** |
| unitary tests : | **test_operator.cpp** |
| header dependences : | **DifferentialOperator.hpp, Operand.hpp, config.h, utils.h** |

## 7.8 The `KernelOperatorOnUnknowns` class

The `KernelOperatorOnUnknowns` class deals with expressions involving two operators on unknown linked with an `OperatorOnKernel`, that is

$$op_u\ aop_l\ op_k\ aop_r\ op_v$$

Such expression appears in integral equation or integral representation, for instance to deal with:

$$\int_\Gamma\int_\Gamma u(x)*G(x,y)*v(y)\,dx\,dy.$$

```
class KernelOperatorOnUnknowns
{
  protected :
    OperatorOnUnknown opu_;
    OperatorOnUnknown opv_;
    AlgebraicOperator aopu_;
    AlgebraicOperator aopv_;
    OperatorOnKernel opker_;
}
```

The class provides one basic constructor and a lot of extern functions building `KernelOperatorOnUnknowns` object:

```
KernelOperatorOnUnknowns(const OperatorOnUnknown&, AlgebraicOperator, const OperatorOnKernel&,
     AlgebraicOperator, const OperatorOnUnknown&);

KernelOperatorOnUnknowns operator*(const OperatorOnUnknown&, const OperatorOnKernel&); //opu *
     opker
KernelOperatorOnUnknowns operator*(const OperatorOnKernel&, const OperatorOnUnknown&); //opker *
     opv
KernelOperatorOnUnknowns operator*(const OperatorOnUnknown&, const Kernel&);          //opu * ker
KernelOperatorOnUnknowns operator*(const Kernel&, const OperatorOnUnknown&);          //ker * opv
KernelOperatorOnUnknowns operator*(const Unknown&, const Kernel&);                    //u * ker
KernelOperatorOnUnknowns operator*(const Kernel&, const Unknown&);                    //ker * v
KernelOperatorOnUnknowns operator*(const OperatorOnUnknown&, const KernelOperatorOnUnknowns&);
    //opu * opker
KernelOperatorOnUnknowns operator*(const KernelOperatorOnUnknowns&, const OperatorOnUnknown&);
    //opker * opv
KernelOperatorOnUnknowns operator*(const Unknown&, const KernelOperatorOnUnknowns&);   //u * opker
KernelOperatorOnUnknowns operator*(const KernelOperatorOnUnknowns&, const Unknown&);   //opker * v
//same for operation inner product |, cross product ^ and contracted product %

template <typename T>
KernelOperatorOnUnknowns operator*(const Unknown& un, T(fun)(const Point&, const Point&,
    Parameters&));//u * fun
template <typename T>
KernelOperatorOnUnknowns operator*(T(fun)(const Point&, const Point&, Parameters&), const
    Unknown& un);//fun * u
template <typename T>
KernelOperatorOnUnknowns operator*(T(fun)(const Vector<Point>&,const Vector<Point>&,
    Parameters&), const Unknown& un); //fun * u
template <typename T>
KernelOperatorOnUnknowns operator*(const Unknown& un, T(fun)(const Vector<Point>&,const
    Vector<Point>&, Parameters&)) //! u * func
//same for operation inner product |, cross product ^ and contracted product %
```

It provides also accessors and print facilities

```
const OperatorOnUnknown& opu() const;
const OperatorOnUnknown& opv() const;
OperatorOnUnknown& opu();
OperatorOnUnknown& opv();
AlgebraicOperator algopu() const;
AlgebraicOperator algopv() const;
AlgebraicOperator& algopu();
AlgebraicOperator& algopv();
const OperatorOnKernel& opker() const;
bool isKernelType() const;
ValueType valueType() const;

void print(std::ostream&) const;
friend std::ostream& operator<<(std::ostream&, const KernelOperatorOnUnknowns&);
```

| | |
|---:|:---|
| library : | **operator** |
| header : | **KernelOperatorOnUnknowns.hpp** |
| implementation : | **KernelOperatorOnUnknowns.cpp** |
| unitary tests : | **test_operator.cpp** |
| header dependences : | **OperatorOnUnknown.hpp, OperatorOnKernel.hpp, config.h, utils.h** |

## 7.9 The `TensorKernel` class

TheTensorKernel class inherited from Kernel handles some particular kernels, say tensor kernels:

$$K(x,y)=\sum_{m,n}\phi_n(y)\mathbb{A}_{mn}\psi_m(x).$$

This kernel is involved in DirichletToNeumann map.

In case of complex basis functions, the TensorKernel is often involved in integral of the following form:

$$\sum_{mn} \mathbb{A}_{mn} \int_\Sigma w_j(y) * \overline{\phi}_n(y) \int_\Gamma \tau_i(x) * \psi_m(x)$$

where appears a conjugate operation on $\phi_n$ functions.
By default, computation functions do not apply the conjugate operation. So if you have to applied to, there is a flag to enforce the conjugate operation.

Because, Kernel class uses SpectralBasis class to handles functions $\phi_n$ and $\psi_n$, it can not be located in *utils* library. It is the reason why it is located in *term* library.

```
class TensorKernel : public Kernel
{
protected :
  const SpectralBasis* phi_p, *psi_p; //pointers to SpectralBasis object
  VectorEntry* matrix_p;              //matrix stored as a vector
public :
  bool isDiag;            //!< true if matrix is diagonal matrix
  Function xmap, ymap;    //!< maps applied to point x and y
  bool isConjugate;       //!< conjugate phi_p in IESP computation (default=false)
```

SpectralBasis class manages either a family of explicit functions given by a Function object or a family of interpolated functions given as a vector of TermVector (see SpectralBasisFun class and SpectralBasisInt defined in *space* library). Stored as a MatrixEntry object, the matrix $\mathbb{A}$ may be of real or complex type.
TheTensorKernel class provides some explicit constructors from SpectralBasis and vector<T> (matrix $\mathbb{A}$) and some implicit constructors from Unknown associated to a spectral space equipped with a spectral basis, and vector<T>.

```
TensorKernel();
template<typename T>
 TensorKernel(const SpectralBasis&, const std::vector<T>&, bool =false);
template<typename T>
 TensorKernel(const SpectralBasis&, const std::vector<T>&, const SpectralBasis&);
template<typename T>
 TensorKernel(const Unknown&, const std::vector<T>&, bool =false);
template<typename T>
  TensorKernel(const Unknown&, const std::vector<T>&, const Unknown&);
template<typename T>
  TensorKernel(const std::vector<TermVector>&, const std::vector<T>&, bool =false);
template<typename T>
  TensorKernel(const std::vector<TermVector>&, const std::vector<T>&, const
       std::vector<TermVector>&);
~TensorKernel();
```

Besides it provides some accessors and properties

```
const VectorEntry& vectorEntry() const {return *matrix_p;}
const SpectralBasis* phip() const {return phi_p;}
const SpectralBasis* psip() const {return psi_p;}
const SpectralBasis& phi()  const {return *phi_p;}
const SpectralBasis& psi()  const {return *psi_p;}
const TensorKernel* tensorKernel() const;
TensorKernel* tensorKernel();

Dimen dimOfPhi() const;
Dimen dimOfPsi() const;
Number nbOfPhi() const;
Number nbOfPsi() const;
bool phiIsAnalytic() const;
bool psiIsAnalytic() const;
virtual KernelType type() const;
virtual bool isSymbolic() const;
virtual ValueType valueType() const;
virtual StrucType structType() const;
bool sameBasis() const;
```

It proposes two template functions that compute the product of $\mathbb{A}_m$ or $\mathbb{A}_{mn}$ by something of type T, expecting a a result of same type!

```
template<typename T>
 T kernelProduct(Number, const T&) const;
template<typename T>
 T kernelProduct(Number, Number, const T&) const;
```

| | |
|---|---|
| library : | **operator** |
| header : | **TensorKernel.hpp** |
| implementation : | **TensorKernel.cpp** |
| unitary tests : | **test_EssentialCondition.cpp** |
| header dependences : | **space.h, config.h, utils.h** |

# 8 The *form* library

This library provides the main LinearForm and BilinearForm classes which are the fundamental user classes to describe variational formulation. Linear and bilinear forms involved in variational formulation may have multiple expressions. For the moment, the library deals with:

- Single integral form involved in standard variational formulation, say

  $$\int_D \mathscr{L}(u) \;\text{ or }\; \int_D \mathscr{L}_1(u)\, O\, \mathscr{L}_2(v)$$

  where $D$ is a geometrical domain, $u$, $v$ are unknowns or test functions, $\mathscr{L}$ are linear operators (see OperatorOnUnknown class) and $O$ is an algebraic operation.

  Canonical examples are:

  $$\int_\Omega f\,u, \;\text{ or }\; \int_\Omega A\nabla(u).\nabla(v)$$

  and for Galerkin Discontinuous approach ($S_\Omega$ the internal sides of elements of $\Omega$):

  $$\int_{S_\Omega} [u]\{v\}.$$

- Double integral form involved in integral representation or integral equation variational formulation, say

  $$\int_{D_1}\int_{D_2} K(x_1,x_2)\, O\, \mathscr{L}(u)(x_1) \;\text{ or }\; \int_{D_1}\int_{D_2} K(x_1,x_2)\, O\, \mathscr{L}(u)(x_1)\, O\, \mathscr{L}(v)(x_2)$$

  where $D_1$ and $D_2$ are geometrical domains, $u$, $v$ are unknowns or test functions, $\mathscr{L}$ are linear operators and $K(x_1,x_2)$ is a kernel function.

Besides, it should be friendly to deal with multiple unknowns formulation. For instance the formulation of Stokes problem involves the pressure and the velocity as unknowns. Thus, linear (resp. bilinear) forms taken into account are lists of linear combination of basic linear (resp. bilinear) forms. A basic linear (resp. bilinear) form is a simple or a double integral of an operator acting on unknown (resp. a "product" of operators acting on unknown), see the OperatorOnUnknown class. Only basic linear (resp. bilinear) forms having the same unknown (resp. couple of unknowns) may be combined in a linear combination. On the other hand, lists of linear combination of basic linear (resp. bilinear) forms may be algebraically combined, combination being done on each unknown (resp. couple of unknowns) separately. A multiple unknowns linear form may be seen as a vector of linear form indexed by unknown and a multiple unknowns bilinear form may be seen as a matrix of linear form indexed by a couple of unknowns. In this way, a single unknown linear form is a vector of size one and a "single" unknown bilinear form is a matrix one by one.

To intend to this organisation, the following classes are provided:

BasicLinearForm **(resp.** BasicBilinearForm**)** class is the abstract base class of basic linear (resp. bilinear) form,

IntgLinearForm **(resp.** IntgBilinearForm**)** class inherits from BasicLinearForm (resp. BasicBilinearForm) and deals with forms defined with an integral on a geometrical domain,

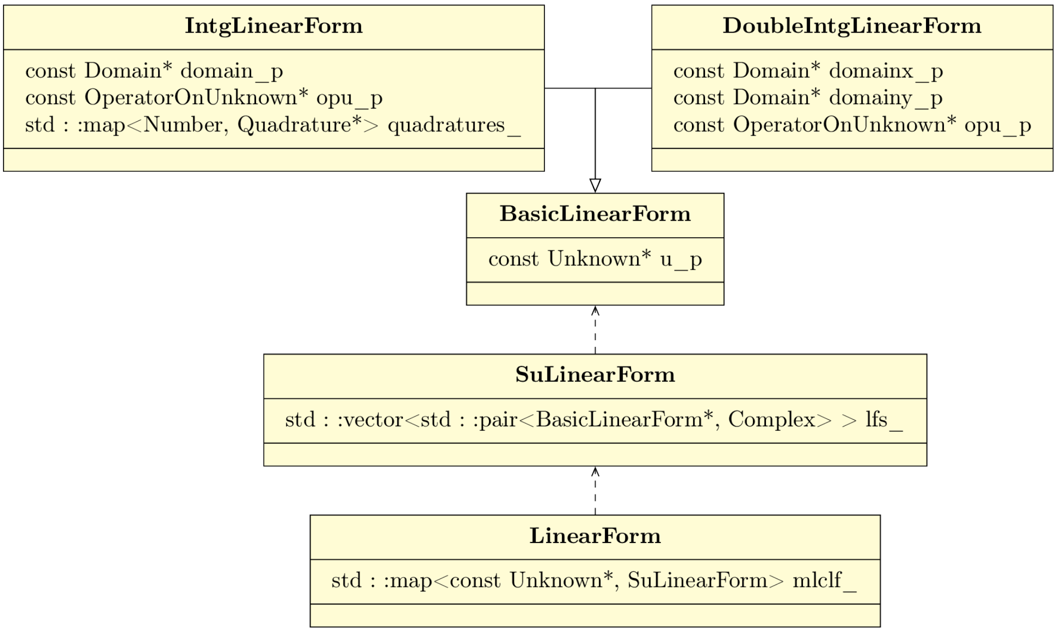
`DoubleIntgLinearForm` **(resp.** `DoubleIntgBilinearForm`**)** class inherits from `BasicLinearForm` (resp. `BasicBilinear`
and deals with forms defined with an integral on a product of geometrical domains (double integral). Such integrals are involved in integral equation formulation,

`UserBilinearForm` class inherits from `BasicBilinearForm` and manages bilinear forms defined from a user function building elementary matrices. Because of the low-level programming and the management of internal classes of XLIFE++, this approach is reserved for advanced users.

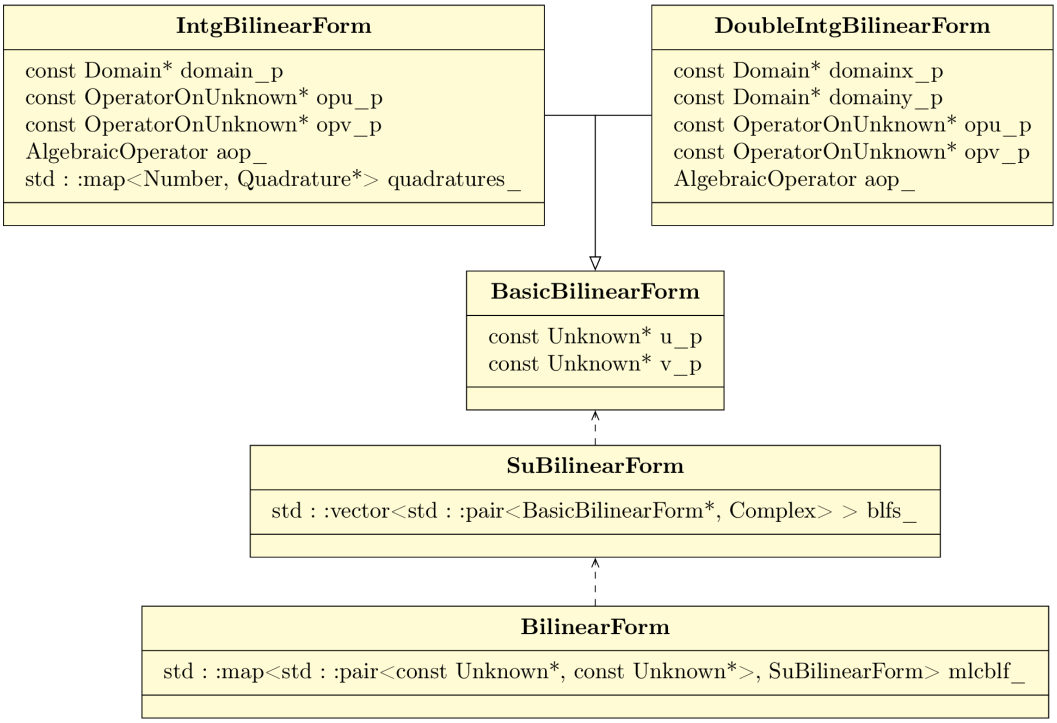
`LcLinearForm` **(resp.** `LcBilinearForm`**)** class stores a linear combination of `BasicLinearForm` (resp. `BasicBilinear`
objects having same unknown (resp. couple of unknowns),

`LinearForm` **(resp.** `BilinearForm`**)** class stores a list of `LcLinearForm` (resp. `LcBilinearForm`) objects using map indexed by unknown (resp. couple of unknowns).

The organisation of linear forms looks like:


IntgLinearForm
const Domain* domain_p
const OperatorOnUnknown* opu_p
std : :map<Number, Quadrature*> quadratures_
DoubleIntgLinearForm
const Domain* domainx_p
const Domain* domainy_p
const OperatorOnUnknown* opu_p
BasicLinearForm
const Unknown* u_p
SuLinearForm
std : :vector<std : :pair<BasicLinearForm*, Complex> > lfs_
LinearForm
std : :map<const Unknown*, SuLinearForm> mlclf_

and the organisation of bilinear forms is similar:


IntgBilinearForm
const Domain* domain_p
const OperatorOnUnknown* opu_p
const OperatorOnUnknown* opv_p
AlgebraicOperator aop_
std : :map<Number, Quadrature*> quadratures_
DoubleIntgBilinearForm
const Domain* domainx_p
const Domain* domainy_p
const OperatorOnUnknown* opu_p
const OperatorOnUnknown* opv_p
AlgebraicOperator aop_
BasicBilinearForm
const Unknown* u_p
const Unknown* v_p
SuBilinearForm
std : :vector<std : :pair<BasicBilinearForm*, Complex> > blfs_
BilinearForm
std : :map<std : :pair<const Unknown*, const Unknown*>, SuBilinearForm> mlcblf_

## 8.1 Linear forms

Linear forms are managed using

- BasicLinearForm abstract class of basic linear form,
- IntgLinearForm class inheriting from BasicLinearForm and dealing with integral form,
- DoubleIntgLinearForm class inheriting from BasicLinearForm and dealing with double integral forms,
- SuLinearForm class storing linear combination of BasicLinearForm objects having the same unknown,
- LinearForm class storing a list of SuLinearForm objects using a map indexed by unknown.

### 8.1.1 The BasicLinearForm class

The BasicLinearForm class is an abstract class having only an unknown as attribute and its associated accessor:

```
class BasicLinearForm
{protected:
   const Unknown* u_p;           //pointer to unknown
 public :
   const Unknown& up() const     //return the unknown
```

The child classes inheriting from BasicLinearForm have to provide the following member functions:

```
virtual ~BasicLinearForm(){};                  //virtual destructor
virtual BasicLinearForm* clone() const =0;  //clone of the linear form
virtual LinearFormType type() const =0;       //return the type of the linear form
virtual ValueType valueType() const=0;        //return the value type of the linear form
virtual void print(std::ostream&) const =0;//print utility
```

The virtual clone function is used to construct a copy of the child objects from parent.

### 8.1.2 The IntgLinearForm class

The IntgLinearForm class handles linear forms defined by a (single) integral over a geometric domain:

$$\int_D \mathscr{L}(u)$$

where $D$ is a geometric domain (Domain class) and $\mathscr{L}$ a linear operator (OperatorOnUnknown class) acting on unknown $u$ (Unknownn class).
This class is defined as follows:

```
class IntgLinearForm : public BasicLinearForm
{protected :
 const GeomDomain* domain_p; //geometric domain of the integral (pointer)
 const OperatorOnUnknown* opu_p; //operator on unknown (pointer)
```

It has some public constructors and some public accessors:

```
IntgLinearForm(const GeomDomain&,const OperatorOnUnknown&);
const OperatorOnUnknown* opu() const;
const GeomDomain* domain() const;
virtual BasicLinearForm* clone() const;
virtual LinearFormType type() const
virtual ValueType valueType() const
virtual void print(std::ostream&) const;
```

### 8.1.3 The DoubleIntgLinearForm class

The DoubleIntgLinearForm class handles linear forms defined by a double integral over a product of geometric domains:

$$\int_{D_x}\int_{D_y} \mathscr{L}(u)$$

where $D_x$, $D_y$ are geometric domain (GeomDomain class) and $\mathscr{L}$ a linear operator (OperatorOnUnknown class) acting on unknown $u$ (Unknown class).
Except, there are two geometric domains, this class is very similar to the IntgLinearForm class:

```
class DoubleIntgLinearForm : public BasicLinearForm
{protected :
 const OperatorOnUnknown* opu_p;  // operator on unknown (pointer)
 const GeomDomain* domainx_p; // first geometric domain (say x variable)
 const GeomDomain* domainy_p; // second geometric domain (say y variable)
```

It provides some public constructors and some public accessors:

```
DoubleIntgLinearForm(const GeomDomain&, const GeomDomain&,const OperatorOnUnknown&);
const OperatorOnUnknown* opu() const;
const GeomDomain* domainx() const;
const GeomDomain* domainy() const;
virtual BasicLinearForm* clone() const;
virtual LinearFormType type() const;
virtual ValueType valueType() const;
virtual void print(std::ostream&)const;
```

### 8.1.4 The SuLinearForm class

BasicLinearForm objects may be lineary combined to produce a linear combination of BasicLinearForm objects stored as a list of pair of BasicLinearForm object and a complex scalar in the SuLinearForm class.

```
typedef std::pair<BasicLinearForm*,complex_t> lfPair;
class SuLinearForm
{protected:
   std::vector<lfPair> lfs_; //list of pairs of basic linear form and coefficient
   ...
```

All theBasicLinearForm objects must have the same unknown ! It is the reason why this class has no pointer to an unknown; it refers to the first basic linear form to get its unknown.

Because BasicLinearForm objects are copied for safety reason, this class provides default and basic constructors but also a copy constructor, a destructor and the overload assignment operator:

```
SuLinearForm(){};
SuLinearForm(const SuLinearForm&);
~SuLinearForm();
SuLinearForm& operator=(const SuLinearForm&);
```

It provides few accessors (some being const and no const):

```
number_t size() const;
std::vector<lfPair>& lfs();
const std::vector<lfPair>& lfs() const;
lfPair& operator()(number_t n);
const lfPair& operator()(number_t n) const;
const Unknown* unknown() const;
const Space* space() const;
LinearFormType type() const;
ValueType valueType() const;
```

It is possible to perform linear combination of linear combinations using the following overloaded operators:

```
SuLinearForm& SuLinearForm::operator +=(const SuLinearForm&);
SuLinearForm& SuLinearForm::operator -=(const SuLinearForm&);
SuLinearForm& SuLinearForm::operator *=(const complex_t&);
SuLinearForm& SuLinearForm::operator /=(const complex_t&);
SuLinearForm operator-(const SuLinearForm&);
SuLinearForm operator+(const SuLinearForm&,const SuLinearForm&);
SuLinearForm operator-(const SuLinearForm&,const SuLinearForm&);
SuLinearForm operator*(const complex_t&,const SuLinearForm&);
SuLinearForm operator*(const SuLinearForm&,const complex_t&);
SuLinearForm operator/(const SuLinearForm&,const complex_t&);
bool SuLinearForm::checkConsistancy(const SuLinearForm&) const;
```

The member function checkConsistancy performs a test to insure that unknown is always the same.

Finally, there are some print facilities:

```
void SuLinearForm::print(std::ostream&)const;
std::ostream& operator<<(std::ostream&,const SuLinearForm&);
```

### 8.1.5 The LinearForm class

The LinearForm class is the end user class dealing with general linear form, either a single unknown linear form (a SuLinearForm object) or a multiple unknown linear form (a list of SuLinearForm objects). In this class, a single unknown linear form is a multiple unknown linear form with one unknown! The list of SuLinearForm objects is stored in a map of SuLinearForm, indexed by the pointer to SuLinearForm unknown:

```
class LinearForm
{protected :
 std::map<const Unknown *,SuLinearForm> mlclf_;  //list of linear combinations of basic forms
 ...
```

To manage the map, the following aliases are defined:

```
typedef std::map<const Unknown *,SuLinearForm>::iterator it_mulc;
typedef std::map<const Unknown *,SuLinearForm>::const_iterator cit_mulc;
```

When the SuLinearForm unknown is an unknown component, the SuLinearForm object is attached to its parent item! In other words, a component unknown is not indexed in the map.

This class provides only one constructor from a linear combination of forms:

```
LinearForm(const SuLinearForm&);
```

and proposes some accessors and facilities:

```
bool isEmpty() const;
bool singleUnknown() const;
SuLinearForm& operator[](const Unknown*);                //protected
const SuLinearForm& operator[](const Unknown*) const; //protected
const SuLinearForm& first() const;
LinearForm operator()(const Unknown&) const;
BasicLinearForm& operator()(const Unknown&,number_t);
const BasicLinearForm& operator()(const Unknown&,number_t) const;
```

Besides, there are three fundamental external end user's function (intg) which constructs LinearForm object:

```
LinearForm intg(const GeomDomain&,const LcOperatorOnUnknown&);
LinearForm intg(const GeomDomain&,const OperatorOnUnknown&);
LinearForm intg(const GeomDomain&,const Unknown&);
LinearForm intg(const GeomDomain&,const GeomDomain&,const OperatorOnUnknown&);
LinearForm intg(const GeomDomain&,const GeomDomain&,const Unknown&);
```

In order to construct any linear forms, the algebraic operators (+= -= *= /= + - * /) are oveloaded for different objects:

```
LinearForm& LinearForm::operator +=(const LinearForm&);
LinearForm& LinearForm::operator -=(const LinearForm&);
LinearForm& LinearForm::operator *=(const complex_t&);
LinearForm& LinearForm::operator /=(const complex_t&);
LinearForm operator+(const LinearForm&,const LinearForm&);
LinearForm operator-(const LinearForm&,const LinearForm&);
LinearForm operator*(const complex_t&,const LinearForm&);
LinearForm operator*(const LinearForm&,const complex_t&);
LinearForm operator/(const LinearForm&,const complex_t&);
```

Finally, the class provides usual print facilities:

```
void LinearForm::print(std::ostream&)const;
std::ostream& operator<<(std::ostream&,const LinearForm&);
```

### Example

To end we show some characteristic examples. In these examples, u is a scalar unknown, w is a vector unknown, f either a scalar or a scalar function, h either a vector or a vector function, g a scalar or a scalar kernel and Omega,Gamma Sigma some geometric domains.

```
LinearForm l1=intg(Omega, f*u);
l1+=intg(Omega,h|grad(u));
l1=intg(Omega, f*u)+intg(Omega,h|grad(u));    //equivalent
l1=l1-2*intg(Gamma,Sigma,g*u);
LinearForm l2=intg(Omega, f*div(w))+intg(Gamma,h|(w^n));
LinearForm l3=l1+l2;         //multiple unknowns
l3=intg(Omega, f*u)+intg(Omega, f*div(w))+intg(Omega,h|grad(u))
  +2*intg(Gamma,Sigma,g*u)+intg(Gamma,h|(w^n));    //same result
```

| | |
|---|---|
| library : | **form** |
| header : | **LinearForm.hpp** |
| implementation : | **LinearForm.cpp** |
| unitary tests : | **test_form.cpp** |
| header dependences : | **config.h, utils.h** |

## 8.2 Bilinear forms

Bilinear forms are managed using

- BasicBilinearForm abstract class of basic linear form,
- IntgBilinearForm class inheriting from BasicBilinearForm and dealing with integral form,
- DoubleIntgBilinearForm class inheriting from BasicBilinearForm and dealing with double integral forms,
- UserBilinearForm class inheriting from BasicBilinearForm and dealing with bilinear forms defined from a user function building elementary matrices,
- SuBilinearForm class storing linear combination of BasicBilinearForm objects having the same unknown,
- BilinearForm class storing a list of SuBilinearForm objects using a map indexed by unknowns.

### 8.2.1 The BasicBilinearForm class

The BasicBilinearForm class is an abstract class having only the unknowns as attribute and their associated accessors:

```
class BasicBilinearForm
{protected:
   const Unknown* u_p;             //pointer to unknown u
   const Unknown* v_p;             //pointer to unknown v (test function)
 public :
   const Unknown& up() const;
   const Unknown& vp() const;
   ...
```

The ’u’ letter refers always to the left unknown of the bilinear form and the ’v’ letter to the right unknown (test function) of the bilinear form. In matrix representation ’u’ stands for columns and ’v’ for rows.

The child classes inheriting from BasicBilinearForm have to provide the following member functions:

```
virtual ~BasicBilinearForm() {};
virtual BasicBilinearForm* clone() const =0;
virtual LinearFormType type() const =0;
virtual ValueType valueType() const=0;
virtual void print(std::ostream&) const =0;
```

The virtual clone() function is used to construct a copy of the child objects from parent.

### 8.2.2 The IntgBilinearForm class

The IntgBilinearForm class handles linear forms defined by a (single) integral over a geometric domain:

$$\int_D \mathscr{L}_1(u) op \mathscr{L}_2(v)$$

where $D$ is a geometric domain (Domain class) and $\mathscr{L}_1$, $\mathscr{L}_2$ are linear operators (OperatorOnUnknown class) acting on unknowns $u$ and $v$ (Unknown class) and $op$ is an algebraic product operator. In case of mesh domain, it handles also the quadrature rules, one rule by shape of elements.
This class is defined as follows:

```
class IntgBilinearForm : public BasicBilinearForm
{protected :
 const GeomDomain* domain_p; //geometric domain of the integral (pointer)
 const OperatorOnUnknown* opu_p; //operator on unknown u (pointer)
 const OperatorOnUnknown* opv_p; //operator on unknown v (pointer)
 AlgebraicOperator aop_;         //algebraic operation between operators
 map<Number, Quadrature*> quadratures_; //!< pointers to quadrature rules
 ...
```

Note that the quadratures_ map may be empty. This, is the case when the domain is not of type mesh domain. Generally, the elements of a mesh domain have the same shape but it may not. It is the reason why a map is used to store the quadratures .

It has one basic constructor, some public accessors and utilities:

```
IntgBilinearForm(const GeomDomain&,const OperatorOnUnknown&, AlgebraicOperator,
                 const OperatorOnUnknown&, QuadRule = _defaultRule, Number =0)
const OperatorOnUnknown* opu() const;
const OperatorOnUnknown* opv() const;
const GeomDomain* domain() const;
virtual BasicBilinearForm* clone() const;
virtual LinearFormType type() const
virtual ValueType valueType() const
void setQuadrature(QuadRule , Number);
virtual void print(std::ostream&) const;
```

The setQuadrature function set the quadrature pointers from a QuadRule (enumeration of type of quadrature rule) and a quadrature number (degree or order of quadrature rule). For a full description of quadrature rules see section 5.6.2. When QuadRule is set to _defaultRule in constructor, the ’best’ rule is chosen regarding the shape element and the degree of integrand (see Quadrature::bestQuadRule function).

### 8.2.3 The DoubleIntgBilinearForm class

The DoubleIntgBilinearForm class handles linear forms defined by a double integral over a product of geometric domains:

$$\int_{D_x}\int_{D_y}\mathscr{L}(u)$$

where $D_x$, $D_y$ are geometric domain (GeomDomain class) and $\mathscr{L}$ a linear operator (OperatorOnUnknown class) acting on unknown $u$ (Unknownn class).
Except, there are two geometric domains, this class is very similar to the IntgBilinearForm class:

```
class DoubleIntgBilinearForm : public BasicBilinearForm
{protected :
 const GeomDomain* domainx_p;      //first geometric domain (say x variable)
 const GeomDomain* domainy_p;      //second geometric domain (say y variable)
 const OperatorOnUnknown* opu_p; //operator on unknown u (pointer)
 const OperatorOnUnknown* opv_p; //operator on unknown v (pointer)
 ...
```

It provides a basic constructor and some public accessors:

```
DoubleIntgBilinearForm(const GeomDomain&,const GeomDomain&,const OperatorOnUnknown&,
                       AlgebraicOperator,const OperatorOnUnknown&);
const OperatorOnUnknown* opu() const;
const OperatorOnUnknown* opv() const;
const GeomDomain* domainx() const;
const GeomDomain* domainy() const;
virtual BasicBilinearForm* clone() const;
virtual LinearFormType type() const;
virtual ValueType valueType() const;
virtual void print(std::ostream&)const;
```

Be cautious in the definition of double integral. The syntax:

```
BilinearForm a=intg(Sigma, Gamma ,u*G*v);
```

has to be interpreted as

$$\int_{\Sigma_x}\int_{\Gamma_y} u(y)G(x,y)v(x)\,dy\,dx$$

where $u$ (the right unknown) stands for the unknown, $v$ (the left unknown) being the test function. In matrix representation, it means that $u$ stands for columns and $v$ for rows.

### 8.2.4 The UserBilinearForm class

The UserBilinearForm class allows users to define general bilinear form. It is based on a BlfFunction providing the computation of elementary matrices. This function has always the following signature:

```
void blfun(BlfDataComputation& blfd);
```

where the BlfDataComputation class encapsulates some useful data updated by computation algorithms:

```
class BlfDataComputation
{ public :
  const Element* elt_u, *elt_v;        // Element pointers (FEM or BEM)
  const Element* elt_u2,*elt_v2;       // additional Element pointers (DG)
  const GeomElement* sidelt;           // side element when DG
  vector<Matrix<real_t>> matels;       // real elementary matrices
  vector<Matrix<complex_t>> cmatels;   // complex elementary matrices
  ...
```

Regarding their own business, users have to fill either real elementary matrices (`matels`) or complex elementary matrices (`cmatels`) from element data (`elt_u`, `elt_v`, ...).

> Up to now, only FEM and DG computation algorithms manage `UserBilinearForm`.

So, the `UserBilinearForm` class handles the following data:

```
class UserBilinearForm : public BasicBilinearForm
{ public :
  BlfFunction blfun_;                        // pointer to an extern blf function (0 by default)
  const IntegrationMethod* intgMethod_p;     // pointer to an integration method
  bool requireInvJacobian_;                  // requiring jacobian  (default=false)
  bool requireNormal_;                       // requiring normal vector (default=false)
```

This class provides two general constructors and a copy constructor:

```
UserBilinearForm(const GeomDomain& dom, const Unknown& u, const Unknown& v, BlfFunction blf,
  ComputationType ct,SymType st,bool rij,bool rno,const IntegrationMethod& im);
UserBilinearForm(const GeomDomain& domv,const GeomDomain& domu,const Unknown& u,const Unknown& v,
  BlfFunction blf,ComputationType ct,SymType st,bool rij,bool rno,const IntegrationMethod& im);
UserBilinearForm(const UserBilinearForm&);
BasicBilinearForm* clone() const;      // clone of the UserBilinearForm
~UserBilinearForm();
```

In practice, it is advised to use external pseudo-constructors with some default arguments :

```
BilinearForm userBlf(const GeomDomain& g, const Unknown& u, const Unknown& v, BlfFunction blf,
             ComputationType ct, SymType=_noSymmetry, bool reqIJ=false, bool reqN=false,
             const IntegrationMethod& im=QuadratureIM(_GaussLegendreRule,3));
BilinearForm userBlf(const GeomDomain& g, const GeomDomain&, const Unknown& u, const Unknown& v,
             BlfFunction blf, ComputationType ct, SymType=_noSymmetry, bool reqIJ=false,
             bool reqN=false, const IntegrationMethod& im=QuadratureIM(_GaussLegendreRule,3));
```

Besides some useful tools are provided:

```
LinearFormType type() const;                  // return the type of the linear form (_userLf)
const IntegrationMethod* intgMethod() const;  // pointer to the integration method object
ValueType valueType() const;                  // return the value type
void requireInvJacobian(bool tf=true);        // set on/off the requireInvJacobian flag
void requireNormal(bool tf=true);             // set on/off the requireNormal flag
SymType setSymType() const ;                  // set the symmetry property (done by analysis)
void print(std::ostream&) const;              // print utility
void print(PrintStream& os) const;            // print utility
string_t asString() const;                    // interpret as string for print purpose
```

The next simple example shows how to deal with `UserBilinearForm`. It deals with the $\int_\Omega \nabla u.\nabla v$ bilinear form that can be handled by standard approach:

```
//compute elementary matrix grad.grad in 2D-P1
void blfGradGrad(BlfDataComputation& blfd)
{ if(blfd.matel().size()==0) blfd.matel() = Matrix<Real>(3,3);
  const Element* elt=blfd.elt_u;    //get element concerned by
  if(elt==0) return;                //no computation
  GeomMapData& mapdata = *elt->geomElt_p->meshElement()->geomMapData_p; //get geometric data
  Matrix<Real> C=(0.5*mapdata.differentialElement)*mapdata.inverseJacobianMatrix
                *tran(mapdata.inverseJacobianMatrix);
  Matrix<Real> G(2,3,0.);G(1,1)=1;G(2,2)=1;G(1,3)=-1;G(2,3)=-1; //gradient in ref element
  blfd.matel()=tran(G)*C*G;   //elementary matrix
}
...
Mesh ms(Rectangle(_xmin=0.,_xmax=1., _ymin=0., _ymax=1.,_nnodes=10,_domain_name="Omega"),
        _triangle, 1,_structured,_alternateSplit);
Domain omega=ms.domain("Omega");
```

```
Space H(omega, Lagrange, 1, "H"); Unknown p(H,"p"); TestFunction t(p,"t");
BilinearForm ublf =
       userBlf(omega,p,t,blfGradGrad,_FEComputation,_symmetric, true, false); // define user blf
TermMatrix Ku(ublf,"Ku"); // use it as usual
```

See the *unit_DG.cpp* file for a more complex example which deals with the discontinuous Galerkin term:

$$\int_\Gamma \{\nabla_h u_h . n\}[v]$$

### 8.2.5 The SuBilinearForm class

BasicBilinearForm objects may be lineary combined to produce a linear combination of BasicBilinearForm objects stored as a list of pair of BasicBilinearForm object and a complex scalar in the SuBilinearForm class.

```
typedef std::pair<BasicBilinearForm*,complex_t> blfPair;
class SuBilinearForm
{protected:
   std::vector<blfPair> blfs_; //list of pairs of basic bilinear form and coefficient
   ...
```

All the BasicBilinearForm objects must have the same pair of unknowns ! It is the reason why this class has no pointer to unknowns; it refers to the first basic bilinear form to get its unknowns.

Because BasicBilinearForm objects are copied for safety reason, this class provides default and basic constructors but also a copy constructor, a destructor and the overload assignment operator:

```
SuBilinearForm() {};
SuBilinearForm(const SuBilinearForm&);
~SuBilinearForm();
SuBilinearForm& operator=(const SuBilinearForm&);
```

It provides few accessors (some being const and no const):

```
number_t size() const;
std::vector<blfPair>& blfs();
const std::vector<blfPair>& blfs() const;
blfPair& operator()(number_t n);
const blfPair& operator()(number_t n) const;
const Unknown* up() const;
const Unknown* vp() const;
const Space* uSpace() const;
const Space* vSpace() const;
LinearFormType type() const;
ValueType valueType() const;
```

It is possible to perform linear combination of linear combinations using the following overloaded operators:

```
SuBilinearForm& SuBilinearForm::operator +=(const SuBilinearForm&);
SuBilinearForm& SuBilinearForm::operator -=(const SuBilinearForm&);
SuBilinearForm& SuBilinearForm::operator *=(const complex_t&);
SuBilinearForm& SuBilinearForm::operator /=(const complex_t&);
SuBilinearForm operator-(const SuBilinearForm&);
SuBilinearForm operator+(const SuBilinearForm&,const SuBilinearForm&);
SuBilinearForm operator-(const SuBilinearForm&,const SuBilinearForm&);
SuBilinearForm operator*(const complex_t&,const SuBilinearForm&);
SuBilinearForm operator*(const SuBilinearForm&,const complex_t&);
SuBilinearForm operator/(const SuBilinearForm&,const complex_t&);
bool SuBilinearForm::checkConsistancy(const SuBilinearForm&) const;
```

The member function `checkConsistancy` performs a test to insure that pair of unknowns is always the same.

Finally, there are some print facilities:

```
void SuBilinearForm::print(std::ostream&)const;
std::ostream& operator<<(std::ostream&,const SuBilinearForm&);
```

### 8.2.6 The `BilinearForm` class

The `BilinearForm` class is the end user class dealing with general bilinear form, either a single unknown bilinear form (a `SuBilinearForm` object) or a multiple unknown bilinear form (a list of `SuBilinearForm` objects). In this class, a single unknown bilinear form is a multiple unknown blinear form with one pair of unknowns! The list of `SuBilinearForm` objects is stored in a map of `SuBilinearForm`, indexed by a pair of pointers to unknown :

```
typedef std::pair<const Unknown *,const Unknown *> uvPair;

class BilinearForm
{protected :
 std::map<uvPair,SuBilinearForm> mlcblf_;  //list of linear combinations of basic forms
 ...
```

To manage the map, the following aliases are defined:

```
typedef std::map<uvPair,SuBilinearForm>::iterator it_mublc;
typedef std::map<uvPair,SuBilinearForm>::const_iterator cit_mublc;
```

When the `SuBilinearForm` unknowns owns an unknown component, the `SuBilinearForm` object is attached to its parent item! In other words, component unknowns are not indexed in the map.

This class provides only one constructor from a linear combination of forms:

```
BilinearForm(const SuBilinearForm&);
```

and proposes some accessors and facilities:

```
bool singleUnknown() const;
bool isEmpty() const;
SuBilinearForm& operator[](const uvPair&);                 //protected
const SuBilinearForm& operator[](const uvPair&) const;  //protected
const SuBilinearForm& first() const;
BilinearForm operator()(const Unknown&,const Unknown&) const;
BasicBilinearForm& operator()(const Unknown&,const Unknown&,number_t);
const BasicBilinearForm& operator()(const Unknown&,const Unknown&,number_t) const;
```

Besides, there are trhee fundamental external enduser's function (`intg` and `intg_intg`) which constructs `BilinearForm` object:

```
BilinearForm intg(const GeomDomain&,const OperatorOnUnknown&,
                  AlgebraicOperator,const OperatorOnUnknown&);
BilinearForm intg(const GeomDomain&,const OperatorOnUnknowns&);
BilinearForm intg(const GeomDomain&,const LcOperatorOnUnknowns&);
BilinearForm intg(const GeomDomain&,const GeomDomain&,
                       const OperatorOnUnknown&,AlgebraicOperator,
                          const OperatorOnUnknown&);
BilinearForm intg(const GeomDomain&,const GeomDomain&,const OperatorOnUnknowns&);
```

`OperatorUnknows` is a simple class used to store the two operators and the algebraic operation.

In order to construct any linear forms, the algebraic operators (`+= -= *= /= + - * /`) are oveloaded for different objects:

```
BilinearForm& BilinearForm::operator +=(const BilinearForm&);
BilinearForm& BilinearForm::operator -=(const BilinearForm&);
BilinearForm& BilinearForm::operator *=(const complex_t&);
BilinearForm& BilinearForm::operator /=(const complex_t&);
BilinearForm operator+(const BilinearForm&,const BilinearForm&);
BilinearForm operator-(const BilinearForm&,const BilinearForm&);
BilinearForm operator*(const complex_t&,const BilinearForm&);
BilinearForm operator*(const BilinearForm&,const complex_t&);
BilinearForm operator/(const BilinearForm&,const complex_t&);
```

Finally, the class provides usual print facilities:

```
void BilinearForm::print(std::ostream&)const;
std::ostream& operator<<(std::ostream&,const BilinearForm&);
```

## Example

To end we show some characteristic examples. In these examples, `u`,`v` are scalar unknowns, `p`, `q` are vector unknowns, `f` either a scalar or a scalar function, `h` either a vector or a vector function, `g` a scalar or a scalar kernel and `Omega`,`Gamma Sigma` some geometric domains.

```
BilinearForm a1=intg(Omega,grad(u)|grad(v));
a1-=k2*intg(Omega,f*u*v);
a1=intg(Omega,grad(u)|grad(v))-intg(Omega,f*u*v);    //same result
BilinearForm a2=intg(Omega,div(p)*q)+eps*intg(Omega,p*q);
BilinearForm a3=a1+a2;
a3=intg(Omega,grad(u)|grad(v))+intg(Omega,div(p)*q)  //same result
  -intg(Omega,f*u*v)+eps*intg(Gamma,p*q);
```

| | |
|---|---|
| library : | **form** |
| header : | **BilinearForm.hpp** |
| implementation : | **BilinearForm.cpp** |
| unitary tests : | **test_form.cpp** |
| header dependences : | **config.h, utils.h** |

# 9 The *largeMatrix* library

The *largeMatrix* library deals with large matrices stored in different ways : dense storages (all the matrix values are stored), skyline storages (values on a row or a column are stored from the first non zero values) and compressed sparse storage (only non zero values are stored). For each of these storages, different "access" methods, driving how the matrix values are stored, are proposed : by rows, by columns, by rows and columns (say dual access) and symmetric access which is like dual access but with same row and column access. The symmetric access is well suited for matrices having symmetry property (symmetric, skew-symmetric, self-adjoint or skew-adjoint), or matrix with symmetric storage property, currently met in finite element approximation. Note that the row dense storage corresponds to the storage used by the `Matrix` class defined in the *utils*. As other access methods may be useful in finite element methods, it is the reason why the *largeMatrix* library provides dense storages.
Large matrices under consideration may be real or complex value matrices, but also matrices of real/complex matrices. This last case allows to deal with vector variational problems where the unknown and test function are vector functions, using the same storage structure as in the scalar case.

More precisely, the *largeMatrix* library is based on the template class `LargeMatrix<T>` which mainly handles a vector to store the matrix values and a pointer to a storage describing how the matrix values are stored. Different storage structures are organized in a hierarchy of classes, terminal classes carrying specific data and methods of storages, in particular the product of a matrix and a vector.

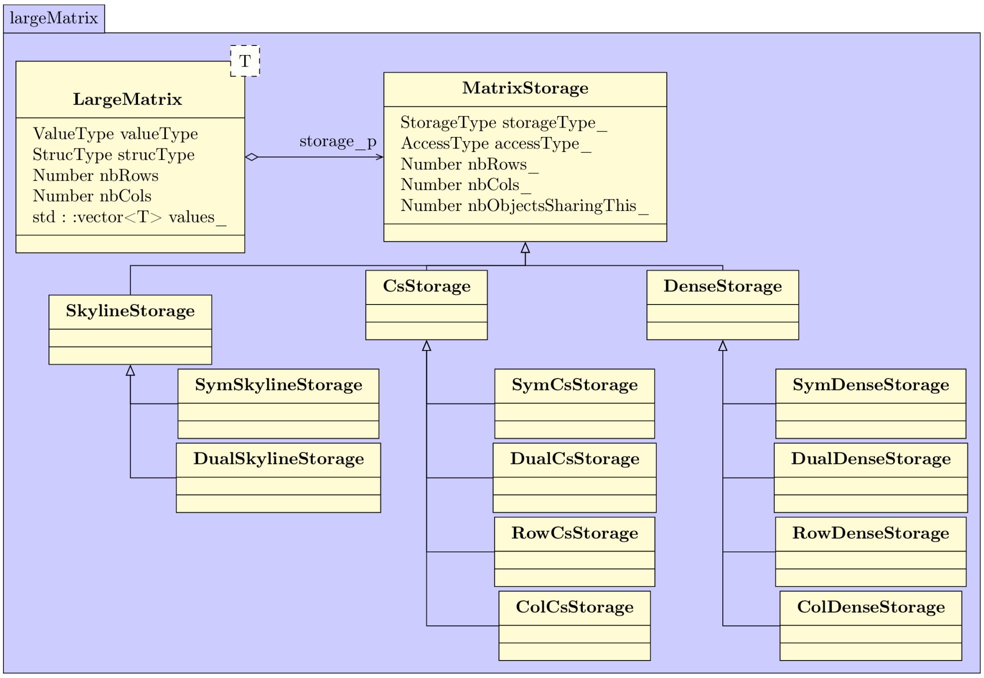


Figure 9.1: The *largeMatrix* library main class diagram

## 9.1 The LargeMatrix class

The LargeMatrix class deals with large matrices with different type of storages. It is a template class LargeMatrix<T> where T is either the type Real, Complex, Matrix<Real> or Matrix<Complex>. Although it is possible to instantiate LargeMatrix<T> with other types, most of functionalities do not work because some member functions are overloaded only for the previous types.

The class mainly manages a vector storing the matrix values and a pointer to a storage structure (MatrixStorage base class):

```
template <typename T>
class LargeMatrix{
public :
  ValueType valueType;      // type of values (real, complex)
  StrucType strucType;      // struc of values (scalar, matrix)
  Number nbRows;            // number of rows counted in T
  Number nbCols;            // number of columns counted in T
  SymType sym;              // type of symmetry
  Dimen nbRowsSub;          // number of rows of submatrices (1 if scalar values)
  Dimen nbColsSub;          // number of columns of submatrices (1 if scalar values)
  String name;              // optionnal name, useful for documentation
protected :
  vector<T> values_;    // list of values ordered along storage method
  MatrixStorage* storage_p; // pointer to the matrix storage
   ...
```

When T=Matrix<Real> or T=Matrix<Complex>, the number of rows and columns are counted in Matrix not in scalar!

The first value (index 0) of the vector values_ is not used for storing a matrix value. It contains the default value (in general T()) returned when trying to access to a matrix value outside the storage. Be care with default Matrix<T>(), its a 0 × 0 matrix!

There are various constructors : three from a existing storage, some from file where the large matrix is loaded from the file and some from matrix dimensions and a default value. A large matrix which is created by the copy constructor (shallow copy) will share a same storage with the input one. Be care with these last constructors, they allocate the vector of values only for dense storage.

```
LargeMatrix();
LargeMatrix(const LargeMatrix<T>&);
LargeMatrix(MatrixStorage*, const T&= T(), SymType= _noSymmetry);
LargeMatrix(MatrixStorage* ms, dimPair dims, SymType sy = _noSymmetry);
LargeMatrix(MatrixStorage*, SymType);
LargeMatrix(Number, Number, StorageType = _dense, AccessType = _row, const T& = T());
LargeMatrix(Number, Number, StorageType = _dense, SymType = _symmetric, const T& = T());
LargeMatrix(const String&, StorageType, Number , Number, StorageType = _dense,
            AccessType = _row,  Number nsr=1, Number nsc=1);
LargeMatrix(const String&, StorageType, Number, StorageType = _dense,
            SymType = _symmetric,  Number nsr=1);
 ~LargeMatrix();

void init(MatrixStorage*, const T&, SymType);
void allocateStorage(StorageType, AccessType, const T& = T());
void setType(const T&);
```

The StorageType, AccessType and SymType are enumerations :

```
enum StorageType{_noStorage=0,_dense,_cs,_skyline,_coo};
enum AccessType {_noAccess=0,_sym,_row,_col,_dual};
enum SymType     {_noSymmetry=0,_symmetric,_skewSymmetric,_selfAdjoint,_skewAdjoint,
                  _diagonal};
```

The storage type _cs means compressed sparse. It refers to the well known CSR/CSC storage (see the next section for details on storage). The storage type _coo means coordinates storage $(i, j, a_{ij})$. So far, it is not proposed as a storage method for large matrix but large matrix may be saved to file in this format. Constructors use the utilities: init, allocateStorage and setType. The SetType function uses some utilities (external functions) to get the dimensions of sub-matrices:

```
pair<Dimen,Dimen> dimsOf(const Real&);
pair<Dimen,Dimen> dimsOf(const Complex&);
pair<Dimen,Dimen> dimsOf(const Matrix<Real>&);
pair<Dimen,Dimen> dimsOf(const Matrix<Complex>&);
bool isDiagonal() const;
bool isId(const double & tol=0.) const;
```

Note that for the moment, it is not possible to load from a file a matrix as a matrix of matrices (use only nsr=1 and nsc=1 arguments in constructors from file).

There are few facilities to access to matrix values :

```
Number pos(Number i, Number j) const;
void positions(const vector<number_t>&, const vector<number_t>&,
               vector<number_t>&, bool = false) const;
vector<pair<number_t, number_t>> getCol(number_t, number_t =1, number_t=0) const;
vector<pair<number_t, number_t>> getRow(number_t, number_t =1, number_t =0) const;
T operator()(number_t adr) const;
T& operator()(number_t adr);
typename vector<T>::iterator at(number_t, number_t);
typename vector<T>::const_iterator at(number_t i, number_t j) const;
T operator() (Number i, Number j) const;
T& operator()(Number i, Number j, bool =true);
Number nbNonZero() const;
void resetZero();
```

The member function pos(i,j) returns the adress in vector values_ of the matrix value $M_{ij}$ for $i, j \geq 1$. The returned adress begins at 1 except when the value is outside the storage where the function returns 0. The access operator (i,j) returns the matrix value or a reference to it with the *non const* version. In that case, it is possible to activate (errorOn=true) an error handler to prevent access to values outside the storage. It is the default behaviour. When errorOn=false, the access operator returns a reference to values_[0], thus you can modify its value. This trick avoids to perform test like if(pos(i,j)!=0)... before writing matrix values. To be safe at end, reset the values_[0] to 0 with resetZero function. Note that the skyline or compressed storage structure can not be dynamically changed when "inserting" a new value.

pos(i,j), getRow and getCol function should not be used in heavy computations because it is time consuming. In heavy computation, write codes based on storage structure!

As LargeMatrix class provides a lot of functions to modify its contents, some being time expansive regarding the storage :

```
void deleteRows(number_t, number_t);
void deleteCols(number_t, number_t);
void setColToZero(number_t c1=0, number_t c2=0);
void setRowToZero(number_t r1=0, number_t r2=0);
void roundToZero(real_t aszero=10*theEpsilon);

LargeMatrix<T>& operator*=(const K&);
LargeMatrix<T>& operator/=(const K&);
LargeMatrix<T>& operator+=(LargeMatrix<T>&);
LargeMatrix<T>& operator-=(LargeMatrix<T>&);
```

```
LargeMatrix<T>& add(iterator&,iterator&);
LargeMatrix<T>& add(const vector<T>&, const vector<number_t>&,const vector<number_t>&);
LargeMatrix<T>& add(const T& c, const vector<number_t>&, const vector<number_t>&);
LargeMatrix<T>& add(const LargeMatrix<K>&, const vector<number_t>&,const vector<number_t>&, C);
void addColToCol(number_t, number_t, complex_t a, bool =false);
void addRowToRow(number_t, number_t, complex_t a, bool =false);
void copyVal(const LargeMatrix<T>&, const vector<number_t>&, const vector<number_t>&);
LargeMatrix<T>& assign(const LargeMatrix<K>&, const vector<number_t>&, const vector<number_t>&);
```

Some functions are provided to change the scalar/matrix representation of the matrix or the storage:

```
void toSkyline();
void toStorage(MatrixStorage*);
LargeMatrix<K>* toScalar(K);
void toScalarEntries(const vector<Matrix<K> >&, vector<K>&, const MatrixStorage&);
void toUnsymmetric(AccessType at=_sym);
void extract2UmfPack(vector<int_t>& colPointer, vector<int_t>& rowIndex, vector<T>& matA) const;
bool getCsColUmfPack(vector<int_t>& colPointer, vector<int_t>& rowIndex, const T*& matA) const;
```

Matrices that are stored as Dense or Skyline can be factorized as LU, LDLt, LDL* and matrices that are stored as Skyline or Sparse can be factorized using UMFpack if it is available. All the stuff related to solve linear system is also available.

```
void ldltFactorize();
void ldlstarFactorize();
void luFactorize(bool withPermutation=true);
void umfpackFactorize();

void ldltSolve(vector<S1>& vec, vector<S2>& res) const;
void ldlstarSolve(vector<S>& vec, vector<T>& res) const;
void luSolve(vector<S1>& vec, vector<S2>& res) const;
void umfluSolve(vector<S1>& vec, vector<S2>& res) const;

void sorLowerMatrixVector(const vector<S1>& vec, vector<S2>& res, real_t) const;
void sorDiagonalMatrixVector(const vector<S1>& vec, vector<S2>& res,real_t) const;
void sorUpperMatrixVector(const vector<S1>& vec, vector<S2>& res,real_t) const;
void sorLowerSolve(const vector<S1>& vec, vector<S2>& res,real_t) const;
void sorDiagonalSolve(const vector<S1>& vec, vector<S2>& res,real_t) const;
void sorUpperSolve(const vector<S1>& vec, vector<S2>& res,real_t ) const;

real_t umfpackSolve(const vector<S>& vec,
vector<typename Conditional<NumTraits<ScalarType>::IsComplex, ScalarType, S>::type>& res,
bool soa=true);
real_t umfpackSolve(const vector<vector<S>*>&,
vector<vector<typename Conditional<NumTraits<ScalarType>::IsComplex, ScalarType,S>::type>* >&,
bool soa=true);
real_t umfpackSolve(const vector<int_t>& colPointer, const vector<int_t>& rowIndex,
const vector<T>& values, const vector<S>& vec,
vector<typename Conditional<NumTraits<ScalarType>::IsComplex, ScalarType, S>::type>& res,
bool soa=true);
```

In a same way, some functions interfaces eigen solvers:

```
friend number_t eigenDavidsonSolve(const LargeMatrix<K>* pA, const LargeMatrix<K>* pB,
          vector<pair<complex_t,Vector<complex_t> > >& res, number_t nev, real_t tol,
          string_t which, bool isInverted, FactorizationType fac, bool isShift);
friend number_t eigenKrylovSchurSolve(const LargeMatrix<K>* pA, const LargeMatrix<K>* pB,
          vector<pair<complex_t,Vector<complex_t> > >& res,number_t nev, real_t tol,
          string_t which, bool isInverted, FactorizationType fac, bool isShift);
```

The Frobenius norm $\sqrt{\sum |a_{ij}|^2}$ and infinity norm $\max_{|a_{ij}|}$ are provided:

```
real_t norm2() const;
real_t norminfty() const;
real_t partialNormOfCol(number_t, number_t, number_t) const;
```

Some operations are available as external functions to the class.

The LargeMatrix supplies methods to add two large matrices, which share a same storage. The matrix result will use the same storage as the two added matrices. If the result doesn't point to the storage of addend, after the addition, it will be forced to use this storage, and the number of object sharing this storage increases by one. Similar to multiplication of matrix-vector, these functions are also external templates, with specializations to mixed real and complex types.

```
friend void addMatrixMatrix(const LargeMatrix<S>& matA, const LargeMatrix<S>& matB,
     LargeMatrix<S>& matC);
friend void addMatrixMatrix(const LargeMatrix<Complex>& matA, const LargeMatrix<Real>& matB,
     LargeMatrix<Complex>& matC);
friend void addMatrixMatrix(const LargeMatrix<Real>& matA, const LargeMatrix<Complex>& matB,
     LargeMatrix<Complex>& matC);
```

The operator + is overloaded for LargeMatrix in the same manner.

```
LargeMatrix<T> operator+(const LargeMatrix<T>& matA, const LargeMatrix<T>& matB);
LargeMatrix<Complex> operator+(const LargeMatrix<Real>& matA, const LargeMatrix<Complex>& matB);
LargeMatrix<Complex> operator+(const LargeMatrix<Complex>& matA, const LargeMatrix<Real>& matB);
```

The symmetry of the result matrix depends on the ones of both addends. If one of these has _noSymmetry as SymType, the result will have the same SymType (i.e: _noSymmetry).

A large matrix can multiply by a scalar with the external templated functions

```
friend LargeMatrix<S> multMatrixScalar(const LargeMatrix<S>&, const S);
friend LargeMatrix<Complex> multMatrixScalar(const LargeMatrix<Complex>&, const Real);
friend LargeMatrix<Complex> multMatrixScalar(const LargeMatrix<Real>&, const Complex);
```

Like addMatrixMatrix, the result of multMatrixScalar shares the same storage of the input large matrix. The operator * can be also overloaded in the same manner.

```
LargeMatrix<T> operator*(const LargeMatrix<T>& mat, const T v);
LargeMatrix<T> operator*(const T v, const LargeMatrix<T>& mat);
LargeMatrix<Complex> operator*(const LargeMatrix<Complex>& mat, const Real v);
LargeMatrix<Complex> operator*(const Real v, const LargeMatrix<Complex>& mat);
LargeMatrix<Complex> operator*(const LargeMatrix<Real>& mat, const Complex v);
LargeMatrix<Complex> operator*(const Complex v, const LargeMatrix<Real>& mat);
```

The product of matrix and vector is one of the most important operation required. The LargeMatrix class interfaces matrix-vector product and the vector-matrix matrix; the product being really done by the storage classes. They are external templated functions to the class (declared friend of class), with specializations to mixed real and complex types (only casting from real to complex is allowed) :

```
void multMatrixVector(const LargeMatrix<S>&, const vector<S>&, vector<S>&);
void multVectorMatrix(const LargeMatrix<S>&, const vector<S>&, vector<S>&);
void multMatrixVector(const LargeMatrix<Matrix<S> >&,
                      const vector<Vector<S> >&, vector<Vector<S> >&);
void multVectorMatrix(const LargeMatrix<Matrix<S> >&,
                      const vector<Vector<S> >&, vector<Vector<S> >&);
```

The operator * is overloaded for LargeMatrix and vector or vector and LargeMatrix in a same way :

```
friend vector<S> operator*(const LargeMatrix<S>&, const vector<S>&);
friend vector<S> operator*(const vector<S>&, const LargeMatrix<S>&);
friend vector<Vector<S> operator*(const LargeMatrix<Matrix<S> >&,
                                  const vector<Vector<S> >&);
friend vector<Vector<S> operator*(const vector<Vector<S> >&,
                                  const LargeMatrix<Matrix<S> >&);
...
```

The product of two matrices is provided, but be cautious, up to now the result matrix is a dense matrix (except if one matrix is a diagonal one):

```
void multMatrixMatrix(const LargeMatrix<SA>&, const LargeMatrix<SB>&, LargeMatrix<SR>&);
```

The `LargeMatrix` also provides some functions to factorize a matrix and solve factorized syste. Like `multMatrixVector`, these functions are external (friend of class), template with hybrid complex-real specialization.

```
void ldltFactorize(LargeMatrix<S>& mat);
void ldlstarFactorize(LargeMatrix<S>& mat);
void luFactorize(LargeMatrix<S>& mat);
```

These functions are available for `SkylineStorage` and `DenseStorage`.

If a matrix is factorized, some other operation are available

```
void multFactMatrixVector(const LargeMatrix<S1>&, const vector<S2>&, vector<S3>&);
void multVectorFactMatrix(const LargeMatrix<S1>&, const vector<S2>&, vector<S3>&);
void multInverMatrixVector(const LargeMatrix<S1>& mat, const vector<S2>& vec,
     vector<typename Conditional<NumTraits<S1>::IsComplex, S1, S2>::type>& res,
     FactorizationType);
```

In order to generate a diagonal matrix which uses an existent matrix as prototype, `LargeMatrix` class provides function

```
LargeMatrix<S> diagonalMatrix(const LargeMatrix<S>&, const S);
```

A special version of this function is a function to generate an identity matrix from an existing one.

```
LargeMatrix<S> identityMatrix(const LargeMatrix<S>&);
```

These functions work with `LargeMatrix` class having all kinds of matrix storage except `RowCsStorage` class and `ColCsStorage` class.

Finally, the class has input/output member functions :

```
void print(ostream&) const;
void viewStorage(ostream&) const;
ostream& operator<<(ostream&, const LargeMatrix<S>&);
void saveToFile(const String &, StorageType, bool encode=false) const;
void loadFromFile(const String&, StorageType);
String encodeFileName(const String&, StorageType) const;
```

Only two formats are allowed for saving matrix to file or loading matrix from file :

- the dense format (`_dense`), where all the matrix values are written row by row (one row by line), space character separates each value :

```
A11 A12 ... A1n                     re(A11) im(A11)  ... re(A1n) im(A1n)
A21 A22 ... A2n   if complex values re(A21) im(A21)  ... re(A2n) im(A2n)
...                                  ...
Am1 Am2 ... Amn                     re(Am1) im(Am1)  ... re(Amn) im(Amn)
```

- the coordinates format (`_coo`)

```
i1 j1 Ai1j1                        i1 j1 re(Ai1j1) im(Ai1j1)
i2 j2 Ai2j2      if complex values i2 j2 re(Ai2j2) im(Ai2j2)
...
```

> For matrix of matrices (`T=Matrix<Real>` or `T=Matrix<Complex>`), submatrix structure is not preserved when writing matrix values!

To keep some general informations about matrix, with the argument `encode=true` in the `saveFile` function, the name of file may be modified by inserting the string :

`(m_n_storageType_valueType_strucType_p_q)`

where `m` and `n` are the "dimensions" of the matrix, `storageType = dense or coo`, `valueType = real or complex` , `strucType = scalar or matrix` and p and q are the dimensions of sub-matrices. In case of scalar value, this parameters are omitted. This trick avoids to include informations in file in order that it is easily loadable by other softwares, in particular Matlab.

### Some examples

Manipulate a 3 × 2 matrix with row dense storage:

```
Vector<Real> x(2,2);
LargeMatrix<Real> A(3,2,_dense,_row,1.);
out<<"matrix A : "<<A;
out<<"access A(1,1)= "<<A(1,1);
out<<"product A*x : "<<A*x;
A.saveToFile("A_dense.mat",_dense);
LargeMatrix<Real> Areload("A_dense.mat",_dense,3,2,_dense,_row);
```

Manipulate a 3 × 2 matrix of 2 × 2 real matrices with dual dense storage:

```
Matrix<Real> I1(2,_idMatrix);
Vector<Real> x(6,3);
LargeMatrix<Matrix<Real> > B(6,3,_dense,_dual,2*I1);
out<<"product X*B : "<<X*B;
```

Manipulate a 9 × 9 symmetric matrix with symmetric compressed storage:

```
//construct storage for a Q1 mesh
Number n=3;
vector<vector<Number> > elts((n-1)*(n-1),vector<Number>(4));
for(Number j=1; j<=n-1; j++)
  for(Number i=1; i<=n-1; i++) {
     Number e=(j-1)*(n-1)+i-1, p=(j-1)*n+i;
     elts[e][0]=p; elts[e][1]=p+1; elts[e][2]=p+n; elts[e][3]=p+n+1;
     }
SymCsStorage* cssym= new SymCsStorage(n*n,elts,elts);
//construct large matrix with symmetric compressed storage
LargeMatrix<Real> C(cssym,1.,_symmetric);
C.viewStorage(out);
```

```
Vector<Real> x(n*n,0.);for(Number i=0;i<n*n;i++) x1[i]=i;
out<<"product C*x : "<<C*x;
C.saveToFile("C_coo.mat"),_coo);
//construct large matrix with symmetric compressed storage
LargeMatrix<Real> C1(cssym,1.,_symmetric);
out<<"addition C+C1 "<< C+C1;
// multiply a matrix with a scalar
out<<"product C*10.0 "<< C*10.0;
// generate a diagonal matrix
out<<"diagonal matrix from matrix C " << diagonalMatrix(C, 10.0);
// generate an identity matrix
out<<"identity matrix from matrix C " << identityMatrix(C);
```

Note that compressed storage has to be built before to instantiate a large matrix with compressed storage. The function viewStorage produced the output:

```
symmetric_compressed sparse (csr,csc), size = 29, 9 rows, 9 columns
 (shared by 1 objects).
          123456789
       1  d........
       2  xd.......
       3  .xd......
       4  xx.d.....
       5  xxxxd....
       6  .xx.xd...
       7  ...xx.d..
       8  ...xxxxd.
       9  ....xx.xd
          123456789
```

LDLt-Factorize a positive definite 3x3 matrix with symmetric skyline storage:

```
LargeMatrix<Real> rResSymSkylineLdlt(inputsPathTo("matrix3x3SymPosDef.data"), _dense, rowNum,
    _skyline, _symmetric);
ldltFactorize(rResSymSkylineLdlt);
out << "The result of LDLt factorizing sym skyline matrix is " << rResSymSkylineLdlt << endl;
```

| | |
|---|---|
| library : | **largeMatrix** |
| header : | **LargeMatrix.hpp** |
| implementation : | **LargeMatrix.cpp** |
| unitary tests : | **test_LargeMatrixDenseStorage.cpp, test_LargeMatrixCsStorage.cpp** |
| header dependences : | **MatrixStorage.hpp, DenseStorage.hpp, CsStorage.hpp, SkylineStorage.hpp, config.h, utils.h** |

## 9.2 The MatrixStorage class

The MatrixStorage is the abstract base class of all supported matrix storages. Vectors carrying storage pointers are defined in child classes and the vector storing the matrix entries is defined outside the storage (see LargeMatrix class for instance). Various matrix storages are defined by three characteristics :

- a StorageType : _dense for dense storage, _cs for compressed sparse storage (CSR/CSC) and _skyline for skyline strorage
- an AccessType : _row for a row wise access, _col for a column wise access,_dual for a row wise access for lower triangular part of the matrix and a column wise access for the upper triangular part of the matrix, and _sym if the storage is symmetric (only the lower triangular part is described with a row wise access).

- a BuildStorageType : describing the way the storage is constructed :`_undefBuild, _feBuild, _dgBuild, _diagBuild, _ecBuild, _globalBuild, _otherBuild`
- a flag telling if the storage comes from a vector to scalar conversion

```
class MatrixStorage
{protected:
   StorageType storageType_;      // storage type
   AccessType accessType_;        // access type
   StorageBuildType buildType_;   // storage build type
   bool scalarFlag_;              // scalar conversion flag
   Number nbRows_;                // number of rows
   Number nbCols_;                // number of columns
   Number nbObjectsSharingThis_;  // number of matrices sharing "this" storage
   ...
```

The number of rows and columns are counted in value type of the matrix.

It manages also a string index to identify the storage (generally encoding the row/col space pointers)

```
 public:
   String stringId;  // string identifier based on characteristic pointers
```

The class provides some constructors which only initialize members of the class.

```
MatrixStorage();
MatrixStorage(StorageType, AccessType at = _noAccess);
MatrixStorage(StorageType, AccessType, Number, Number);
virtual ~MatrixStorage();
```

Protected members may be read by accessors :

```
String name() const;
StorageType storageType() const;
AccessType accessType() const;
StorageBuildType buildType() const;
Number nbOfRows() const;
Number nbOfColumns() const;
Number numberOfObjects() const
void objectPlus() ;
void objectMinus();
```

All storage object pointers are stored in a static vector

```
static vector<MatrixStorage*> theMatrixStorages; // list of all matrix storages
static void clearGlobalVector();                 // delete all MatrixStorage objects
static void printAllStorages(ostream&);          // print the list of MatrixStorage in memory
static void printAllStorages(PrintStream& os);
```

and some static functions dealing with are available.

When building a new storage, it is possible to look for an existing storage by using the external function:

```
MatrixStorage* findMatrixStorage(const String& id, StorageType st, AccessType at,
                StorageBuildType sb, bool scal=false, Number nbr=0, Number nbc=0);
```

Travelling `theMatrixStorages` vector this function checks if it exists a storage having the same characteritics (id, storage type, access type, build type) and may check the scalar flag and the number of rows or columns if non zero values are given.

The class provides virtual member functions returning the sizes of storage (number of matrix entries stored) :

```
virtual Number size() const = 0;
Number diagonalSize() const;
virtual Number lowerPartSize() const=0;
virtual Number upperPartSize() const=0;
```

Most of the member functions depend on type of storage, so they are virtual member functions. Besides, as storages do not depend on value type of matrix, the storage classes are not templated by the matrix value type. Because virtual template functions are not allowed in C++, all the value type specializations are explicit in base class and in child classes. Up to now, the supported specialisations are `Real`, `Complex`, `Matrix<Real>` and `Matrix<Complex>`. We describe here only the `Real` specialisation.

There are two functions related to matrix entry position in storage, the first one gives the position of entry $(i, j)$ with $i, j \geq 1$ and the second one compute the positions of the entries of the submatrix given by its row indices and column indices. These functions give **positions from index 1** if the entry is inside the storage else the returned position is 0. In the second function, it is possible to activate an error when entry index is outside the storage. In both functions, the symmetry has to be specified if the matrix has a symmetry property, in that case the position is always in lower triangular part. Be care with the fact that a matrix with no symmetry may have a symmetric storage!

```
virtual Number pos(Number i, Number j, SymType sym=_noSymmetry) const;
virtual void positions(const std::vector<Number>&, const std::vector<Number>&,
                       std::vector<Number>&, bool errorOn=true, SymType=_noSymmetry) const;
```

To print, to save to file or load from file large matrices, the following functions are proposed :

```
virtual void printEntries(std::ostream&, const std::vector<Real>&,
                          Number vb = 0, SymType sym = _noSymmetry) const;
template<typename T>
  void printDenseMatrix(std::ostream&, const std::vector<T>&, SymType s=_noSymmetry) const;
  void printCooMatrix(std::ostream&, const std::vector<T>&, SymType s=_noSymmetry) const;
virtual void loadFromFileDense(std::istream&, std::vector<Real>&, SymType, bool);
virtual void loadFromFileCoo(std::istream&, std::vector<Real>&, SymType, bool);
virtual void visual(std::ostream&) const;
```

The `printEntries` function print on output stream the stored matrix entries in a well suited presentation, the `printDenseMatrix` function print the matrix entries in a dense format as it was dense and the `printCooMatrix` function print the matrix entries in a coordinates format $(i, j, A_{ij}$. A $m \times n$ matrix saved as dense produced a file like :

```
A11 A12 ... A1n                      re(A11) im(A11)  ... re(A1n) im(A1n)
A21 A22 ... A2n   if complex values  re(A21) im(A21)  ... re(A2n) im(A2n)
...                                   ...
Am1 Am2 ... Amn                      re(Am1) im(Am1)  ... re(Amn) im(Amn)
```

and when saved as coordinates format :

```
i1 j1 Ai1j1                          i1 j1 re(Ai1j1) im(Ai1j1)
i2 j2 Ai2j2      if complex values   i2 j2 re(Ai2j2) im(Ai2j2)
...                                  ...
```

Note that `printDenseMatrix` and `printCooMatrix` functions are templated functions. Their coding is not optimal because they use the virtual `pos` function and other extern utilities which "interpret" the type of the template :

```
void printDense(ostream&, const Real&, Number);
void printDense(ostream&, const Complex&, Number);
template<typename T>
```

```
  void printDense(ostream&, const Matrix<T>&, Number);
  void printCoo(ostream&, const Matrix<T>&, Number);
void printCoo(ostream&, const Real&, Number);
void printCoo(ostream&, const Complex&, Number);
Number numberOfRows(const Real&);
Number numberOfRows(const Complex&);
Number numberOfCols(const Real&);
Number numberOfCols(const Complex&);
template<typename T> Number numberOfRows(const Matrix<T>&);
template<typename T> Number numberOfCols(const Matrix<T>& m);
```

The `visual` function prints only the matrix entries inside the storage as ’x’ characters (d for diagonal entries):

```
matrix storage :row_compressed sparse (csr,csc), size = 49, 9 rows, 9 columns (shared by 0
    objects).
          123456789
      1   dx.xx....
      2   xdxxxx...
      3   .xd.xx...
      4   xx.dx.xx.
      5   xxxxdxxxx
      6   .xx.xd.xx
      7   ...xx.dx.
      8   ...xxxxdx
      9   ....xx.xd
          123456789
```

The `MatrixStorage` class provides the product matrix × vector and the product vector × matrix:

```
virtual
 void multMatrixVector(const vector<Real>&, const vector<Real>&, vector<Real>&, SymType) const;
 void multMatrixVector(const vector< Matrix<Real> >&, const vector<Vector<Real>>&, vector
     Vector<Real>>&, SymType) const;
 void multVectorMatrix(const vector<Real>&, const vector<Real>&, vector<Real>&, SymType) const;
 void multVectorMatrix(const vector<Matrix<Real>>&, const vector<Vector<Real>>&,
     vector<Vector<Real>>&, SymType) const;
```

Note that mixing real vector/matrix and complex vector/matrix is also provided. Each child class implements the best algorithm for the product.
The addition of two matrices is supplied with:

```
virtual void addMatrixMatrix(const vector<Real>&, const vector<Real>&,
                             vector<Real>&) const;
```

Similar to multiplication of matrix-vector, this function is implemented in each child class. The `MatrixStorage` class also provides the matrix factorizations

```
virtual
 void ldlt(vector<Real>&, vector<Real>&, const SymType sym = _symmetric) const;
 void ldlt(vector<Complex>&, vector<Complex>&, const SymType sym = _symmetric) const;
 void lu(vector<Real>&, vector<Real>&, const SymType sym = _noSymmetry) const;
 void lu(vector<Complex>&, vector<Complex>&, const SymType sym = _noSymmetry) const;
 void ldlstar(vector<Real>&, vector<Real>&) const;
 void ldlstar(vector<Complex>&, vector<Complex>&) const;
```

as well as some special solvers

```
virtual
 void lowerD1Solver(const vector<Real>&, vector<Real>&, vector<Real>&) const;
 void diagonalSolver(const vector<Real>&, vector<Real>&, vector<Real>&) const
 void upperD1Solver(const vector<Real>&, vector<Real>&, vector<Real>&,
                    const SymType sym = _noSymmetry) const;
```

```
void upperSolver(const vector<Real>&, vector<Real>&, vector<Real>&,
                 const SymType sym = _noSymmetry) const;
void sorDiagonalMatrixVector(const vector<Real>&, const vector<Real>&, vector<Real>&,
                             const Real) const;
void sorLowerMatrixVector(const vector<Real>&, const vector<Real>&, vector<Real>& ,Real,
                          const SymType = _noSymmetry) const;
void sorUpperMatrixVector(const vector<Real>&, const vector<Real>&, vector<Real>&, Real,
                          const SymType = _noSymmetry) const;
void sorDiagonalSolve(const vector<Real>&, const vector<Real>&, vector<Real>&, Real) const;
void sorLowerSolve(const vector<Real>&, const vector<Real>&, vector<Real>&, Real) const;
void sorUpperSolve(const vector<Real>&, const vector<Real>&, vector<Real>&, Real,
                   const SymType sym = _noSymmetry) const;
```

Each descendant will implement the specific algorithm for these virtual functions. Values on the diagonal of a matrix is set with the function

```
virtual void setDiagValue(vector<Real>&, Real);
```

| | |
|---:|:---|
| library : | **largeMatrix** |
| header : | **MatrixStorage.hpp** |
| implementation : | **MatrixStorage.cpp** |
| unitary tests : | **test_LargeMatrix...Storage.cpp** |
| header dependences : | **config.h, utils.h** |

## 9.3 Dense storages

Dense storages are proposed as childs of `MatrixStorage` class in order to be consistent with other storages. Contrary to the `Matrix` class (see *utils* lib) which is a row dense storage, several dense storages are offered for a $m \times n$ matrix (say $A$) :

- the row dense storage (`RowDenseStorage` class)

$$(A_{11}, A_{12}, ..., A_{1n}, A_{21}, A_{22}, ..., A_{2n}, ..., A_{m1}, A_{m2}, ..., A_{mn})$$

- the column dense strorage (`ColDenseStorage` class)

$$(A_{11}, A_{21}, ..., A_{2m}, A_{12}, A_{22}, ..., A_{m2}, ..., A_{1n}, A_{2n}, ..., A_{mn})$$

- the dual dense storage (`DualDenseStorage` class), diagonal part is first stored, then strict lower triangular part and strict upper triangular part :

$$(A_{11}, A_{22}, ..., A_{mm}, A_{21}, ..., A_{i1}, ...A_{i,i-1}, ..., A_{12}, ..., A_{1j}, ...A_{j-1,j}, ...) \text{ case } m = n$$

- the symmetric dense storage (`SymDenseStorage` class), diagonal part is first stored, then strict lower triangular part :

$$(A_{11}, A_{22}, ..., A_{mm}, A_{21}, ..., A_{i1}, ...A_{i,i-1}, ...) \text{ case } m = n$$

Dual storage works also for non square matrices. Obviously, symmetric storage works only for square matrices!

All dense storages inherit from the `DenseStorage` abstract class which inherits from `MatrixStorage` abstract class.

### 9.3.1 The DenseStorage class

The DenseStorage class has no member attribute.There are some basic constructors just calling MatrixStorage constructors:

```
class DenseStorage : public MatrixStorage
{public :
  DenseStorage();
  DenseStorage(AccessType);
  DenseStorage(AccessType, Number);
  DenseStorage(AccessType, Number, Number);
  virtual ~DenseStorage() {}
  ...
```

DenseStorage objects do not have to be instantiated. This class acts as an interface to particular dense storages and gathers all common functionalities of dense storages, some being virtuals:

- pubic size functions:

```
Number size() const;
virtual Number lowerPartSize() const;
virtual Number upperPartSize() const;
```

- protected input/output functions (template line is written once):

```
template<typename Iterator>
void printScalarEntries(Iterator&, Number, Number, Number, Number, Number,
                        const String&, Number, std::ostream&) const;
void printScalarEntriesTriangularPart(Iterator& , Iterator&, Number, Number,
                                      Number, Number, Number, const String&,
                                      Number, std::ostream&) const;
void printMatrixEntries(Iterator&, Number, Number, const String&, Number,
                        std::ostream&) const;
void printMatrixEntriesTriangularPart(Iterator&, Iterator&, Number, Number,
                                      const String&, Number, std::ostream&) const;
void loadFromFileDense(std::istream&, std::vector<Real>&, SymType, bool);
void loadFromFileDense(std::istream&, std::vector<Complex>&, SymType, bool);
void loadFromFileCoo(std::istream&, std::vector<Real>&, SymType, bool);
void loadFromFileCoo(std::istream&, std::vector<Complex>&, SymType, bool);
```

- product of matrix and vector (template line is written once):

```
template<typename MatIterator, typename VecIterator, typename ResIterator>
  void diagonalMatrixVector(MatIterator&, VecIterator&, ResIterator&,
                            ResIterator&) const;
  void diagonalVectorMatrix(MatIterator&, VecIterator&, ResIterator&,
                            ResIterator&) const;
  void lowerMatrixVector(MatIterator&, VecIterator&, VecIterator&,
                         ResIterator&, ResIterator&, SymType) const;
  void lowerVectorMatrix(MatIterator&, VecIterator&, VecIterator&,
                         ResIterator&, ResIterator&, SymType) const;
  void upperMatrixVector(MatIterator&, VecIterator&, VecIterator&,
                         ResIterator&, ResIterator&, SymType) const;
  void upperVectorMatrix(MatIterator&, VecIterator&, VecIterator&,
                         ResIterator&, ResIterator&, SymType) const;
  void rowMatrixVector(MatIterator&, VecIterator&, VecIterator&,
                       ResIterator&, ResIterator&)  const;
  void rowVectorMatrix(MatIterator&, VecIterator&, VecIterator&,
                       ResIterator&, ResIterator&)  const;
  void columnMatrixVector(MatIterator&, VecIterator&, VecIterator&,
                          ResIterator&, ResIterator&)  const;
```

```
void columnVectorMatrix(MatIterator&, VecIterator&, VecIterator&,
                        ResIterator&, ResIterator&)  const;
```

Note that the product of matrix and vector are performed either by row or column access, for diagonal part, lower part or upper part. They use iterators to by-pass the templated matrix values vector! With this trick, product algorithms are all located in `DenseStorage` class.

- addition of two matrices:

```
template<typename Mat1Iterator, typename Mat2Iterator, typename ResIterator>
void sumMatrixMatrix(Mat1Iterator&, Mat2Iterator&, ResIterator&, ResIterator&) const;
```

| | |
|---|---|
| library : | **largeMatrix** |
| header : | **DenseStorage.hpp** |
| implementation : | **DenseStorage.cpp** |
| unitary tests : | **test_LargeMatrixDenseStorage.cpp** |
| header dependences : | **MatrixStorage.hpp, config.h, utils.h** |

### 9.3.2 `Row/Col/Dual/SymDenseStorage` classes

All child classes (`RowDenseStorage`, `ColDenseStorage`, `DualDenseStorage` and `SymDenseStorage`) of `DenseStorage` class have the same structure. We give here only the description of `RowDenseStorage` class.
`RowDenseStorage` class manages dense storage where matrix values are stored row by row in values vector. It has no member attribute and has constructors just calling `DenseStorage` constructors:

```
class RowDenseStorage : public DenseStorage
{public :
  RowDenseStorage();
  RowDenseStorage(Number);
  RowDenseStorage(Number, Number);
  virtual ~RowDenseStorage() {}
  ...
```

The class provides all the virtual methods declared in `MatrixStorage` class :

```
Number pos(Number i, Number j, SymType s=_noSymmetry) const;
void positions(const std::vector<Number>&, const std::vector<Number>&,
               std::vector<Number>&, bool errorOn=true, SymType=_noSymmetry ) const;
void printEntries(std::ostream&, const std::vector<Real>&,
                  Number vb = 0, SymType sym = _noSymmetry) const;
template<typename M, typename V, typename R>
  void multMatrixVector(const std::vector<M>&, const std::vector<V>&,
                        std::vector<R>&) const;
  void multVectorMatrix(const std::vector<M>&, const std::vector<V>&,
                        std::vector<R>&) const;
template<typename T>
  void setDiagValueColDense(std::vector<T>& m, const T k);
template<typename M1, typename M2, typename R>
  void addMatrixMatrix(const std::vector<M1>&, const std::vector<M2>&, std::vector<R>&) const;
  ...
```

Only version of `multMatrixVector` and `multVectorMatrix` are written here for `Real` type but versions for `Complex`, `Matrix<Real>`, `Matrix<Complex>` and mixed types are also provided.

`DualDenseStorage` and `SymDenseStorage` classes provides also the size of strict lower and strict upper triangular part:

```
Number lowerPartSize() const;
Number upperPartSize() const;
```

XXX=Row, Col, Dual or Sym

| | |
|---|---|
| library : | **largeMatrix** |
| header : | **XXXDenseStorage.hpp** |
| implementation : | **XXXDenseStorage.cpp** |
| unitary tests : | **test_LargeMatrixDenseStorage.cpp** |
| header dependences : | **DenseStorage.hpp, MatrixStorage.hpp, config.h, utils.h** |

## 9.4 Compressed sparse storages

Compressed sparse storages are designed to store only non zero values of a matrix. It exists several methods to do it. The well known CSR/CSC storage being the most common one, we chose it. It consists in storing non zero values of a row (resp. column) in a compressed vector and their column indices (resp. row indices) in a compressed vector. A vector of addresses where begin rows (resp. columns) is also required. More precisely, for a $m\times n$ matrix

- row compressed storage is defined by the three vectors :
  values = $(0, A_{1\mathscr{C}_1}, ..., A_{i\mathscr{C}_i}, ..., A_{m\mathscr{C}_m})$
  colIndex = $(\mathscr{C}_1, ..., \mathscr{C}_i, ..., \mathscr{C}_m)$
  rowPointer = $(p_1,...,p_i,..., p_m,\ p_{m+1})$
  where $\mathscr{C}_i$ is the set of index $j$ where $A_{ij}\neq 0$ and $p_i$ is the position in vector colIndex of the first entry of row $i\leq m$; $p_{m+1}$ gives the number of non zero values. By convention, all the indices begins at 0 and first entry of values vector is always 0!
  For instance, the following $5\times 6$ non symmetric matrix

$$A=\begin{bmatrix} 11 & 12 & 0 & 14 & 0 & 16\\ 0 & 22 & 23 & 0 & 0 & 26\\ 31 & 32 & 33 & 0 & 0 & 0\\ 0 & 0 & 43 & 44 & 0 & 0\\ 51 & 0 & 53 & 54 & 55 & 0 \end{bmatrix}$$

  has the row compressed storage vectors:

  values = ( 0 11 12 14 16  22 23 26  31 32 33  43 44  51 53 54 55 )
  colIndex = ( 0 1 3 5  1 2 5  0 1 2  2 3  0 2 3 4 )
  rowPointer = ( 0 4 7 10 12 16)

- row compressed storage is defined by the three vectors :
  values = $(0, A_{\mathscr{R}_1 1}, ..., A_{\mathscr{R}_j j}, ..., A_{\mathscr{R}_n n})$
  rowIndex = $(\mathscr{R}_1, ..., \mathscr{R}_j, ..., \mathscr{R}_n)$
  colPointer = $(p_1,...,p_j,..., p_n,\ p_{n+1})$
  where $\mathscr{R}_j$ is the set of index $i$ where $A_{ij}\neq 0$ and $p_j$ is the position in rowIndex vector of the first entry of column $j\leq n$; $p_{n+1}$ gives the number of non zero values. By convention, all the indices begins at 0 and first entry of values vector is always 0!
  For instance, the previous $5\times 6$ non symmetric matrix $A$ has the column compress storage vectors:
  values = ( 0 11 31 51  12 22 32  23 33 43 53  55  16 26 )
  rowIndex = ( 0 2 4  0 1 2  1 2 3 4  0 3 4  4  0 1)

colPointer = ( 0 4 7 10 12 16)

- dual compressed storage is defined by the five vectors :
  values = (0,diag(A), $A_{\mathscr{C}_1 1}$, ..., $A_{\mathscr{C}_i i}$, ..., $A_{\mathscr{C}_m m}$, $A_{\mathscr{R}_1 1}$, ..., $A_{\mathscr{R}_j j}$, ..., $A_{\mathscr{R}_n n}$)
  colIndex = ($\mathscr{C}_1$, ..., $\mathscr{C}_i$, ..., $\mathscr{C}_m$)
  rowPointer = ($p_1$,...,$p_i$,..., $p_m$, $p_{m+1}$)
  rowIndex = ($\mathscr{R}_1$, ..., $\mathscr{R}_j$, ..., $\mathscr{R}_n$)
  colPointer = ($q_1$,...,$q_j$,..., $q_n$, $q_{n+1}$)
  where $\mathscr{C}_i$ is the set of index $j$ where $A_{ij} \neq 0$ and $j \leq \min(i-1,n)$, $\mathscr{R}_j$ is the set of index $i$ where $A_{ij} \neq 0$ and $i \leq \min(j-1,m)$, $p_i$ (resp. $q_j$) is the position in colIndex (resp. rowIndex) vector of the first entry of row $i \leq m$ (resp. column $j \leq n$). The colIndex and rowPointer vectors describes the row compressed storage of the strict lower part of matrix while the rowIndex and colPointer vectors describes the column compressed storage of the strict upper part of matrix. In this storage, all the diagonal entries of matrix are always first stored even the null entries!
  For instance, the previous 5 × 6 non symmetric matrix $A$ has the column compress storage vectors:
  values = ( 0 11 22 33 44 55 31 32 43 51 53 54 23 14 44 16 26 )
  colIndex = (0 1 2 0 2 3)
  rowPointer = (0 0 0 2 3 6)
  rowIndex = (0 1 0 0 1)
  colPointer = ( 0 0 1 2 2 3 5)
  Note that for an empty row $i$ (resp. column $j$), rowPointer($i$)=rowPointer($i-1$) (resp. colPointer($j$)=colPointer($j-1$)). By the way, rowPointer($i$)-rowPointer($i-1$) gives the number of stored entries on row $i-1$.

- symmetric compressed storage is devoted to square matrix with symmetric storage, the matrix may be not symmetric.. In that case, only the storage of lower triangular part of matrix is described by the three vectors (those of row part of dual storage):
  values = (0,diag(A), $A_{\mathscr{C}_1 1}$, ..., $A_{\mathscr{C}_i i}$, ..., $A_{\mathscr{C}_m m}$) if $A$ has a symmetry property
  values = (0,diag(A), $A_{\mathscr{C}_1 1}$, ..., $A_{\mathscr{C}_i i}$, ..., $A_{\mathscr{C}_m m}$,$A_{\mathscr{C}_1 1}$, ..., $A_{\mathscr{C}_j j}$, ..., $A_{\mathscr{C}_m m}$) if $A$ has no symmetry property
  colIndex = ($\mathscr{C}_1$, ..., $\mathscr{C}_i$, ..., $\mathscr{C}_m$)
  rowPointer = ($p_1$,...,$p_i$,..., $p_m$, $p_{m+1}$)
  where the meaning of $\mathscr{C}_i$ and $p_i$ is the same as dual storage.
  For instance, the 5 × 5 non symmetric matrix with symmetric storage

$$B = \begin{bmatrix} 11 & 0 & 13 & 0 & 15 \\ 0 & 22 & 23 & 0 & 0 \\ 31 & 32 & 33 & 34 & 35 \\ 0 & 0 & 43 & 44 & 45 \\ 51 & 0 & 53 & 54 & 55 \end{bmatrix}$$

  has the symmetric compressed storage vectors:
  values = ( 0 11 22 33 44 55 31 32 43 51 53 54 13 23 34 15 35 45)
  colIndex = (0 1 2 0 2 3)
  rowPointer = (0 0 0 2 3 6)

Be care with the fact that actual matrix values begins at adress 1 in values vector defined outside the storage stuff.

### 9.4.1 The `CsStorage` class

The `CsStorage` class has no member attribute. There are some basic constructors just calling `MatrixStorage` constructors:

```
class CsStorage : public MatrixStorage
{public :
  CsStorage(AccessType = _dual);
  CsStorage(Number, AccessType = _dual);
  CsStorage(Number, Number, AccessType = _dual);
  virtual ~CsStorage() {}
 protected :
  void buildCsStorage(const std::vector<std::vector<Number> >&,
                      std::vector<Number>&, std::vector<Number>&);
```

The `buildCsStorage` is a general member function building storage vectors from lists of column indices by row. It is used by any child class of `CsStorage` class. `CsStorage` objects do not have to be instantiated. This class acts as an interface to particular compressed storages and gathers all common functionalities of dense storages, some being virtuals (some template line declaration are omitted):

```
virtual Number size() const = 0;
virtual Number lowerPartSize() const;
virtual Number upperPartSize() const;
template<typename Iterator>
  void printEntriesAll(StrucType, Iterator& , const std::vector<Number>&,
                       const std::vector<Number>&, Number, Number, Number,
                       const String&, Number, std::ostream&) const;
  void printEntriesTriangularPart(StrucType, Iterator&, Iterator&,
                       const std::vector<Number>&, const std::vector<Number>&,
                       Number, Number, Number, const String&, Number,
                       std::ostream&) const;
  void printCooTriangularPart(std::ostream&, Iterator&, const std::vector<Number>&,
                              const std::vector<Number>&, bool,
                              SymType sym = _noSymmetry) const;
  void printCooDiagonalPart(std::ostream&, Iterator&, Number) const;

template <typename T>
    void loadCsFromFileDense(std::istream&, std::vector<T>&, std::vector<Number>&,
                             std::vector<Number>&, SymType, bool);
    void loadCsFromFileCoo(std::istream&, std::vector<T>&, std::vector<Number>&,
                           std::vector<Number>&, SymType, bool);
    void loadCsFromFileDense(std::istream&, std::vector<T>&, std::vector<Number>&,
                             std::vector<Number>&, std::vector<Number>&,
                             std::vector<Number>&, SymType, bool);
    void loadCsFromFileCoo(std::istream&, std::vector<T>&, std::vector<Number>&,
                           std::vector<Number>&, std::vector<Number>&,
                           std::vector<Number>&, SymType, bool);
```

The `CsStorage` class provides the real code of product of matrix and vector, using iterators as arguments to by-pass the template type of matrix values. For dual and symmetric storage, the computation is performed by splitting the matrix in its diagonal, lower and upper part (template line are omitted):

```
template<typename MatIterator, typename VecIterator, typename ResIterator>
  void diagonalMatrixVector(MatIterator&, VecIterator&, ResIterator&,
                            ResIterator&) const;
  void lowerMatrixVector(const std::vector<Number>&, const std::vector<Number>&,
                         MatIterator&, VecIterator&, ResIterator&, SymType sym) const;
  void upperMatrixVector(const std::vector<Number>&, const std::vector<Number>&,
                         MatIterator&, VecIterator&, ResIterator&, SymType) const;
  void rowMatrixVector(const std::vector<Number>&, const std::vector<Number>&,
                       MatIterator&, VecIterator&, ResIterator&)  const;
  void columnMatrixVector(const std::vector<Number>&, const std::vector<Number>&,
                          MatIterator&, VecIterator&, ResIterator&)  const;
  void diagonalVectorMatrix(MatIterator&, VecIterator&, ResIterator&,
                            ResIterator&) const;
  void lowerVectorMatrix(const std::vector<Number>&, const std::vector<Number>&,
                        MatIterator&, VecIterator&, ResIterator&, SymType sym) const;
void upperVectorMatrix(const std::vector<Number>&, const std::vector<Number>&,
                        MatIterator&, VecIterator&, ResIterator&, SymType) const;
void rowVectorMatrix(const std::vector<Number>&, const std::vector<Number>&,
                      MatIterator&, VecIterator&, ResIterator&)  const;
void columnVectorMatrix(const std::vector<Number>&, const std::vector<Number>&,
                         MatIterator&, VecIterator&, ResIterator&)  const;
```

Besides the product of matrix and vector, the `CsStorage` provides solvers for matrix in its diagonal, lower and upper part

```
template<typename MatIterator, typename VecIterator, typename ResIterator>
void bzSorDiagonalMatrixVector(MatIterator& itd, const VecIterator& itvb,
                               ResIterator& itrb, const Real w) const;

template<typename MatIterator, typename VecIterator, typename XIterator>
void bzSorLowerSolver(const MatIterator&, const MatIterator&,
                      VecIterator&, XIterator&, XIterator&,
                      const std::vector<Number>&, const std::vector<Number>&, const Real)
                          const;

template<typename MatIterator, typename VecIterator, typename XIterator>
void bzSorDiagonalSolver(const MatIterator& itdb, VecIterator& itbb,
                         XIterator& itxb, XIterator& itxe, const Real w) const;

template<typename MatRevIterator, typename VecRevIterator, typename XRevIterator>
void bzSorUpperSolver(const MatRevIterator&, const MatRevIterator&,
                      VecRevIterator&, XRevIterator&, XRevIterator&,
                      const std::vector<Number>&, const std::vector<Number>&, const Real)
                          const;
```

Addition of two matrices are implemented by

```
template<typename Mat1Iterator, typename Mat2Iterator, typename ResIterator>
void sumMatrixMatrix(Mat1Iterator&, Mat2Iterator&, ResIterator&, ResIterator&) const;
```

| | |
|---|---|
| library : | **largeMatrix** |
| header : | **CsStorage.hpp** |
| implementation : | **CsStorage.cpp** |
| unitary tests : | **test_LargeMatrixCstorage.cpp** |
| header dependences : | **MatrixStorage.hpp, config.h, utils.h** |

### 9.4.2 `Row/ColCsStorage` classes

As mentioned before, row compressed storage are based on the column indices vector and the row pointers vector. So the `RowCsStorage` class carries this two vectors:

```
class RowCsStorage : public CsStorage
{protected :
  std::vector<Number> colIndex_;   //vector of column index of non zero value
  std::vector<Number> rowPointer_; //vector of positions of begining of rows
  ...
```

The class provides a default constructor with no construction of storage vectors and constructors from a list of $(i,j)$ index (coordinates) or a lists of column indices by row, constructing the compressed storage vectors:

```
RowCsStorage(Number nr=0, Number nc=0);
RowCsStorage(Number, Number, const std::vector< std::vector<Number> >&,
             const std::vector< std::vector<Number> >&);
RowCsStorage(Number, Number, const std::vector< std::vector<Number> >&);
~RowCsStorage() {};
```

The class provides most of the virtual methods declared in `MatrixStorage` class. For sake of simplicity, we report here only function with `Real` type but versions with `Complex`, `Matrix<Real>`, `Matrix<Complex>` and mixed types are also provided. Some template line declarations are also omitted.

```
Number size() const;
Number pos(Number i, Number j, SymType s=_noSymmetry) const;
void positions(const std::vector<Number>&, const std::vector<Number>&,
               std::vector<Number>&, bool errorOn=true,
               SymType s=_noSymmetry) const;
void printEntries(std::ostream&, const std::vector<Real>&, Number, SymType) const;
void printCooMatrix(std::ostream&, const std::vector<Real>&,
                    SymType s=_noSymmetry) const;
void loadFromFileDense(std::istream&, std::vector<Real>&, SymType, bool );
void loadFromFileCoo(std::istream& , std::vector<Real>&, SymType, bool);
template<typename M, typename V, typename R>
  void multMatrixVector(const std::vector<M>&, const std::vector<V>&,
                        std::vector<R>&) const;
  void multVectorMatrix(const std::vector<M>&, const std::vector<V>&,
                        std::vector<R>&) const;
  void multMatrixVector(const std::vector<Real>&, const std::vector<Real>&,
                        std::vector<Real>&, SymType) const;
  void multVectorMatrix(const std::vector<Real>&, const std::vector<Real>&,
                        std::vector<Real>&, SymType) const;
template<typename M1, typename M2, typename R>
  void addMatrixMatrix(const std::vector<M1>&, const std::vector<M2>&, std::vector<R>&) const;
      //!< templated row dense Matrix + Matrix
  void addMatrixMatrix(const std::vector<Real>& m, const std::vector<Real>& v, std::vector<Real>&
      rv) const
    { addMatrixMatrix<>(m, v, rv);}
```

There is no `printDenseMatrix` function because the general one defined in `MatrixStorage` class is sufficiently efficient.

The `ColCsStorage` class is very similar to the `RowCsStorage` class, except that it manages a row indices vector and a column pointers vector:

```
class ColCsStorage : public CsStorage
{protected :
  std::vector<Number> rowIndex_;   //!< vector of row index of non zero value
  std::vector<Number> colPointer_; //!< vector of positions of begining of cols
  ...
```

Its constructors have a similar structure (same arguments) and all prototypes of member functions are the same as `ColCsStorage` member functions. We do not repeat them. XXX=Row or Col

| | |
|---:|:---|
| library : | **largeMatrix** |
| header : | **XXXCsStorage.hpp** |
| implementation : | **XXXCsStorage.cpp** |
| unitary tests : | **test_LargeMatrixCsStorage.cpp** |
| header dependences : | **CsStorage.hpp, MatrixStorage.hpp, config.h, utils.h** |

### 9.4.3 Dual/SymCsStorage classes

Dual compressed storage travels the matrix as diagonal, strict lower and upper parts. Column indices and row pointers vectors are attached to strict lower part and row indices and column pointers vectors are attached to strict upper part:

```
class DualCsStorage : public CsStorage
{protected :
  std::vector<Number> colIndex_;    //vector of column index of non zero value
  std::vector<Number> rowPointer_;  //vector of positions of begining of rows
  std::vector<Number> rowIndex_;    //vector of row index of non zero value
  std::vector<Number> colPointer_;  //vector of positions of begining of cols
  ...
```

DualCsStorage class provides basic constructor (no construction of storage vectors), constructor from a pair of global numbering vectors or list of column indices by rows. Both of them create the compressed storage vector using the auxiliary function buildStorage:

```
DualCsStorage(Number nr=0, Number nc=0);
DualCsStorage(Number, Number, const std::vector< std::vector<Number> >&,
              const std::vector< std::vector<Number> >&);
DualCsStorage(Number, Number, const std::vector<std::vector<Number> >&);
void buildStorage(const std::vector<std::vector<Number> >&);
~DualCsStorage() {};
```

The class provides most of the virtual methods declared in MatrixStorage class. For sake of simplicity, we report here only function with Real type but versions with Complex, Matrix<Real>, Matrix<Complex> and mixed types are also provided. Some template line declarations are also omitted.

```
Number size() const;
Number lowerPartSize() const ;
    Number upperPartSize() const;
Number pos(Number i, Number j, SymType s=_noSymmetry) const;
void positions(const std::vector<Number>&, const std::vector<Number>&,
               std::vector<Number>&, bool errorOn=true,
               SymType s=_noSymmetry) const;
void printEntries(std::ostream&, const std::vector<Real>&, Number, SymType) const;
void printCooMatrix(std::ostream&, const std::vector<Real>&,
                    SymType s=_noSymmetry) const;
void loadFromFileDense(std::istream&, std::vector<Real>&, SymType, bool );
void loadFromFileCoo(std::istream& , std::vector<Real>&, SymType, bool);
template<typename M, typename V, typename R>
  void multMatrixVector(const std::vector<M>&, const std::vector<V>&,
                        std::vector<R>&) const;
  void multVectorMatrix(const std::vector<M>&, const std::vector<V>&,
                        std::vector<R>&) const;
  void multMatrixVector(const std::vector<Real>&, const std::vector<Real>&,
                        std::vector<Real>&, SymType) const;
  void multVectorMatrix(const std::vector<Real>&, const std::vector<Real>&,
                        std::vector<Real>&, SymType) const;
template<typename M1, typename M2, typename R>
  void addMatrixMatrix(const std::vector<M1>&, const std::vector<M2>&, std::vector<R>&) const;
  void addMatrixMatrix(const std::vector<Real>& m, const std::vector<Real>& v, std::vector<Real>&
      rv) const
    { addMatrixMatrix<>(m, v, rv);}
```

The SymCsStorage class is very similar to the DualCsStorage class, except that it addresses only square matrix with symmetric storage and, thus, does not manage row indices vector and column pointers vectors because the upper part has same storage as lower part (transposed). Note that matrix may be have no symmetry property but a symmetric storage. In that case, the upper part is stored.

```
class SymCsStorage : public CsStorage
{protected :
  std::vector<Number> colndex_;    //!< vector of row index of non zero value
  std::vector<Number> rowPointer_; //!< vector of positions of begining of cols
  ...
```

Contrary to the row compressed storage, in the SymCsStorage, the diagonal is first stored then the lower part of the matrix.
Its constructors have a similar structure (same arguments) to the `DualCsStorage` constructors and all prototypes of member functions are the same as `DualCsStorage` member functions. We do not repeat them.
Different from other `CsStorage` classes, the `SymCsStorage` class provides some functions to deal with the `SorSolver` class and `SsorSolver` class. Only specialized functions with `Real` are listed in the following

```
void sorDiagonalMatrixVector(const std::vector<Real>& m, const std::vector<Real>& v,
    std::vector<Real>& rv, const Real w) const
{ sorDiagonalMatrixVector<>(m, v, rv, w); }
void sorLowerMatrixVector(const std::vector<Real>& m, const std::vector<Real>& v,
    std::vector<Real>& rv, const Real w, const SymType sym) const
{ sorLowerMatrixVector<>(m, v, rv, w, sym); }
void sorUpperMatrixVector(const std::vector<Real>& m, const std::vector<Real>& v,
    std::vector<Real>& rv, const Real w, const SymType sym) const
{ sorUpperMatrixVector<>(m, v, rv, w, sym); }
void sorDiagonalSolve(const std::vector<Real>& m, const std::vector<Real>& b, std::vector<Real>&
    x, const Real w) const
{ sorDiagonalSolve<>(m, b, x, w); }
void sorLowerSolve(const std::vector<Real>& m, const std::vector<Real>& b, std::vector<Real>& x,
    const Real w) const
{ sorLowerSolve<>(m, b, x, w); }
void sorUpperSolve(const std::vector<Real>& m, const std::vector<Real>& b, std::vector<Real>& x,
    const Real w, const SymType sym) const
{ sorUpperSolve<>(m, b, x, w, sym); }
```

XXX=Dual or Sym

| | |
|---:|:---|
| library : | **largeMatrix** |
| header : | **XXXCsStorage.hpp** |
| implementation : | **XXXCsStorage.cpp** |
| unitary tests : | **test_LargeMatrixCsStorage.cpp** |
| header dependences : | **CsStorage.hpp, MatrixStorage.hpp, config.h, utils.h** |

## 9.5 Skyline storages

With dense storages, skyline storages are the only storages that are compatibles with factorisation methods like LU. Skyline storages consist in storage rows or columns from its first non zero value up to its last non zero value. When lower triangular part is addressed, the last non zero value on a row is the diagonal matrix entry. When upper triangular part is addressed, the last non zero value on a column is the diagonal matrix entry. Only dual and symmetric skyline storages are proposed here (resp. `DualSkylineStorage` and `SymSkylineStorage` classes).

- Dual skyline stores first the diagonal of the matrix, then the strict lower "triangular" part and the strict upper "triangular" part of the matrix using the following storage vectors ($A$ is a $m \times n$ matrix):

  values=(0, $A_{11}, ..., A_{ii}, ..., A_{il}, ..., A_{i,p_i}, ..., A_{i,l_i}, ..., A_{q_j,j}, ..., A_{q_j,c_j}$)
  rowPointer=($s_1, ..., s_i, ..., s_m, s_{m+1}$)
  colPointer=($t_1, ..., t_j, ..., t_n, t_{n+1}$)

where

$$\begin{aligned}
&l_i = \min(i-1, n-1),\ c_j = \min(j-1, m-1)\\
&p_i = \min 0 < j < l_i,\ A_{ij} \neq 0 \text{ and } q_j = \min 0 < i < c_j,\ A_{ij} \neq 0\\
&s_1 = 0;\ s_i = s_{i-1} + i - s_{i-1}\ \forall i = 2, m, \text{ and } t_1 = 0;\ t_j = s_{j-1} + j - t_{j-1}\ \forall j = 2, n
\end{aligned}$$

The rowPointer (resp. colPointer) vector gives the position in lower (resp. upper) part of the first non zero entry of a row (resp. a column); $s_{m+1}$ (resp.$t_{n+1}$) gives the number of entries stored in lower part (resp. upper part).

For instance, the following 5 × 6 non symmetric matrix

$$A = \begin{bmatrix} 11 & 12 & 0 & 14 & 0 & 16\\ 0 & 22 & 23 & 0 & 0 & 26\\ 31 & 32 & 33 & 0 & 0 & 0\\ 0 & 0 & 43 & 44 & 0 & 0\\ 51 & 0 & 53 & 54 & 55 & 0 \end{bmatrix}$$

has the following storage vectors:

values = ( 0 11 22 33 44 45  22  31 32  43  51 0 53 54   12  23  14 0 0   16 26 0 0 )<br>
rowPointer = ( 0 0 0 2 3 7 )<br>
colPointer = ( 0 0 1 2 5 5 8 )

The lengh of row $i$ (resp. column $j$) is given by $s_{i+1} - s_i$ (resp. $t_{t+1} - t_j$). The position in values vector of entry $(i, j)$ is given by the following relations ($1 \leq i \leq m$, $1 \leq j \leq n$):

$$\begin{aligned}
&\text{if } i = j\ \ \mathrm{adr}(i,j) = i\\
&\text{if } p_i \leq j \leq l_i\ \ \mathrm{adr}(i,j) = \min(m,n) + s_{i+1} + j - i\\
&\text{if } q_j \leq i \leq c_j\ \ \mathrm{adr}(i,j) = \min(m,n) + s_{m+1} + t_{j+1} + i - j
\end{aligned}$$

### 9.5.1 The SkylineStorage class

The SkylineStorage class has no member attribute. It has some basic constructors just calling MatrixStorage constructors:

```
class SkylineStorage : public MatrixStorage
{public :
  SkylineStorage(AccessType = _dual);
  SkylineStorage(Number, AccessType = _dual);
  SkylineStorage(Number, Number, AccessType = _dual);
  virtual ~SkylineStorage() {}
```

SkylineStorage objects do not have to be instantiated. This abstract class acts as an interface to particular skyline storages and gathers all common functionalities of skyline storages, some being virtuals (some template line declarations are omitted):

```
virtual Number size() const = 0;
virtual Number lowerPartSize() const = 0;
virtual Number upperPartSize() const {return 0;}
template<typename Iterator>
 void printEntriesTriangularPart (StrucType, Iterator&, Iterator&, const std::vector<Number>&,
      Number, Number, Number, const String&, Number, std::ostream&) const;
 void printCooTriangularPart(std::ostream&, Iterator&, const std::vector<Number>&, Number,
      Number, bool, SymType sym = _noSymmetry) const;
 void printCooDiagonalPart(std::ostream&, Iterator&, Number) const;

template <typename T>
```

```
 void loadSkylineFromFileDense(std::istream&, std::vector<T>&, std::vector<Number>&,
      std::vector<Number>&, SymType, bool);
 void loadSkylineFromFileCoo(std::istream&, std::vector<T>&, std::vector<Number>&,
      std::vector<Number>&, SymType, bool);

template<typename MatIterator, typename VecIterator, typename ResIterator>
 void diagonalMatrixVector(MatIterator&, VecIterator&, ResIterator&, ResIterator&) const;
 void lowerMatrixVector(const std::vector<Number>&, MatIterator&, VecIterator&, ResIterator&,
      SymType sym) const;
 void upperMatrixVector(const std::vector<Number>&, MatIterator&, VecIterator&, ResIterator&,
      SymType) const;
 void diagonalVectorMatrix(MatIterator&, VecIterator&, ResIterator&, ResIterator&) const;
 void lowerVectorMatrix(const std::vector<Number>&, MatIterator&, VecIterator&, ResIterator&,
      SymType sym) const;
 void upperVectorMatrix(const std::vector<Number>&, MatIterator&, VecIterator&, ResIterator&,
      SymType) const;
 void sumMatrixMatrix(Mat1Iterator&, Mat2Iterator&, ResIterator&, ResIterator&) const;
```

The SkylineStorage class provides the real code of product of matrix and vector, using iterators as arguments to by-pass the template type of matrix values.
In order to deal with some specific solvers, this class also comes with several following functions. For simplicity, we only declare template line once.

```
template<typename MatIterator, typename VecIterator, typename XIterator>
void bzLowerSolver(const MatIterator&, const MatIterator&, const VecIterator&,  const XIterator&,
    const XIterator&, const std::vector<size_t>::const_iterator) const;
void bzLowerD1Solver(const MatIterator&, const VecIterator&, const XIterator&, const XIterator&,
    const std::vector<size_t>::const_iterator) const;
void bzLowerConjD1Solver(const MatIterator&, const VecIterator&,  const XIterator&, const
    XIterator&,  const std::vector<size_t>::const_iterator) const;
void bzDiagonalSolver(const MatIterator&, const VecIterator&,  const XIterator&, const
    XIterator&) const;
void bzUpperSolver(const MatRevIterator&, const MatRevIterator&, const VecRevIterator&,  const
    XRevIterator&, const XRevIterator&, const std::vector<size_t>::const_reverse_iterator) const;
void bzUpperD1Solver(const MatRevIterator&, const VecRevIterator&, const XRevIterator&, const
    XRevIterator&, const std::vector<size_t>::const_reverse_iterator) const;
void bzUpperConjD1Solver(const MatRevIterator&, const VecRevIterator&, const XRevIterator&, const
    XRevIterator&, const std::vector<size_t>::const_reverse_iterator) const;
```

Like the product of matrix and vector, these functions take advantage of iterators as arguments to by-pass the template type of matrix values.

| | |
|---|---|
| library : | **largeMatrix** |
| header : | **SkylineStorage.hpp** |
| implementation : | **SkylineStorage.cpp** |
| unitary tests : | **test_LargeMatrixSkylinetorage.cpp** |
| header dependences : | **MatrixStorage.hpp, config.h, utils.h** |

### 9.5.2 Dual/SymSkylineStorage classes

Dual skyline storage travels the matrix as diagonal, strict lower and upper parts. Row pointers vectors are attached to strict lower part and column pointers vectors are attached to strict upper part:

```
class DualSkylineStorage : public SkylineStorage
{protected :
  std::vector<Number> rowPointer_; // vector of positions of begining of rows
  std::vector<Number> colPointer_; // vector of positions of begining of cols
  ...
```

DualSkylineStorage class provides basic constructor (no construction of storage vectors), constructor from a pair of global numbering vectors or list of column indices by rows. Both of them create the compressed storage vector using the auxiliary function buildStorage:

```
DualSkylineStorage(Number nr = 0, Number nc = 0);
DualSkylineStorage(Number, Number, const std::vector< std::vector<Number> >&,
                   const std::vector< std::vector<Number> >&);
DualSkylineStorage(Number, Number, const std::vector< std::vector<Number> >&);
~DualSkylineStorage() {};
```

The class provides most of the virtual methods declared in MatrixStorage class. For sake of simplicity, we report here only function with Real type but versions with Complex, Matrix<Real>, Matrix<Complex> and mixed types are also provided. Some template line declarations are also omitted.

```
Number size() const;
Number lowerPartSize() const ;
Number upperPartSize() const;
Number pos(Number i, Number j, SymType s=_noSymmetry) const;
void positions(const std::vector<Number>&, const std::vector<Number>&,
               std::vector<Number>&, bool errorOn=true,
               SymType s=_noSymmetry) const;
void printEntries(std::ostream&, const std::vector<Real>&, Number, SymType) const;
void printCooMatrix(std::ostream&, const std::vector<Real>&,
                    SymType s=_noSymmetry) const;
void loadFromFileDense(std::istream&, std::vector<Real>&, SymType, bool );
void loadFromFileCoo(std::istream& , std::vector<Real>&, SymType, bool);
template<typename M, typename V, typename R>
  void multMatrixVector(const std::vector<M>&, const std::vector<V>&,
                        std::vector<R>&) const;
  void multVectorMatrix(const std::vector<M>&, const std::vector<V>&,
                        std::vector<R>&) const;
  void multMatrixVector(const std::vector<Real>&, const std::vector<Real>&,
                        std::vector<Real>&, SymType) const;
  void multVectorMatrix(const std::vector<Real>&, const std::vector<Real>&,
                        std::vector<Real>&, SymType) const;
template<typename M1, typename M2, typename R>
  void addMatrixMatrix(const std::vector<M1>&, const std::vector<M2>&, std::vector<R>&) const;
template<typename T>
  void setDiagValueDualSkyline(std::vector<T>&, const T);
template<typename M>
void lu(std::vector<M>& m, std::vector<M>& fa) const;
template<typename M, typename V, typename X>
  void lowerD1Solver(const std::vector<M>&, std::vector<V>&, std::vector<X>&) const;
  void diagonalSolver(const std::vector<M>&, std::vector<V>&, std::vector<X>&) const;
  void upperD1Solver(const std::vector<M>&, std::vector<V>&, std::vector<X>&, const SymType)
      const;
  void upperSolver(const std::vector<M>&, std::vector<V>&, std::vector<X>&) const;
```

The SymSkylineStorage class is very similar to the DualSkylineStorage class, except that it adresses only square matrix with symmetric storage and, thus, does not manage column pointers vectors because the upper part has same storage as lower part (with transposition) :

```
class SymSkylineStorage : public SkylineStorage
{protected :
  std::vector<Number> rowPointer_; //!< vector of positions of begining of cols
  ...
```

Note that the matrix may be not symmetric. In that case its upper part is stored.
Besides some similar functions to DualSkylineStorage class', the SymSkylineStorage provides more several functions to factorize matrix: LDLt and LDL* factorization

```
template<typename M>
    void ldlt(std::vector<M>& m, std::vector<M>& fa, const SymType sym = _symmetric) const;
    void ldlstar(std::vector<M>& m, std::vector<M>& fa) const;
```

XXX=Dual or Sym

| | |
|---|---|
| library : | **largeMatrix** |
| header : | **XXXSkylineStorage.hpp** |
| implementation : | **XXXSkylineStorage.cpp** |
| unitary tests : | **test_LargeMatrixSkylineStorage.cpp** |
| header dependences : | **SkylineStorage.hpp, MatrixStorage.hpp, config.h, utils.h** |

# 10 The *hierarchicalMatrix* library

The *hierarchicalMatrix* library deals with large matrices that are represented by a hierarchical tree, each tree node being either a real submatrix (leaf) or a virtual submatrix adressing up to four nodes:

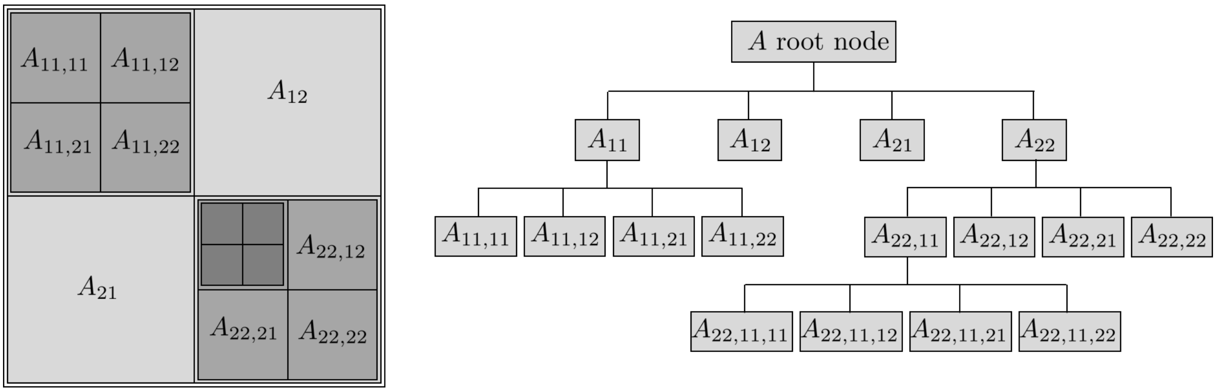


Figure 10.1: Hierachical matrix

The matrix may be not squared and therefore the submatrices too.

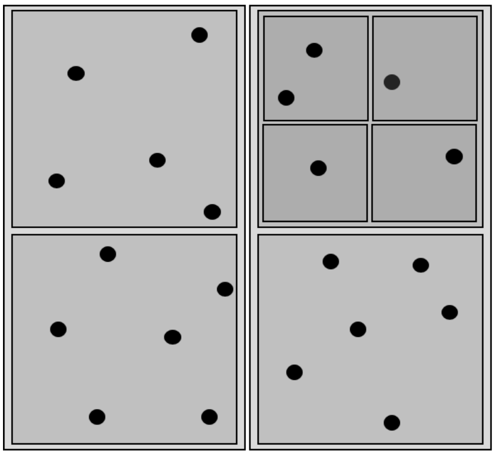
Such representation comes from mesh partition (clustering) where far interactions in BEM may be approximated by low rank matrices, so reducing the storage of matrix and making the matrix vector product faster. The *hierarchicalMatrix* library proposes

- some templated classes to deal with clusters of Points, FeDofs, Elements, ... : `ClusterTree<I>` and `ClusterNode<I>`
- some templated classes to deal with approximated matrices : `ApproximateMatrix<T>` and `LowRankMatrix<T>`
- some templated classes addressing hierarchical matrices : `HMatrix<T,I>`, `HMatrixNode<T,I>` and `HMatrixEntry<I>`

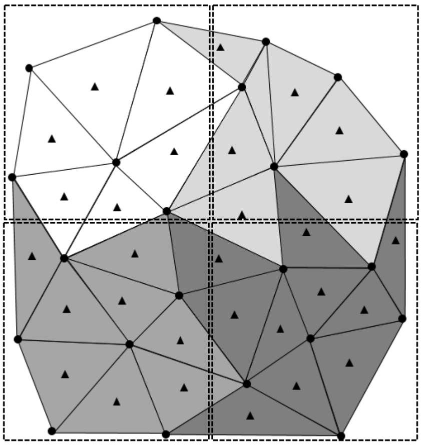
## 10.1 Cluster tree

The clustering of a set of objects consists in a partition of this set with a hierarchical structure. Each node of the cluster being a subset of the parent node subset. The partitioning of a subset is done according to some rules depending of the purpose of the cluster.

In the case of a mesh, we are interested in clusters of points (mesh nodes) or in clusters of elements where the partitioning rule aims to separate geometrically the points or the elements.



Cluster of points



Clustering of triangles using centroids

XLIFE++ provides two classes templated by the type T of objects to be clustered :

- ClusterNode<T> managing one node of the tree representation
- ClusterTree<T> managing the tree representation from the root node

### 10.1.1 The ClusterNode class

The ClusterNode<T> class describes one node of the tree representing the cluster where T is the type of objects to be clustered. It is assumed that T is a geometric object and that the three following functions are available:

```
dimen_t dim(const T&) const;                 //dimension of T object
real_t coords(const T&, number_t i) const    //i-th coordinates of T object
BoundingBox boundingBox(const T &)           //xy(z) bounding box of T object
```

For instance, these functions are provided for the XLIFE++ classes : Point, FeDof, Element allowing to cluster mesh using either some points of mesh (vertices), some finite element dofs or some finite elements.

The class manages standard informations:

```
vector<T>* objects_;       //pointer to the list of all objects
vector<number_t> numbers_; //object numbers related to objects_ vector
ClusterNode* parent_;      //pointer to its parent (0 for root node)
ClusterNode* child_;       //pointer to its first child (0 = no child)
ClusterNode* next_;        //pointer to its brother, (0 = no brother)
number_t depth_;           //depth of node/leaf in tree (0 for root node)
BoundingBox boundingBox_;        //bounding box from characteristic points
BoundingBox realBoundingBox_;    //bounding box from bounding boxes of objects
```

The list of objects belonging to the cluster node is given by the numbers_ vector that stores the indices of objects in the vector objects_. The clusters we deal with are supposed to be geometrical clusters and the clustering methods are mainly based on splitting of boxes, it is the reason why the class deals explicitly with bounding boxes. In the context of finite element, some additional data (mutable) can be handled :

```
vector<number_t> dofNumbers_;  //list of dof numbers related to the node
vector<Element*> elements_;    //list of element numbers related to the node
```

The class provides only one constructor assigning fundamental data (objects_, parent_, child_, next_, depth_) and a clear method that deletes recursively the subtree from the current node:

```
ClusterNode(vector<T>*,ClusterNode*,number_t, ClusterNode*=0, ClusterNode*=0);
void clear();
```

The copy constructor and assignment operator are the default ones, so the tree structure is not duplicated but only shared. Be cautious, when you use copy or assignment.

The class provides some functions to get some properties or data:

```
number_t dimSpace() const;    //geometric dimension
number_t size() const;        //number of objects
bool isVoid() const;          //true if void node
vector<ClusterNode*> getLeaves() const; //list of leave pointers
list<number_t> getNumbers(bool) const;  //list of Numbers (recursive)
const BoundingBox& box() const;     //return the real bounding box if allocated
real_t boxDiameter() const;         //diameter ot the (real) bounding box
```

The main member function that builds the tree structure from a division process is:

```
void divideNode(ClusteringMethod cm, number_t mininleaf,
                number_t maxdepth=0, bool store = true);
```

where

- ClusteringMethod is the enumeration of clustering methods:

```
enum ClusteringMethod { _regularBisection, _boundingBoxBisection,
                        _cardinalityBisection, _uniformKdtree, _nonuniformKdtree };
```

  Except the _uniformKdtree and _nonuniformKdtree methods, each others are bisection method in the direction where the boxes is larger, so the tree is a binary one. _regularBisection split boxes in two boxes of the same size, _boundingBoxBisection split bounding boxes of objects in two boxes of the same size, _cardinalityBisection split boxes in two boxes such that each new boxes have the same number of objects. The trees produced by this last method are better balanced. The _uniformKdtree and _nonuniformKdtree methods split any boxes in 2, 4 or 8 sub-boxes regarding the space dimension (1, 2 or 3); the sub-boxes are of the same size in any direction. Thus it produces binary tree in 1D, quadtree in 2D and octree in 3D. With _uniformKdtree method, all the boxes at the same level have the same size whereas with _nonuniformKdtree method, all the boxes are the minimal bounding boxes defined from the objects that they embed.

- maxinleaf is the maximum of objects in a leaf node, more precisely, a node is divided when its number of objects is greater than maxinleaf

- maxdepth, if not null, allows to stop the division process when maxdepth is reached. This stopping criteria has priority over the previous criteria.

- if store parameter is true, data (numbers_, bounding boxes, ...) are stored for each node else they are only stored for each leaves. By default its value is true, but if cluster is too large, not storing some data may save memory but some algorithms working on clusters could be slower.

Up to now, only three clustering methods are offered, but it is quite easy to add a new one by handling a new case in divideNode function. Bisection methods build binary tree but there is not limitation of the number of children in the ClusterNode class!

When some data (numbers_, bounding boxes, ...) are not available it is possible to build or update it:

```
void setBoundingBox();            //set the bounding box
void setRealBoundingBox();        //set the real bounding box
void updateRealBoundingBoxes();   //update recursively real bounding boxes
void updateNumbers();             //update numbers_ vector
```

When dealing with finite elements some additional data may be useful, in particular the link between dofs and elements. To avoid costly re-computation, it may be clever to store it. The following member functions do the job on demand when working with a `ClusterNode<FeDof>` or a `ClusterNode<Element>`:

```
const vector<number_t>& dofNumbers() const; //access to dofNumbers
const vector<Element*>& elements() const;   //access to elt pointers
vector<number_t> getDofNumbers(bool=false) const; //list of dof numbers
vector<Element*> getElements(bool=false) const;   //list of elt numbers
void updateDofNumbers();                     //update recursively dofNumbers
void updateElements();                       //update recursively elements
number_t nbDofs() const;                     //number of dofs
```

Finally, there are some stuff to print and save to file node informations:

```
void printNode(std::ostream&, bool shift=true) const; //print node
void print(std::ostream&) const;          //print tree from current node (recursive)
void printLeaves(std::ostream&) const;    //print leaves of the tree
void saveToFile(const string_t&, bool) const; //save bounding boxes to file
friend ostream& operator<<(std::ostream&, const ClusterNode<T>&);
```

### 10.1.2 The `ClusterTree` class

The `ClusterTree<T>` class is the front end of `ClusterNode<T>` class which supports the tree structure of the cluster. Because the `ClusterTree<T>` class interfaces most data and functionnalities of the `ClusterNode<T>` class, for explanation go to the previous section.

The `ClusterTree<T>` class manages the parameters and informations required or provided by the the `ClusterTree<T>` class. It handles the tree structure (the cluster) through the root node pointer:

```
template <typename T = FeDof> class ClusterTree
{public:
vector<T>* objects_;          //pointer to a list of objects
ClusteringMethod method_;     //clustering method
number_t maxInBox_;           //maximum number of objects in a leaf
number_t depth;               //depth of the tree
bool storeNodeData_;          //store data on each node if true
bool clearObjects_;           //if true deallocate vector objects_ when clear
number_t nbNodes;             //number of nodes (info)
number_t nbLeaves;            //number of leaves (info)
bool withOverlap_;            //true if dof numbering of nodes overlap
bool noEmptyBox_;             //do not keep empty boxes in tree
 private:
ClusterNode<T>* root_;        //root node of cluster
...
```

Note that the `ClusterTree` has `FeDof` object as template default argument. This is the standard cluster used by the `HMatrix` class presented in a next section.
This class provides a unique constructor, building the cluster from a list of geometric object, a clustering method, the maximal depth of the tree, the maximal number of objects in leaf node and a flag telling if empty leaf nod are removed from the tree :

```
ClusterTree(const vector<T>&, ClusteringMethod, number_t depth,
            number_t maxinleaf=0, bool store=true, bool noemptybox = true);
```

The copy constructor and assignment operator are the default ones, so the tree structure is not duplicated but only shared. Be cautious, when you use copy or assignment. In particular avoid destruction of `ClusterTree` object, except if you set the member data `clearObjects_` to `false` before destroy it.

Almost all the member functions are interface to their equivalent in `ClusterNode` class:

```
ClusterNode<T>* root();
void setOverlap();
void updateBoundingBoxes();            //update recursively bounding boxes
void updateRealBoundingBoxes();        //update recursively real bounding boxes
void updateNumbers();                  //update recursively Numbers_ vector
void updateDofNumbers();               //update recursively DofNumbers_ vector
void updateElements();                 //update recursively Elements_ vector
void updateInfo();                     //update tree info (depth, ...)
number_t nbDofs() const;
void print(ostream&) const;            //print tree
void printLeaves(ostream&) const;      //print only leaves
void saveToFile(const string_t&,
     bool withRealBox= false) const; //save (real) bounding boxes to file
ostream& operator<<(ostream& out, const ClusterTree<T>&);
```

For instance, to generate a cluster of a disk mesh, write :

```
Disk disk(_center=Point(0.,0.),_radius=1.,_nnodes=16,_domain_name="Omega");
Mesh mesh(disk,_triangle,1,_gmsh);
Domain omg=mesh.domain("Omega");
Space V(omg,P0,"V",false);
ClusterTree<FeDof> clt(V.feSpace()->dofs,_regularBisection,10);
clt.saveToFile("cluster_disk.txt");
```

As the dofs of P0 approximation are virtually located at the centroids of triangles, clustering of FeDof is equivalent to the clustering of centroids. We show on the figure 10.2 the clustering of a disk mesh (1673 nodes) with maximum of 10 nodes by box, using regular method, boundingbox, cardinality bisection methods. Only boxes of leaves are displayed; different colors correspond to different node depths.

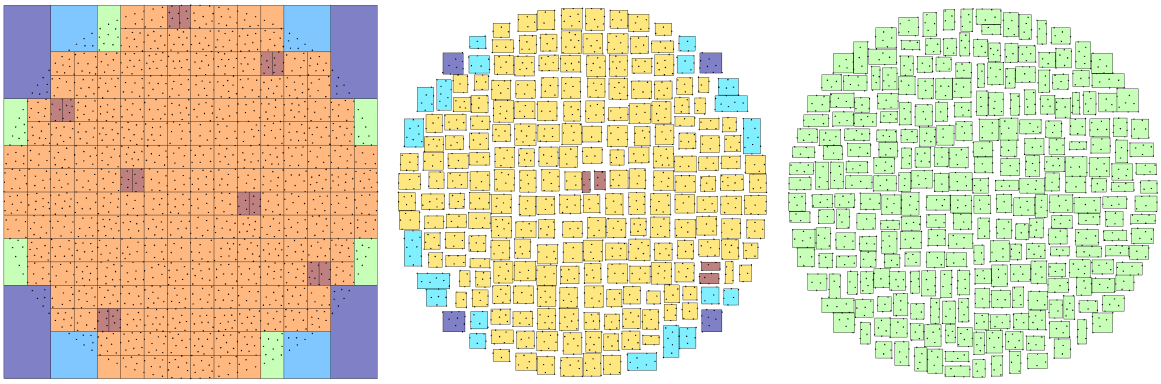


Figure 10.2: clustering of a disk mesh using regular, boundingbox and cardinality bisection methods

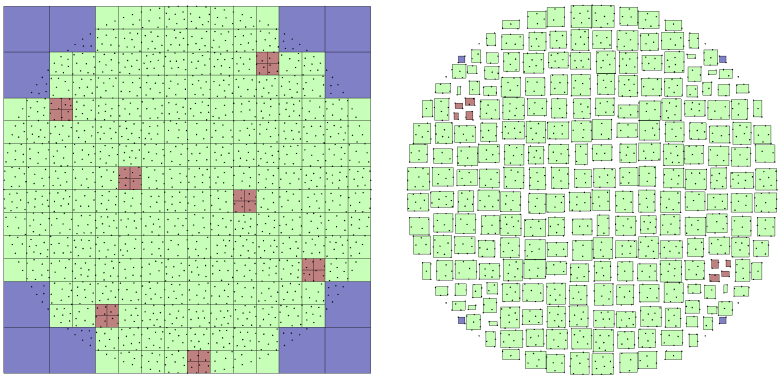


Figure 10.3: clustering of a disk mesh using `_uniformKdtree` and `_nonuniformKdtree` methods

| | |
|---|---|
| library : | **hierarchicalMatrix** |
| header : | **clusterTree.hpp** |
| implementation : | **clusterTree.cpp** |
| unitary tests : | **test_clusterNode.cpp** |
| header dependences : | **space.h, config.h, utils.h** |

## 10.2 Approximate matrix

In the context of hierarchical matrix, some sub-matrices may be "compressed" to save memory and time computation. XLiFE++ provides a general class `ApproximateMatrix` to deal with real or complex approximate matrix that can be

- low rank matrix represented as the product $UDV^*$ (`LowRankMatrix`)
- sinus cardinal decomposition (`SCDMatrix`), not yet available
- fast multipole representation (`FMMMatrix`), not yet available

### 10.2.1 The `ApproximateMatrix` class

The `ApproximateMatrix` class is a template abstract class (templated by the type of coefficients) that manages only the type of approximation, the name of the approximate matrix and defines all virtual functions that children has to implement:

```
template <typename T>
class ApproximateMatrix
{public :
MatrixApproximationType approximationType;      //type of approximation
string_t name;                                  //optional name useful for doc
virtual ~ApproximateMatrix() {};                //virtual destructor
virtual ApproximateMatrix<T>* clone() const=0;  //creation of a clone
virtual number_t numberOfRows() const =0;       //nb of rows
virtual number_t numberOfCols() const =0;       //nb of columns
virtual number_t nbNonZero() const =0;          //nb of non zeros coefficient
virtual number_t rank() const =0;               //rank of matrix
virtual vector<T>& multMatrixVector(const vector<T>&, vector<T>&) const = 0;
virtual vector<T>& multVectorMatrix(const vector<T>&, vector<T>&) const = 0;
virtual real_t norm2() const =0;                   //Frobenius norm
virtual real_t norminfty() const=0;                //infinite norm
virtual LargeMatrix<T> toLargeMatrix() const = 0;  //convert to LargeMatrix
virtual void print(std::ostream&) const =0;        //print to stream
};
```

Up to now, the only children available is the templated `LowRankMatrix<T>` class.

### 10.2.2 The `LowRankMatrix` class

A low rank matrix is a matrix of the form

$$UDV^*$$

where $U$ is a $m \times r$ matrix, $V$ is a $n \times r$ matrix and $D$ is a $r \times r$ diagonal matrix. The rank of a such matrix is at most $r$. So it is a low rank representation of a $m \times n$ matrix if $r$ is small compared to $m$, $n$. Contrary to the class name suggests, some matrix may be not low rank representation. Think about the SVD (singular value decomposition) of a $m \times n$ matrix that can be handled by this class ($r = \min(m, n)$).

The `LowRankMatrix` class is derived from the `ApproximateMatrix` and handles the $U, V$ matrices as `Matrix` objects of XLiFE++ (dense matrix with major row access) and the diagonal matrix $D$ as a `Vector` object of XLiFE++:

```
template <typename T>
class LowRankMatrix : public ApproximateMatrix<T>
{public :
 Matrix<T> U_, V_;
 Vector<T> D_;
 ...
}
```

Different constructors are available:

```
LowRankMatrix();      //default constructor
//constructor from explicit matrices and vector
LowRankMatrix(const Matrix<T>&, const Matrix<T>&, const Vector<T>&,
              const string_t& na="");
LowRankMatrix(const Matrix<T>&, const Matrix<T>&, const string_t& na="");
//constructor from dimensions
LowRankMatrix(number_t m, number_t n, number_t r, const string_t& na="");
LowRankMatrix(number_t m, number_t n, number_t r, bool noDiag,
              const string_t& na="");
//constructor from matrix iterators and vector iterator
template <typename ITM, typename ITV>
LowRankMatrix(number_t m, number_t n, number_t r,
              ITM itmu, ITM itmv, ITV itd, const string_t& na="");
template <typename ITM>
LowRankMatrix(number_t m, number_t n, number_t r,
              ITM itmu, ITM itmv, const string_t& na="");
```

The `LowRankMatrix` class provides all virtual functions declared by the `ApproximateMatrix` class:

```
ApproximateMatrix<T>* clone() const;
number_t numberOfRows() const;
number_t numberOfCols() const;
number_t nbNonZero() const;
number_t rank() const;
bool hasDiag() const;
vector<T>& multMatrixVector(const vector<T>&, vector<T>&) const;
vector<T>& multVectorMatrix(const vector<T>&, vector<T>&) const;
LargeMatrix<T> toLargeMatrix() const;
real_t norm2() const;
real_t norminfty() const;
void print(std::ostream&) const;
```

In addition, the class offers specific algebraic operations as member functions:

```
LowRankMatrix<T> svd(real_t eps) const;
LowRankMatrix<T>& operator+=(const LowRankMatrix<T>&);
LowRankMatrix<T>& operator-=(const LowRankMatrix<T>&);
LowRankMatrix<T>& operator*=(const T&);
LowRankMatrix<T>& operator/=(const T&);
LowRankMatrix<T>& add(const LowRankMatrix<T>&, const T&, real_t eps=0);
```

and as extern functions to the class (template declaration is omitted):

```
LowRankMatrix<T> combine(const LowRankMatrix<T>&, const T&,
                         const LowRankMatrix<T>&, const T&, real_t eps=0);
LowRankMatrix<T> operator+(const LowRankMatrix<T>&, const LowRankMatrix<T>&);
LowRankMatrix<T> operator-(const LowRankMatrix<T>&, const LowRankMatrix<T>&);
LowRankMatrix<T> operator-(const LowRankMatrix<T>&);
LowRankMatrix<T> operator+(const LowRankMatrix<T>&);
LowRankMatrix<T> operator*(const LowRankMatrix<T>&, const T&);
LowRankMatrix<T> operator/(const LowRankMatrix<T>&, const T&);
LowRankMatrix<T> operator*(const T&, const LowRankMatrix<T>&);
```

Note that the combination of a low rank matrix $L_1 = U_1 D_1 V_1$ of rank $r_1$ and a low rank matrix $L_2 = U_2 D_2 V_2$ of rank $r_2$ produces a low rank matrix $L = U\,D\,V$ of rank $r = r_1 + r_2$ because

$$L = a_1 L_1 + a_2 L_2 = \begin{bmatrix} U_1 & U_2 \end{bmatrix} \begin{bmatrix} a_1 D_1 & 0 \\ 0 & a_2 D_2 \end{bmatrix} \begin{bmatrix} V_1 \\ V_2 \end{bmatrix}.$$

When non zero, the `eps` argument in the `LowRankMatrix::add` and `combine` functions is used to re-compress the combined matrix with a truncated svd.

Finally, some compression methods based on SVD are implemented too. These compression methods "produce" a `LowRankMatrix` from a dense matrix stored in major column access and passed by a pointer to its first coefficient (template declaration is omitted):

```
void svdCompression(T* mat, number_t m, number_t n, number_t r,
                    LowRankMatrix<T>& lrm);
void svdCompression(T* mat, number_t m, number_t n, real_t eps,
                    LowRankMatrix<T>& lrm);
void rsvdCompression(T* mat, number_t m, number_t n, number_t r,
                     LowRankMatrix<T>& lrm);
void rsvdCompression(T* mat, number_t m, number_t n, real_t eps,
                     LowRankMatrix<T>& lrm);
void r3svdCompression(T* mat, number_t m, number_t n, real_t eps,
                      LowRankMatrix<T>& lrm,
                      number_t t = 0, number_t p = 0, number_t q = 0,
                      number_t maxit = 0)
```

The SVD compression functions do the full svd of the given matrix and then truncate the number of singular values and singular vectors keeping either the $r$ largest singular values/vectors or the singular values greater than a given `eps`. The fact that this process leads to a good approximate matrix results from the Eckart–Young–Mirsky theorem.

As the full svd is an expansive algorithm time computation, some alternative methods based on the random svd are also available. Random svd consists in capturing the matrix range using only few gaussian random vectors and doing a svd on a smaller matrix. Again, two versions of random svd are available, one providing a low rank matrix of a given rank, the other one providing a low rank matrix with a control on the approximate error. This last method iterates on the rank, so it is more expansive. The r3svd is a more sophisticated iterative method (see https://arxiv.org/ftp/arxiv/papers/1605/1605.08134.pdf).

As svd and qr algorithms have not been implemented for the Matrix class, XLiFE++ uses the Eigen library that is provided when installing XLiFE++.

svd, rsvd and aca compression does not work for matrix of matrices!

| | |
|---|---|
| library : | **hierarchicalMatrix** |
| header : | **ApproximateMatrix.hpp** |
| implementation : | **ApproximateMatrix.cpp** |
| unitary tests : | **test_HMatrix.cpp** |
| header dependences : | **largeMatrix.h, config.h, utils.h** |

## 10.3 HMatrix

Hierarchical matrix is a tree representation of a matrix, each node representing a sub-matrix being either split in sub-matrices (tree nodes) or not if the node is a leaf of the tree. The hierarchical division in sub-matrices is based on hierarchical division of row and column matrix indices or dofs if it is a FE matrix (ClusterTree objects).

To manage this tree representation, three template classes are provided:

- the HMatrixNode<T,I> class dealing with a node of the matrix tree
- the HMatrix<T,I> front end class
- the HMatrixEntry<I> interface class that handles some pointers to HMatrix<real_t,I>, HMatrix<complex_t,I>, … .

These classes are templated by the type of matrix coefficients (T=real_t, complex_t, ...) and the type of row and column clustering (I=Point, FeDof, Element). Let us start by describing the HMatrixNode class supporting the main material.

### 10.3.1 The HMatrixNode class

```
template <typename T, typename I>
class HMatrixNode
{public :
 HMatrixNode<T,I>* parent_;      //pointer to its parent, if 0 root node
 HMatrixNode<T,I>* child_;       //pointer to its first child, if 0 no child
 HMatrixNode<T,I>* next_;        //pointer to its brother, if 0 no brother
 ClusterNode<I>* rowNode_;       //row cluster node to access to row numbering
 ClusterNode<I>* colNode_;       //column cluster node to access to col numbering
 LargeMatrix<T>* mat_;           //pointer to a LargeMatrix
 ApproximateMatrix<T>* appmat_;  //pointer to an ApproximateMatrix
 bool admissible_;               //block can be approximated
 number_t depth_;                //depth of node in tree, root has 0 depth
 number_t rowSub_, colSub_;      //sub block numbering (i,j)
 bool isDiag_;                   //true if matrix node is located on the diagonal
```

Each node refers to its parent node, its first child node, its first brother node and access to its row and column numbering using some pointers to ClusterNode object. If node is a leaf (no child), it stores the node sub-matrix either as a LargeMatrix (pointer mat_) or as a ApproximateMatrix (pointer appmat_). If node is not a leaf, both the pointers mat_ and appmat_ are 0. Besides, HMatrixNode manages some additional useful informations that are set during construction of the tree such as depth_, rowSub_, colSub_, isDiag_.

It manages also the particular data admissible_ that tells from some geometrical rule if the sub-matrix attached to the node can be approximated, generally using compression methods. This property is mainly relevant in the context of BEM matrix where all interactions between distant dof sets can be reduced to few interactions. The choice of admissibility rule is governed by the HMatrix front end class using the enumerations:

```
enum HMatrixMethod {_standardHM, _denseHM};
enum HMAdmissibilityRule {_boxesRule};
```

The HMatrixNode class has few constructors:

```
HMatrixNode();                                           //default constructor
HMatrixNode(HMatrixNode<T,I>*, HMatrixNode<T,I>*, HMatrixNode<T,I>*, number_t,
            ClusterNode<I>*, ClusterNode<I>*,  number_t, number_t,
            LargeMatrix<T>* , ApproximateMatrix<T>* );//full constructor
HMatrixNode(HMatrixNode<T,I>*, number_t);                //node constructor
HMatrixNode(LargeMatrix<T>*, HMatrixNode<T,I>*,
            number_t);                     //LargeMatrix leaf constructor
HMatrixNode(ApproximateMatrix<T>*, HMatrixNode<T,I>*,
            number_t);                     //ApproximateMatrix leaf constructor
HMatrixNode(const HMatrixNode<T,I>&);                    //copy constructor
HMatrixNode<T,I>& operator=(const HMatrixNode<T,I>&); //assign operator
void copy(const HMatrixNode<T,I>&);                      //copy function
```

and some stuff related to destructor or cleaner:

```
~HMatrixNode();               //destructor
void clear();                 //clear all except ClusterNode pointers
void clearMatrices();         //clear (deallocate) only matrices
```

Be cautious when copying HMatrixNode object, if allocated, the large matrix or the approximate matrix are copied, but not the ClusterNode objects (shared pointers!). In the same way, when a HMatrixNode object is cleared or deleted, matrix or approximate matrix are deleted if they have been allocated but the ClusterNode objects are not deallocated.

The most important function is

```
void divide(number_t rmin, number_t cmin, number_t maxdepth = 0,
            HMAdmissibilityRule=_boxesRule, bool sym=false);
```

that creates recursively the sub-tree of the current node according to the admissibility rule given by the enumeration

```
enum HMAdmissibilityRule {_boxesRule};
```

Up to now, only one rule is available, the standard boxes rule used in BEM computation telling that a HMatrixNode is admissible if the bounding box $B_r$ of the row cluster node and the bounding box $B_c$ of the column cluster node satisfy:

$$\mathrm{diam}(B_r) \leq 2 * \eta * \mathrm{dist}(B_r, B_c).$$

Note that in the case of a matrix having symmetry property (symmetric, skew-symmetric, self-adjoint or skew-adjoint), the division process may take it into account (argument sym=true). In that case, it does not generate sub-matrix nodes that are located above the diagonal, so saving memory.

Once the tree is built, some various member functions are available:

```
number_t numberOfRows() const;          //number of rows counted in T
number_t numberOfCols() const;          //number of columns counted in T
dimPair dimValues() const;              //dimensions of matrix values
void setClusterRow(ClusterNode<I>*);    //update row cluster node pointers
void setClusterCol(ClusterNode<I>*);    //update col cluster node pointers
number_t nbNonZero() const;             //number of T coefficients used
void getLeaves(list<HMatrixNode<T,I>* >&,
               bool = true) const;      //get leaves as a list
```

The HMatrixNode class implements all the stuff required by algebraic operations on HMatrix class:

```
vector<T>& multMatrixVectorNode(const vector<T>&, vector<T>&,
                                SymType symt=_noSymmetry) const;
vector<T>& multMatrixVector(const vector<T>&, vector<T>&,
                            SymType symt=_noSymmetry) const;
real_t norm2() const;                                 //Frobenius norm
real_t norminfty() const;                             //infinite norm
```

and by printing operations

```
void printNode(ostream&) const;           //print current node contents
void print(ostream&) const;               //print tree from current node
void printStructure(ostream&, number_t, number_t,
                    bool all=false, bool shift=false) const;
```

Finally, for performance measurement purpose, the class manages also some static data and static functions:

```
static bool counterOn;          //flag to activate the operations counter
static number_t counter;        //operations counter
static void initCounter(number_t n=0); //init the counter and enable it
static void stopCounter();             //disable counter
```

### 10.3.2 The HMatrix class

The HMatrix class is the front end class of hierarchical matrices. It is templated by the type of matrix coefficients and the type of cluster objects. It manages the parameters of the matrix clustering , some general informations and handles the root node of the tree:

```
template <typename T, typename I>
class HMatrix
{private :
 HMatrixNode<T,I>* root_;   //root node of the tree representation
 ClusterTree<I>* rowCT_;    //row cluster tree
 ClusterTree<I>* colCT_;    //col cluster tree
 public :
 string_t name;             //optional name, useful for doc
 ValueType valueType_;      //type of values (real, complex)
 StrucType strucType_;      //structure of values (scalar, vector, matrix)
 HMatrixMethod method_;     //method to define admissible block
 HMAdmissibilityRule admRule_; //block admissible rule
 real_t eta_;               //ratio in the admissibility criteria
 number_t rowmin_, colmin_; //minimum size of block matrix
 SymType sym_;              //type of symmetry
 number_t depth;            //maximal depth (info)
 number_t nbNodes;          //number of nodes (info)
 number_t nbLeaves;         //number of leaves (info)
 number_t nbAdmissibles;    //number of admissible blocks (info)
 number_t nbAppMatrices;    //number of approximate matrices (info)
 ...
```

The data member depth, nbNodes, nbLeaves, nbAdmissibles, nbAppMatrices are set by the division algorithm or computed on demand.

The class redefines the default constructor (initializing data members) and an explicit constructor filling the cluster parameters and building the tree structure recursively:

```
HMatrix();
HMatrix(ClusterTree<I>&, ClusterTree<I>&,  number_t, number_t, number_t =0,
        const string_t& = "", SymType =_noSymmetry,
        HMatrixMethod =_standardHM, HMAdmissibilityRule=_boxesRule, real_t =1.);
void buildTree();                           //build the tree
void updateInfo();                          //update tree info (depth, ...)
HMatrix(const HMatrix<T,I>&);               //copy constructor
HMatrix<T,I>& operator=(const HMatrix<T,I>&); //assign operator
~HMatrix();                                 //destructor
void copy(const HMatrix<T,I>&);             //copy all
void clear();                               //clear all
void clearMatrices();                       //deallocate matrix pointers
```

To preserve integrity of HMatrix object, the copy constructor and the assign operator do a hard copy of the tree and of the matrices attached to HMatrixNode objects but the row and col cluster trees are not copied ! When a HMatrix object is deleted or cleared, all the nodes of the tree and node matrices are deleted but not the row and col cluster trees!

The HMatrix class provides some stuff to get or extract various informations about the tree structure:

```
number_t numberOfRows() const;          //number of rows counted in T
number_t numberOfCols() const;          //number of cols counted in T
dimPair dimValues() const;              //dimensions of values, (1,1) when scalar
number_t nbNonZero() const;             //number of coefficients used
const ClusterTree<I>* rowTree() const;  //access to row ClusterTree pointer
const ClusterTree<I>* colTree() const;  //access to col ClusterTree pointer
void setClusterRow(ClusterTree<I>*);    //change the row ClusterTree pointer
void setClusterCol(ClusterTree<I>*);    //change the col ClusterTree pointer
pair<number_t, number_t> averageSize() const; //average size of leaves
number_t averageRank() const;           //average rank of admissible leaves
list<HMatrixNode<T,I>* > getLeaves(bool = true) const;   //get all leaves
```

It is possible to import a LargeMatrix in a Hmatrix only if the tree structure already exists and to export a Hmatrix to a LargeMatrix (dense storage).

```
void load(const LargeMatrix<T>&,HMApproximationMethod = _noHMApproximation);
LargeMatrix<T> toLargeMatrix(StorageType st=_dense, AccessType at=_row) const;
```

Some algebraic operations on HMatrix are available:

```
vector<T>& multMatrixVector(const vector<T>&, vector<T>&) const;
vector<T>& multMatrixVectorOmp(const vector<T>&, vector<T>&) const;
void addFELargeMatrix(const LargeMatrix<T>&); //add FE LargeMatrix to current
real_t norm2() const;                        //Frobenius norm
real_t norminfty() const;                      //infinite norm
```

Note that the multMatrixVector function is recursive so it is not safe in multithread computation. This is the reason why there exists a non recursive function multMatrixVectorOmp that implements omp pragma to parallelize the computation.

The Hmatrix class provides the following print stuff:

```
void print(std::ostream&) const;
void printSummary(std::ostream&) const;
void printStructure(std::ostream&,bool all=false, bool =false) const;
void saveStructureToFile(const string_t&) const;
ostream& operator<<(ostream& os, const HMatrix<X,J>& hm);
```

As an illustration, we show on figure 10.4 the structure of a HMatrix based on the clustering of a mesh of a sphere, get by the following XLIFE++ code

```
Mesh meshd(Sphere(_center=Point(0.,0.,0.),_radius=1.,_nnodes=2,
                 _domain_name="Omega"),_triangle,1,_subdiv);
Domain omega=meshd.domain("Omega");
Space V(omega,P0,"V",false);
ClusterTree<FeDof> ct(V.feSpace()->dofs,_cardinalityBisection,10);
HMatrix<Real,FeDof> hm(ct,ct,nbox,nbox);
hm.saveStructureToFile("hmatrix.dat");
```

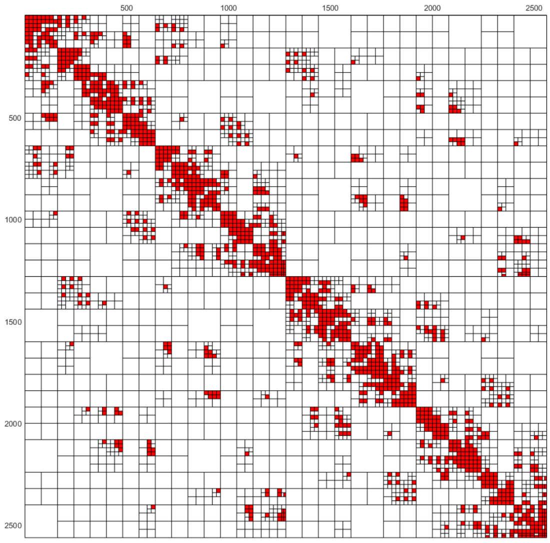


Figure 10.4: HMatrix with a sphere cluster, non admissible blocks in red

### 10.3.3 The HMatrixEntry class

The template HMatrixEntry<I> class is similar to the MatrixEntry class. In order to shadow the type of the HMatrix coefficients it handles pointers to HMatrix<real_t,I>, HMatrix<complex_t,I>, HMatrix<Matrix<real_t>,I> and HMatrix<Matrix<complex_t>,I>:

```
class HMatrixEntry
{
public :
ValueType valueType_;                       //entries value type
StrucType strucType_;                       //entries structure type
HMatrix<real_t,I>* rEntries_p;              //pointer to real HMatrix
HMatrix<complex_t,I>* cEntries_p;           //pointer to complex HMatrix
HMatrix<Matrix<real_t>,I>* rmEntries_p;     //pointer to HMatrix of real matrix
HMatrix<Matrix<complex_t>,I>* cmEntries_p;  //pointer to HMatrix of cmplx matrix
dimPair nbOfComponents;                //nb of rows and columns of matrix values
...
```

The following constructor/destructor stuff is available:

```
HMatrixEntry(ValueType, StrucType, ClusterTree<I>&, ClusterTree<I>&,
             number_t, number_t, number_t =1, number_t=1,
             SymType sy = _noSymmetry);
HMatrixEntry(const HMatrixEntry<I>&);                //copy constructor
HMatrixEntry<I>& operator=(const HMatrixEntry<I>&); //assign operator
~HMatrixEntry(){clear();}                           //destructor
void copy(const HMatrixEntry<I>&);                  //full copy of members
void clear();                                       //deallocate memory used
```

To preserve integrity of HMatrixEntry class, the copy constructor and assignment operator do a hard copy of HMatrix objects pointed as soon as the pointer is not null.

The class provides some useful functionalities:

```
void setClusterRow(ClusterTree<I>*);  //change the ClusterTree row pointer
void setClusterCol(ClusterTree<I>*);  //change the ClusterTree col pointer
template <typename T>
HMatrix<T,I>& getHMatrix() const      //get HMatrix object
real_t norm2() const;                 //Frobenius norm
real_t norminfty() const;             //infinite norm
void print(ostream&) const;           //print HMatrixEntry
void printSummary(ostream&) const;    //print HMatrixEntry in brief
```

The member function getHMatrix has real_t, complex_t, Matrix<real_t> and Matrix<complex_t> specializations.

| | |
|---:|---|
| library : | **hierarchicalMatrix** |
| header : | **HMatrix.hpp** |
| implementation : | **HMatrix.cpp** |
| unitary tests : | **test_HMatrix.cpp** |
| header dependences : | **ApproximateMatrix.hpp, ClusterTree.hpp, largeMatrix.h ,config.h, utils.h** |

### 10.3.4 The HMatrixIM class

In order to inform the code that HMatrix has to be used, a special class of integration method has been developed : HMatrixIM . It inherits from the DoubleIM class inheriting itself from the IntegrationMethod class. Attaching such integration method to a BEM bilinear form, HMatrix computation algorithm will be involved.

```
class HMatrixIM : public DoubleIM
{public:
 ClusterTree<FeDof>* rowCluster_;    //row cluster pointer
 ClusterTree<FeDof>* colCluster_;    //col cluster pointer
 mutable bool deletePointers_;       //flag enabling pointers deallocation
 ClusteringMethod clusterMethod;     //clustering method
 HMApproximationMethod hmAppMethod;  //type of approximation of admissible blocks
 number_t minRowSize, minColSize;    //minimum row/col size of leaf matrix
 number_t maxRank;                   //maximal rank of approximate matrices
 real_t epsRank;                     //precision used in compression
 IntegrationMethod* intgMethod;      //real integration method
 ...
};
```

This class provides some constructors

```
HMatrixIM(ClusteringMethod clm, number_t minRow, number_t minCol,
          HMApproximationMethod hmap, number_t maxr, IntegrationMethod& im);
HMatrixIM(ClusteringMethod clm, number_t minRow, number_t minCol,
          HMApproximationMethod hmap,  real_t epsr, IntegrationMethod& im);
HMatrixIM(HMApproximationMethod hmap,  number_t maxr, IntegrationMethod& im,
          ClusterTree<FeDof>& rowC, ClusterTree<FeDof>& colC);
HMatrixIM(HMApproximationMethod hmap,  real_t epsr, IntegrationMethod& im,
          ClusterTree<FeDof>& rowC, ClusterTree<FeDof>& colC);
```

The two last constructors allow to load some row/column clusters whereas the two first ones provide the parameters to build them. When building `HMatrixIM` object from clustering parameters, the `deletePointers` flag is true, so destroying the `HMatrixIM` object induces the deallocation of the cluster pointers. When building `HMatrixIM` object from cluster pointers, these pointers will not be deallocated by destructor.

The class has also a clear method to delete the cluster pointers and a destructor that clears the cluster pointers if `deletePointers` is true:

```
~HMatrixIM();
 void clear();
```

The `HMatrixIM` class is used as following:

```
Mesh meshd(Sphere(_center=Point(0.,0.,0.),_radius=1.,_nnodes=9,
           _domain_name="Omega"), _triangle,1,_subdiv);
Domain omega=meshd.domain("Omega");
Space W(omega,P0,"V",false);
Unknown u(W,"u"); TestFunction v(u,"v");
Kernel G=Laplace3dKernel();
SauterSchwabIM ssim(5,5,4,3,2.,4.);
HMatrixIM him(_cardinalityBisection, 20, 20,_acaplus,0.00001,ssim);
BilinearForm alf=intg(omega,omega,u*Gl*v,him);
TermMatrix A(alf,"A");
```

Because the compression methods do not work yet for matrix of matrices, `HMatrix` is not fully operational when dealing with some problems with vector unknown.

| | |
|---|---|
| library : | **hierarchicalMatrix** |
| header : | **HMatrix.hpp** |
| implementation : | **HMatrix.cpp** |
| unitary tests : | **test_HMatrix.cpp** |
| header dependences : | **ApproximateMatrix.hpp, ClusterTree.hpp, largeMatrix.h ,config.h, utils.h** |

# 11 The *term* library

This library addresses the Term class and its inherited classes that handle the numerical representations of linear and bilinear forms involved in problems to be solved, say vectors and matrices (LargeMatrix class). The Term class is an abstract class collecting general data (name, computing informations) and has four children :

TermVector class to represent linear forms involving multiple unknowns,

SuTermVector class to represent linear forms involving only one unknown,

TermMatrix to represent bilinear forms involving multiple pairs of unknowns,

SuTermMatrix to represent bilinear forms involving only one pair of unknowns,

TermVector class is linked to a LinearForm object (defined on multiple unknowns) and handles a map of SuTermVector object indexed by unknown. In a same way, TermMatrix class is linked to a BiLinearForm object (defined on multiple unknown pairs) and handles a map of SuTermMatrix object indexed by unknown pair. SuTermVector and SuTermMatrix are related to SuLinearForm and SuBiLinearForm and carries the numerical representations as vector or matrix. This is a block representation.

For instance, consider the following two unknowns $(u,p)\in V\times H$ problem:

$$\left\{\begin{array}{lcl} a(u,v)+b(p,v) & = & f(v) \\ c(u,q)+d(p,q) & = & g(q) \end{array}\right.$$

where $a$, $b$, $c$, $d$ are bilinear forms defines respectively on $V\times V$, $H\times V$, $V\times H$, $H\times H$ and $f$, $g$ are linear forms defined on $V$ and $H$. The block representation is

$$\left[\begin{array}{cc} \mathbb{A} & \mathbb{B} \\ \mathbb{C} & \mathbb{D} \end{array}\right]\left(\begin{array}{c} U \\ P \end{array}\right)=\left(\begin{array}{c} F \\ G \end{array}\right)$$

matrices being stored with their own storages. In order to shadow the type of coefficients (real, complex, scalar, vector, matrix) the vector and matrix representations are managed through the VectorEntry class (see *utils* library) and MatrixEntry class (see *largeMatrix* library).

In certain circumstances the block representation is not well adapted (matrix factorisation, essential condition to apply). So the representation is moved to a scalar global representation, block representation may be or not kept.

This library collects the main algorithms of vector and matrix computation, in particular

- computation from linear and bilinear form (see the *computation* subdirectory)
- computation from explicit vector, matrix or function (nodal computation)
- linear combination of TermVector or TermMatrix (see LcTerm class)
- the elimination process due to essential conditions (in relation with *essentialConditions* library)
- the interface to solvers (direct solvers, iterative solvers or eigen solvers defined in *largeMatrix*, *solvers*, *eigenSolvers* libraries )

- some import and export facilities (see the *ioTerms* subdirectory)

*TermMatrix and TermVector are end user classes, therefore the functions that interact with users has to be simply designed!*

## 11.1 The Term class

The Term class is the abstract basis class of TermVector, TermMatrix, SuTermVector, SuTermMatrix classes. It collects general informations:

```
class Term
{
protected :
 String name_;                   //term name
 TermType termType_;             //type of term
 ComputingInfo computingInfo_;   //computing information
public :
 Parameters params;              //a free zone to store additional data
 static std::vector<Term *> theTerms;
}
```

where *TermType* enumerates the child types :

```
enum TermType {_termUndef,_termVector,_termMatrix,_sutermVector,_sutermMatrix};
```

and ComputingInfo collect various computing informations:

```
class ComputingInfo
{
public :
bool isComputed;
bool noAssembly;
bool multithreading;
bool useGpu;
StorageType storageType;              //_cs,_skyline,_dense
AccessType storageAccess;             //_row,_col,_dual,_sym
EliminationMethod elimination;        //_noElimination, _pseudoElimination, _realElimination
};
```

Using a static vector of Term pointers, the class maintains a list of all terms.

This class provides a default constructor, declared *protected* to forbid instantiation by user, and some basic functions (mainly accessors)

```
Term(const String& na="", ComputingInfo ci=ComputingInfo()); //protected
virtual ~Term();
const String& name() const;
String& name();
TermType termType() const;
TermType& termType();
ComputingInfo computingInfo() const;
ComputingInfo& computingInfo();
bool& computed();
bool computed() const;
virtual void compute()=0;
virtual void clear()=0;
virtual void print(std::ostream&) const=0;
friend std::ostream& operator<<(std::ostream&,const Term&);
static void clearGlobalVector();
};
```

Finally, some general functions (to compute and clear terms) are provided:

```
void compute(Term&);
void compute(Term&, Term&);
...
void clear(Term&);
void clear(Term&, Term&);
...
```

| | |
|---|---|
| library : | **term** |
| header : | **Term.hpp** |
| implementation : | **Term.cpp** |
| unitary tests : | **test_TermVector.cpp** |
| header dependences : | **essentialConditions.h, config.h, utils.h** |

## 11.2 The TermVector class

The TermVector class carries numerical representation of a linear form and more generally any vector attached to an approximation space:

```
class TermVector : public Term
{
 protected :
 LinearForm linForm_;
 map<const Unknown*, SuTermVector*> suTerms_;
 VectorEntry* entries_p;
 VectorEntry* scalar_entries_p;
 vector<DofComponent> cdofs_;
```

The linear form is a multiple unknowns form, may be reduced to a single unknown form (see *form* library). This linear form is void if TermVector is not explicitly construct from a linear form (linear combination, nodal construction). The map *suTerms_* carries each vector block related to an unknown. When there is only one element in map, it means that the TermVector is actually a single unknown term vector. The *scalar_entries_p* pointer may be allocated to concatenate the block vectors. When unknowns are vector unknowns, the representation may be not suited in certain cases (direct solver), so it is possible to create its scalar representation using the *scalar_entries_p* (VectorEntry pointer). The VectorEntry object created has to be of real scalar or complex scalar type. In that case, a non block row numbering consisting in vector of DofComponent (Unknown pointer, dof number, component number) is also defined (*cdofs_*).

The TermVector class provides useful constructors and assign operators designed for end users :

```
//default constructor
TermVector(const String& na = "", bool noass = false);

//from linear form with options and no essential conditions
TermVector(const LinearForm&, const string_t& na="");
TermVector(const LinearForm&, TermOption, const string_t& na="");
TermVector(const LinearForm&, TermOption, TermOption, const string_t& na="");
TermVector(const LinearForm&, TermOption, TermOption, TermOption,
           const string_t& na="");

//from linear form with options and one essential condition
TermVector(const LinearForm&, const EssentialConditions&,
           const string_t& na="");
TermVector(const LinearForm&, const EssentialConditions&, TermOption,
           const string_t& na="");
```

```
TermVector(const LinearForm&, const EssentialConditions&, TermOption,
           TermOption, const string_t& na="");
TermVector(const LinearForm&, const EssentialConditions&, TermOption,
           TermOption, TermOption, const string_t& na="");

void build(const LinearForm &, const EssentialConditions*,
           const vector<TermOption>&, const string_t&);

//from value or function (interpolation)
template <typename T>
  TermVector(const Unknown&, const Domain&, const T&, const String& na = "");

//copy like
TermVector(const TermVector&, const String& na = "");
template <typename T>
  TermVector(const TermVector&, const T&, const String& na);
TermVector(const SuTermVector &, const String& na="");
TermVector(SuTermVector *, const String& na="");
void copy(const TermVector&, const String &);

//constructor from explicit function of TermVector's
TermVector(const TermVector&, funSR1_t& f, const string_t& na="");
TermVector(const TermVector&, TermVector&, funSR2_t& f, const string_t& na="");
TermVector(const TermVector&, funSC1_t& f, const string_t& na="");
TermVector(const TermVector&, TermVector&, funSC2_t& f, const string_t& na="");  single unknown

//constructor from symbolic function of TermVector's
TermVector(const TermVector&, const SymbolicFunction& , const string_t& na="");
TermVector(const TermVector&, const TermVector&, const SymbolicFunction& fs,
const string_t& na="");
TermVector(const TermVector&, const TermVector&, const TermVector&,
const SymbolicFunction& fs, const string_t& na="");

//constructor of a vector TermVector from scalar TermVector's (single unknown, same space)
TermVector(const Unknown&, const TermVector&, const TermVector&, const string_t& ="");
TermVector(const Unknown&, const TermVector&, const TermVector&, const TermVector&, const
    string_t& ="");
TermVector(const Unknown&, const TermVector&, const TermVector&, const TermVector&, const
    TermVector&, const string_t& ="");

//from linear combination
TermVector(const LcTerm&);
//assignment
TermVector& operator=(const TermVector&);
TermVector& operator=(const LcTerm&);
//insert SuTermVector in TermVector
void insert(const SuTermVector &);
void insert(SuTermVector *);
void insert(const Unknown*, SuTermVector*);
//destructor, clear
virtual ~TermVector();
void clear();
```

When TermVector is constructed from linear form, it is automatically computed except if it has set to be not computed using a the `TermOption` *_notCompute* in its construction.
`TermOption`s are managed as an enumeration :

```
enum TermOption
{
 //general
 _compute,                  //default behaviour
 _notCompute,
 _assembled,                //default behaviour
 _unassembled,             //not yet available
 //only for TermMatrix
 _nonSymmetricMatrix,      //to force symmetry property
 _symmetricMatrix,
 _selfAdjointMatrix,
 _skewSymmetricMatrix,
 _skewAdjointMatrix,
 _csRowStorage,            //to force storage
 _csColStorage,
 _csDualStorage,
 _csSymStorage,
 _denseRowStorage,
 _denseColStorage,
 _denseDualStorage,
 _skylineSymStorage,
 _skylineDualStorage,
 _pseudoReduction,         //default behaviour
 _realReduction,           //not yet available
 _penalizationReduction    //not yet available
};
```

Constructors involving `SuTermVector` class are reserved to developers. End users should not have to acces to `SuTermVector` class, but we decide to let this access free to advanced users. Constructors involving `LcTerm` class are implicitly used by users when they write combination of terms in a symbolic way (see `LcTerm` class). The class provides some useful accessors (for users or developers):

```
//user accessors
const LinearForm& linearForm() const;
Number nbOfUnknowns() cons;
bool isSingleUnknown() const;
set<const Unknown*> unknowns() const;
ValueType valueType() const;
Number size() const;
Number nbDofs() const;
Number nbDofs(const Unknown&) const;
const vector<DofComponent>& cdofs() const;
vector<DofComponent>& cdofs();
const Dof& dof(const Unknown&, Number ) const;

//developer accessors
cit_mustv begin() const;
it_mustv begin();
cit_mustv end() const;
it_mustv end();
SuTermVector* firstSut() const;
SuTermVector* firstSut();
const Unknown* unknown() const;
VectorEntry*& entries();
const VectorEntry* entries() const;
VectorEntry*& scalar_entries();
const VectorEntry* scalar_entries() const;
VectorEntry* actual_entries() const;
```

*it_mustv* and *cit_mustv* are iterator aliases:

```
typedef map<const Unknown*, SuTermVector*>::iterator it_mustv;
typedef map<const Unknown*, SuTermVector*>::const_iterator cit_mustv;
```

Access to a block of `TermVector` say a `SuTermVector` is proposed in two ways : either using `subVector` functions returning reference or pointer to `SuTermVector` objects or using `operator()` returning a new `TermVector` object, the `SuTermVector` object being copied. This last method is adressed to end users. For particular purpose, is is also possible to reinterpret a TermVector as a raw vector or a raw vector of vectors (say a Vector<S> or a Vector<Vector<S> > with S a Real or a Complex).

```
const SuTermVector& subVector() const;
SuTermVector& subVector(const Unknown*);
const SuTermVector& subVector(const Unknown*) const;
SuTermVector& subVector(const Unknown&);
const SuTermVector& subVector(const Unknown&) const;
SuTermVector* subVector_p(const Unknown*);
const SuTermVector* subVector_p(const Unknown*) const;
TermVector operator()(const Unknown&) const; //user usage
template<typename T>
  Vector<T>& asVector(Vector<T>&) const;
```

The main computing operations are related to the construction of TermVector from linear form and construction from linear combination TermVector:

```
void compute();
void compute(const LcTerm&);    //implicit
TermVector& operator+=(const TermVector&);
TermVector& operator-=(const TermVector&);
template<typename T>
 TermVector& operator*=(const T&);
template<typename T>
 TermVector& operator/=(const T&);
```

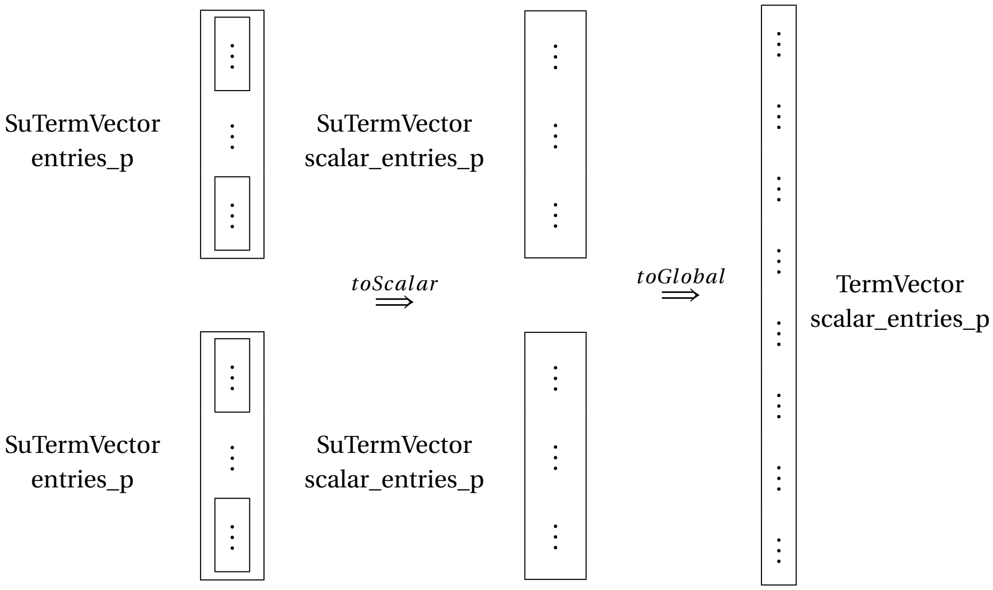
Note that the evaluation of TermVector defined by a value or a function is done during creation of TermVector. The algebraic operators +=, -=, *=, /= do the computation, it is not delayed as it is the case for +,-,* and / operators. The linear combination is based on LcTerm class which manages a list of pairs of Term and coefficient. Algebraic operators on TermVector's produce LcTerm object carrying the linear combination that will be computed by TermVector constructor or assignment operator:

```
const TermVector& operator+(const TermVector&);
LcTerm operator-(const TermVector&);
LcTerm operator+(const TermVector&, const TermVector&);
LcTerm operator-(const TermVector&, const TermVector&);
LcTerm operator+(const LcTerm&, const TermVector&);
LcTerm operator-(const LcTerm&, const TermVector&);
LcTerm operator+(const TermVector&, const LcTerm&);
LcTerm operator-(const TermVector&, const LcTerm&);
template<typename T>
 LcTerm operator*(const TermVector&, const T&);
template<typename T>
 LcTerm operator*(const T&, const TermVector& )
template<typename T>
 LcTerm operator/(const TermVector&, const T&)
```

To manage different representation of TermVector, the following function are provided :

```
void toScalar(bool keepEntries=false);
void toVector(bool keepEntries=false);
void toGlobal(bool keepSuTerms=false);
void toLocal(bool keepGlobal=false);
void adjustScalarEntries(const vector<DofComponent>&);
```

Note the difference between *toScalar* and *toGlobal*. *toScalar* forces the scalar representation of SuTermVector's and *toGlobal* go to non block representation, allocating the *scalar_entries_p* pointer of TermVector. *toGlobal* operation induces *toScalar* operation. *toLocal* reconstructs block representation from global representation (inverse of *toGlobal*) and *toVector* returns to vector representation (inverse of *toScalar*).



In some circonstances, to avoid recomputation, it may be usefull to change the unknowns of a TermVector without changing its content, with an optional management of components of unknown:

```
void changeUnknown(const Unknown&, const Unknown&,
                   const Vector<Number>& = Vector<Number>());
void changeUnknown(const Unknown&,
                   const Vector<Number>& = Vector<Number>());
void changeUnknown(const Unknown&, Number);              //shortcut
void changeUnknown(const Unknown&, Number, Number);    //shortcut
void changeUnknown(const Unknown&, Number, Number, Number); //shortcut
```

The principle of changeUnknown functions is the following :

- when two unknows (u,v) are specified, the unknown u is replaced by the unknown v and the reference to unknown u does no longer exists in TermVector
- when a renumbering components vector (rc) is given too, components are re-settled along this vector
- when v is not specified, only components are re-settled

Here are some exemples :

- u a scalar unknown, v a scalar unknown, replace unknown u by unknown v
- u a scalar unknown, v a 3-vector unknown, rc=[2] leads to sutv = [0 sutv 0]
- u a 4-vector unknown, v a 2-vector unknown, rc=[2,4] leads to sutv = [0 sutv1 0 sutv2]
- u a 3-vector unknown, rc=[3,0,1], re-settle components as [sutu3 0 sutu1]

⚠ Be cautious that there is no check of the space consistancy! So use it with care.

It is possible to adress values of a TermVector by unknown and index, to get it or to set it:

```
Value getValue(const Unknown&, Number) const;
void setValue(const Unknown&, Number, const Value&);
void setValue(const Unknown&, Number, const Real&);
void setValue(const Unknown&, Number, const Complex&);
void setValue(const Unknown&, Number, const vector<Real>&);
void setValue(const Unknown&, Number, const vector<Complex>&);
```

The `Value` class handles different type of values, in particular `Real` and `Complex` values.

It is also possible to change some values of a `TermVector` by specifying the unknown that it is concerned, the geometrical part where values will be changed and the values that can be given either by a constant, a function or a `TermVector`:

```
number_t dofRank(const Unknown&, const Dof&)const;
number_t dofRank(const Dof&) const;
Value getValue(const Unknown&, number_t) const;
Value getValue(const Unknown& u, const Dof& dof) const
void setValue(const Unknown&, number_t, const Value&);
void setValue(const Unknown& u, const Dof& dof, const Value& v)
void setValue(const Unknown&, number_t, const real_t&);
void setValue(const Unknown&, number_t, const complex_t&);
void setValue(const Unknown&, number_t, const std::vector<real_t>&);
void setValue(const Unknown&, number_t, const std::vector<complex_t>&);
template <typename T>
void setValue(const Unknown&, const GeomDomain&, const T&);
void setValue(const Unknown&, const GeomDomain&, const TermVector&);
void setValue(const Unknown&, const TermVector&);
```

In all `setValue` and `getValue` functions, the unknown may be omitted. In that case, the first unknown is assumed.

Most powerful functions are functions that can evaluate any function of approximation space ($V_h$) (representing by a `TermVector` U) at any point, using space interpolation :

$$u_h(x) = \sum_{i=1,n} U_{u,i}\, w_i(x)$$

where $U_{u,i}$ is the $i^{th}$ components related to the unknown $u$ of `TermVector` $U$ and $(w_i)_{i=1,n}$ the basis functions of approximation space $V_h$.

```
Value evaluate(const Unknown&, const Point&) const;
template<typename T>
 T& operator()(const vector<Real>&, T&) const;
template<typename T>
 T& operator()(const Unknown&, const vector<Real>&, T&) const;
```

Some additional computational tools are available:

```
TermVector& toAbs();
TermVector& toReal();
TermVector& toImag();
TermVector& toComplex();
TermVector& toConj();
TermVector& roundToZero(real_t aszero=10*theEpsilon);
Real norm2() const;
Complex maxValAbs() const;
```

`TermVector` may be related to essential conditions either by defining an essential condition from a `TermVector` (e.g `u=TU`) or by applying some essential conditions (`SetOfConstraints` or `EssentialConditiopns` objects) to it:

```
EssentialCondition operator = (const complex_t &);
TermVector& applyEssentialConditions(const SetOfConstraints&,const ReductionMethod&
     =ReductionMethod());
TermVector& applyEssentialConditions(const EssentialConditions&,const ReductionMethod&
     =ReductionMethod());
TermVector& applyBoundaryConditions(const EssentialConditions& ecs,const ReductionMethod&
     rm=ReductionMethod());
```

In order to use a `TermVector` as an interpolated function, the `toFunction()` builds a new function where the `TermVector` is passed to the `Parameters` of some particular functions that implements the interpolation:

```
const Function& toFunction() const;
real_t fun_EC_SR(const Point& P, Parameters& pars);
real_t fun_EC_SC(const Point& P, Parameters& pars);
real_t fun_EC_VR(const Point& P, Parameters& pars);
real_t fun_EC_VC(const Point& P, Parameters& pars);
```

The following functions produce new `TermVector`'s that are defined on an other domain, one mapping the values using a predefined map between two domains the other restricting the values to one domain (included in the current one):

```
TermVector mapTo(const GeomDomain&, const Unknown&, bool errOutDom =true) const;
TermVector onDomain(const GeomDomain&) const;
```

The class proposes some basic output functions:

```
void print(ostream&) const;
void saveToFile(const String&, bool encode=false) const;
```

Besides, some of the functionalities are also provides as extern functions:

```
//linear combination
const TermVector& operator+(const TermVector&);
LcTerm operator-(const TermVector&);
LcTerm operator+(const TermVector&, const TermVector&);
LcTerm operator-(const TermVector&, const TermVector&);
LcTerm operator+(const LcTerm&, const TermVector&);
LcTerm operator-(const LcTerm&, const TermVector&);
LcTerm operator+(const TermVector&, const LcTerm&);
LcTerm operator-(const TermVector&, const LcTerm&);
template<typename T>
 LcTerm operator*(const TermVector&, const T&);
template<typename T>
 LcTerm operator*(const T&, const TermVector&);
template<typename T>
 LcTerm operator/(const TermVector&, const T&)

//inner, hermitian product, norm, ...
TermVector abs(const TermVector&);
TermVector real(const TermVector&);
TermVector imag(const TermVector&);
TermVector conj(const TermVector&);
Complex innerProduct(const TermVector&, const TermVector&);
Complex hermitianProduct(const TermVector&, const TermVector&);
Complex operator|(const TermVector&, const TermVector&);
Real norm(const TermVector&, Number l=2);
Real norm1(const TermVector&);
Real norm2(const TermVector&);
Real norminfty(const TermVector&);

//output functions
```

```
void print(ostream&) const;
void saveToFile(const String&, bool encode=false) const;
void saveToFile(const String&, const list<const TermVector*>&, IOFormat iof=_raw);
void saveToFile(const String&, const TermVector&, IOFormat iof=_raw);
void saveToFile(const String&, const TermVector&, const TermVector&,
                IOFormat iof=_raw);
void saveToFile(const String&, const TermVector&, const TermVector&,
                const TermVector&, IOFormat iof=_raw);
void saveToFile(const String&, const TermVector&, const TermVector&,
                const TermVector&, const TermVector&, IOFormat iof=_raw);
```

Available export format are

- `_raw` : export only the values in a raw format
- `_vtk` : export mesh and values displayable with Paraview
- `_vtu` : export mesh and values displayable with Paraview
- `_matlab` : export mesh and values as an executable Matlab file
- `_xyzv`: export mesh nodes and values as x y z v1 v2 ...

Integral represention is a particular operation mixing numerical quadrature and interpolation :

$$u(x_i) = \int_{\Gamma} opk(K)(x_i, y)\, aop\, opu(p)(y)dy \quad i = 1, n.$$

where $K$ is a kernel, $opk$ an operator on kernel (`OperatorOnKernel`), $p$ a layer potential, $opu$ an operator on unknown (`OperatorOnUnknown`) and $aop$ an algebraic operator.

```
template<typename T>
Vector<T>& integralRepresentation(const vector<Point>& xs,
           const LinearForm& lf, const TermVector& U, Vector<T>& val)
TermVector integralRepresentation(const Unknown&, const GeomDomain&,
           const LinearForm&, const TermVector&);
```

For instance, the single layer integral representation on a list of points is computed as follows:

```
Vector<Point>Points;
...
Vector<Real> val;
integralRepresentation(Points, intg(gamma,G(_y) * u), U, val);
```

or if the list of points is the list of nodes of a domain:

```
 TermVector IR=integralRepresentation(Omega, intg(gamma,G(_y) * u), U, val);
```

For most of functions of TermVector, the algorithms travel the map of `SuTermVector`, calling `SuTermVector`'s functions. For instance, the compute function looks like:

```
void TermVector::compute()
{
  for(it_mustv it = suTerms_.begin(); it != suTerms_.end(); it++)
    {
      if (!it->second->computed()) it->second->compute();
    }
  computed() = true;
}
```

| | |
|---|---|
| library : | **term** |
| header : | **TermVector.hpp** |
| implementation : | **TermVector.cpp** |
| unitary tests : | **test_TermVector.cpp** |
| header dependences : | **SuTermVector.hpp, termUtils.hpp, Term.hpp, form.h, config.h, utils.h** |

## 11.3 The SuTermVector class

The SuTermVector class carries numerical representation of a single linear form and more generally any vector attached to an approximation space.

```
class SuTermVector : public Term
{
protected :
    SuLinearForm* sulf_p;
    const Unknown* u_p;
    mutable Space* space_p;
    std::vector<Space*> subspaces;
    VectorEntry* entries_p;
    VectorEntry* scalar_entries_p;
    std::vector<DofComponent> cdofs_;
    }
```

The sulf_p contains a pointer to a SuLinearForm (single unknown linear form). It may be null, that means there is no explicit linear form attached to the SuTermVector.
The space_p pointer points to the largest subspace involved in SuTermVector. This pointer should not be null because it carries the dofs numbering of vector. For this reason too, the largest subspace has to be correctly updated during any operation on SuTermVector. The Space* vector subspaces contains the subspaces (as subspace of largest space) attached to basic linear forms defined in the SuLinearForm pointer (if defined), see buildSubspaces function.

⚠ Do not confuse the space_p pointer and u_p->space_p pointer that specifies the whole space. They may be the same!

The numerical representation of vector is defined in the entries_p VectorEntry pointer as a real/complex vector or a real/complex vector of vectors, regarding the value type (real or complex) and the structure of the unknown (scalar or vector). If required, vector of vectors representation may be expanded to a vector of scalars stored in the scalar_entries_p VectorEntry pointer. In that case the cdofs_ vector of DofComponent gives the numbering (in DofComponent ) of entries. Note that if SuTermVector is of scalar type, scalar_entries_p = entries_p.

The SuTermVector class provides one constructor from linear form, some constructors from constant value, functions or symbolic functions, one constructor from linear combination and some copy constructors:

```
//constructor from linear form
SuTermVector(SuLinearForm* sulf = 0, const String& na = "", bool noass = false);
//constructors from constant value or function (no linear form)
SuTermVector(const String&, const Unknown*, Space*, ValueType vt = _real, Number n = 0, Dimen nv
    = 0, bool noass = false); //vector of zeros
template <typename T>
SuTermVector(const Unknown&, const GeomDomain&, const Vector<T>&,
             const String&, bool);
template <typename T>
SuTermVector(const Unknown&, const GeomDomain&, const T&,
             const String&, bool);
SuTermVector(const Unknown&, const GeomDomain&, funSR_t&,
             const String& na="", bool noass=false);
SuTermVector(const Unknown&, const GeomDomain&, funSC_t&,
             const String& na="", bool noass =false);
SuTermVector(const Unknown&, const GeomDomain&, funVR_t&,
             const String& na="", bool noass =false);
SuTermVector(const Unknown&, const GeomDomain&, funVC_t&,
             const String& na="", bool noass =false);
//constructor from explicit function of SuTermVector's
SuTermVector(const SuTermVector&, funSR1_t& f, const string_t& na="");
SuTermVector(const SuTermVector&, const SuTermVector&, funSR2_t& f, const string_t& na="");
SuTermVector(const SuTermVector&, funSC1_t& f, const string_t& na="");
SuTermVector(const SuTermVector&, const SuTermVector&, funSC2_t& f, const string_t& na="");
//constructor from symbolic function of SuTermVector's
SuTermVector(const SuTermVector&, const SymbolicFunction& , const string_t& na="");
SuTermVector(const SuTermVector&, const SuTermVector&, const SymbolicFunction&,
             const string_t& na="");
SuTermVector(const SuTermVector&, const SuTermVector&, const SuTermVector&,
             const SymbolicFunction&, const string_t& na="");
//constructor of a vector SuTermVector from scalar SutermVector's
SuTermVector(const Unknown&, const SuTermVector&, const SuTermVector&, const string_t& ="");
SuTermVector(const Unknown&, const std::list<const SuTermVector*>&, const string_t& ="");
//constructor from linear combination (no linear form)
SuTermVector(const LcTerm&);
//copy constructors and assign operator
SuTermVector(const SuTermVector&);
template<typename T>
SuTermVector(const SuTermVector&, const T&);
SuTermVector& operator=(const SuTermVector&);
//other useful stuff
virtual ~SuTermVector();
void copy(const SuTermVector&);     //full copy
void initFromFunction(const Unknown&, const GeomDomain&, const Function&,
                      const String& na="", bool noass=false);
void clear();
```

A lot of useful accessors and shortcuts to some properties are proposed:

```
string_t name();
void name(const string_t&);
SuLinearForm* sulfp() const;
SuLinearForm*& sulfp();
VectorEntry*& entries();
const VectorEntry* entries() const;
TermType termType() const;
ValueType valueType() const;
StrucType strucType() const;
const Unknown* up() const;
const Unknown*& up();
number_t nbOfComponents() const;
const Space* spacep() const;
Space*& spacep();
set<const Space*> unknownSpaces() const;
number_t nbDofs() const;
number_t size() const;
VectorEntry*& scalar_entries();
const VectorEntry* scalar_entries() const;
VectorEntry* actual_entries() const;
const vector<DofComponent>& cdofs() const;
vector<DofComponent>& cdofs();
const Dof& dof(number_t n) const;
const GeomDomain* domain() const;
```

SuTermVector may be modified by the following operators and functions:

```
SuTermVector& operator+=(const SuTermVector&);
SuTermVector& operator-=(const SuTermVector&);
template<typename T>
 SuTermVector& operator*=(const T&);
template<typename T>
 SuTermVector& operator/=(const T&);
SuTermVector& merge(const SuTermVector&);
SuTermVector& toAbs();
SuTermVector& toReal();
SuTermVector& toImag();
SuTermVector operator()(const ComponentOfUnknown&) const;
SuTermVector& toComplex();
complex_t maxValAbs() const;
void setValue(number_t, const Value&);
void setValue(const Value&, const GeomDomain&);
void setValue(const Function&, const GeomDomain&);
void setValue(const SuTermVector&, const GeomDomain&);
void setValue(const SuTermVector&);
```

The operator () extracts unknown component term vector as a SuTermVector when Unknown is a vector unknown. For instance if u is a vector unknown, T(u[2]) returns a SuTermVector containing the elements of T corresponding to second component.

Some values can be extracted or computed from:

```
Value getValue(number_t) const;
SuTermVector* onDomain(const GeomDomain& dom) const;
template<typename T>
 T& operator()(const vector<real_t>&, T&) const;
SuTermVector* interpolate(const Unknown&, const GeomDomain&);
Value evaluate(const Point&) const;
template<typename T>
 Vector<T>& asVector(Vector<T>&) const;
```

SuTermVector provides real computation algorithms, in particular FE computation ones:

```
void buildSubspaces();
void compute();                 //!< compute from linear form
void compute(const LcTerm&);
template<typename T, typename K>
void computeFE(const SuLinearForm&, Vector<T>&, K&);
template<typename T, typename K>
void computeIR(const SuLinearForm&, Vector<T>&, K& vt, const vector<Point>&,
               const Vector<T>&, const vector<Vector<real_t> >* nxs=0);
```

Some particular member functions allow to change the internal representation:

```
void toScalar(bool keepVector=false);
void toVector(bool keepEntries=false);
void extendTo(const SuTermVector&);
void extendTo(const Space&);
void extendScalarTo(const vector<DofComponent>&, bool useDual = false);
SuTermVector* mapTo(const GeomDomain&, const Unknown&, bool =true) const;
void changeUnknown(const Unknown&, const Vector<number_t>&);
void adjustScalarEntries(const vector<DofComponent>&);
```

Some extern function are provided to compute norms, ...

```
Complex innerProduct(const SuTermVector&, const SuTermVector&);
Complex hermitianProduct(const SuTermVector&, const SuTermVector&);
```

```
Real norm1(const SuTermVector&);
Real norm2(const SuTermVector&);
Real norminfty(const SuTermVector&);
```

Finallys, there are some print and export stuff:

```
void print(ostream&) const;
void print(ostream&, bool r, bool h) const; // raw and header option
void saveToFile(const String&, bool encode=false) const;

//extern save functions
void saveToFile(const string_t&, const Space*, const list<SuTermVector*>&,
                IOFormat iof=_raw, bool withDomName=true);
void saveToMsh(ostream&, const Space*, const list<SuTermVector*>&,
               vector<Point>, splitvec_t, const GeomDomain*);
void saveToMtlb(ostream&, const Space*, const list<SuTermVector*>&,
                vector<Point>, splitvec_t, const GeomDomain*);
void saveToVtk(ostream&, const Space*, const list<SuTermVector*>&,
               vector<Point>,splitvec_t, const GeomDomain*);
void saveToVtkVtu(ostream&, const Space*, const list<SuTermVector*>&,
                  vector<Point>, splitvec_t, const GeomDomain*);
pair<vector<Point>, map<number_t, number_t> > ioPoints(const Space* sp);
splitvec_t ioElementsBySplitting(const Space*, map<number_t, number_t>);
```

| | |
|---|---|
| library : | **term** |
| header : | **SuTermVector.hpp** |
| implementation : | **SuTermVector.cpp** |
| unitary tests : | **test_TermVector.cpp** |
| header dependences : | **Term.hpp, LcTerm.hpp, termUtils.hpp, form.h, config.h, utils.h** |

## 11.4 The TermVectors class

The TermVectors is simply an encapsulation of a list of TermVector. It implements a small interface to std::vector<TermVector> and it is adressed to beginners.

```
class TermVectors: public std::vector<TermVector>
{
  public :
  TermVectors(Number n=0);
  TermVectors(const std::vector<TermVector>& vs);
  const TermVector& operator()(Number n) const;
  TermVector& operator()(Number n);
  void print(std::ostream&) const;
};
std::ostream& operator<<(std::ostream&, const TermVectors&);
```

| | |
|---|---|
| library : | **term** |
| header : | **TermVector.hpp** |
| implementation : | **TermVector.cpp** |
| unitary tests : | **test_TermVector.cpp** |
| header dependences : | **Term.hpp, LcTerm.hpp, termUtils.hpp, form.h, config.h, utils.h** |

## 11.5 The KernelOperatorOnTermVector class

To deal with integral representation, say for instance

$$v(x) = \int_\Gamma K(x,y)\,\varphi(y)$$

where $\varphi$ will be represented by a TermVector object F, the user can define the linear form

$$\int_\Gamma K(x,y)\,u(y)$$

and then call the integralRepresentation function to link its TermVector object F to the linear form. To make the user life easier, XLiFE++ provides a small class KernelOperatorOnTermVector that relates a OperatorOnKernel and a TermVector. So, writing intg(gamma, K*F) will be interpreted as the linear form acting to the TermVector F by handling in the back a KernelOperatorOnTermVector:

```
class KernelOperatorOnTermvector
{
 protected:
 OperatorOnKernel opker_; //Kernel operator
 AlgebraicOperator aop_;  //operation (*,|,%,^) between kernel and TermVector
 const TermVector*   tv_; //TermVector involved
 public:
 bool termAtLeft;         //if true : opker aop tv else :  tv aop opker
}
```

The class provides one basic constructor and some accessors:

```
KernelOperatorOnTermvector(const OperatorOnKernel&, AlgebraicOperator,
                           const TermVector&, bool atleft);
AlgebraicOperator algop();
AlgebraicOperator& algop();
const OperatorOnKernel& opker() const;
const TermVector*  termVector();
ValueType valueType() const;
bool xnormalRequired() const;
bool ynormalRequired() const;
```

Besides, extern functions to the class manage the various operation involving kernel and TermVector:

```
KernelOperatorOnTermvector operator*(const TermVector&, const Kernel&);
KernelOperatorOnTermvector operator|(const TermVector&, const Kernel&);
KernelOperatorOnTermvector operator^(const TermVector&, const Kernel&);
KernelOperatorOnTermvector operator%(const TermVector&, const Kernel&);
KernelOperatorOnTermvector operator*(const Kernel&, const TermVector&);
...
KernelOperatorOnTermvector operator*(const TermVector&, const OperatorOnKernel&);
...
KernelOperatorOnTermvector operator*(const OperatorOnKernel&, const TermVector&);
...
OperatorOnUnknown toOperatorOnUnknown(const KernelOperatorOnTermvector&);
```

Finally, to build integral involving KernelOperatorOnTermvector some pseudo-constructors are provided

```
std::pair<LinearForm,const TermVector*>
intg(const GeomDomain&, const KernelOperatorOnTermvector&,const IntegrationMethod&);
std::pair<LinearForm,const TermVector*>
intg(const GeomDomain&, const KernelOperatorOnTermvector&,const IntegrationMethods&);
std::pair<LinearForm,const TermVector*>
intg(const GeomDomain&, const KernelOperatorOnTermvector&,QuadRule = _defaultRule, number_t =0);
```

| | |
|---|---|
| library : | **term** |
| header : | **KernelOperatorOnTermVector.hpp** |
| implementation : | **KernelOperatorOnTermVector.cpp** |
| unitary tests : | **test_operator.cpp** |
| header dependences : | **OperatorOnKernel.hpp, TermVector.hpp, config.h, utils.h** |

## 11.6 The TermMatrix class

The TermMatrix class carries numerical representation of a bilinear form and more generally any matrix attached to a pair of unknowns. It follows a similar organization to TermVector class but manages row and column information:

```
class TermMatrix : public Term
{protected :
BilinearForm bilinForm_;                        //bilinear form if exists
map<uvPair, SuTermMatrix*> suTerms_;   //list of SuTermMatrix
MatrixEntry* scalar_entries_p;                  //scalar entries representation
vector<DofComponent> cdofs_c;          //column scalar dofs
vector<DofComponent> cdofs_r;          //row scalar dofs
SetOfConstraints* constraints_u_p;              //constraints to apply to row
SetOfConstraints* constraints_v_p;              //constraints to apply to column
MatrixEntry* rhs_matrix_p;       //matrix used by right hand side correction
}
```

The bilinear form is a multiple unknown pairs form, may be reduced to a single unknown pair form (see *form* library). This bilinear form is void if TermMatrix is not explicitly construct from a bilinear form (linear combination, nodal construction, ...). In particular, this bilinear form is not updated when TermMatrix objects are combined.
The map  suTerms_ carries each matrix block related to a pair of unknowns. When there is only one element in map, it means that the TermMatrix is actually a single unknown pair term matrix.
As block representation may be too restrictive in certain cases, it is possible to create its non block representation in *scalar_entries_p* (MatrixEntry pointer). The MatrixEntry object created has to be of real scalar or complex scalar type. In that case, non block row and non block column numbering, consisting in vectors of DofComponent (Unknown pointer, dof number, component number), are also defined (cdofs_r and cdofs_c).

Essential conditions (conditions on space functions) induce special treatments in computation of TermMatrix. It is the reason why they are handled with SetOfConstraints objects which are the algebraic representations of essential conditions (see *essentialConditions* for details). SetOfConstraints on row may differ from SetOfConstraints on column (it is often the same). In case of non homogeneous essential condition, the part of matrix that is eliminated contributes to the right hand side; this part is stored into rhs_matrix_p MatrixEntry pointer. Obviously, the pointers constraints_u_p, constraints_v_p, rhs_matrix_p are null pointer whenever no essential conditions are imposed.

The TermMatrix class provides useful constructors and assign operators designed for end users :

```
TermMatrix(const string_t & na="?");

//constructors with no essential boundary conditions and options
TermMatrix(const BilinearForm&, const string_t& na="");
TermMatrix(const BilinearForm&, TermOption, const string_t& na="");
TermMatrix(const BilinearForm&, TermOption, TermOption, const string_t& na="");
...
//constructor with one essential boundary condition (on u and v)
TermMatrix(const BilinearForm&, const EssentialConditions&, const string_t& na="");
TermMatrix(const BilinearForm&, const EssentialConditions&, TermOption,
           const string_t& na="");
...
//constructor with one essential boundary condition and explicit reduction method
TermMatrix(const BilinearForm&, const EssentialConditions&, const ReductionMethod&,
           const string_t& na="");
TermMatrix(const BilinearForm&, const EssentialConditions&, const ReductionMethod&,
           TermOption, const string_t& na="");
...
//constructor with  two essential boundary conditions (on u and v)
TermMatrix(const BilinearForm&, const EssentialConditions&,
           const EssentialConditions&, const string_t& na="");
TermMatrix(const BilinearForm&, const EssentialConditions&,
           const EssentialConditions&, TermOption, const string_t& na="");
...
//constructor with two essential boundary conditions and explicit reduction method
TermMatrix(const BilinearForm&, const EssentialConditions&, const EssentialConditions&,
           const ReductionMethod&, const string_t& na="");
TermMatrix(const BilinearForm&, const EssentialConditions&, const EssentialConditions&,
           const ReductionMethod&, TermOption, const string_t& na="");
...
//effective constructor
void build(const BilinearForm& blf, const EssentialConditions* ecu,
           const EssentialConditions* ecv, const vector<TermOption>&,
           const string_t& na);

//copy constructors
TermMatrix(const TermMatrix &, const string_t& na="");
// diagonal TermMatrix from a TermVector or a vector
TermMatrix(const TermVector &, const string_t& na="");
template<typename T>
TermMatrix(const Unknown&, const GeomDomain&, const Vector<T> &,
           const string_t& na="");
//TermMatrix from a SuTermMatrix
TermMatrix(const SuTermMatrix &, const string_t& na=""); //full copy
TermMatrix(SuTermMatrix *, const string_t& na="");        //pointer copy
//TermMatrix of the form opker(xi,yj)
TermMatrix(const Unknown&, const GeomDomain&, const Unknown&,
           const GeomDomain&, const OperatorOnKernel&,
           const string_t& na="");
//TermMatrix from a row dense matrix (Matrix)
TermMatrix(const Matrix<T>& mat,const string_t& ="");
TermMatrix(const vector<T>& mat, number_t m, number_t n=0, const string_t& ="");
void buildFromRowDenseMatrix(const vector<T>&, number_t, number_t, const string_t&);
// TermMatrix from a linear combination
TermMatrix(const LcTerm&,const string_t& na="");

//assign operator
TermMatrix& operator=(const TermMatrix&);
TermMatrix& operator=(const LcTerm&);
```

The ReductionMethod class allows the user to specify the reduction method he wants, one of the enumeration ReductionMethodType: *_pseudoReduction, _realReduction, _penalizationReduction, _dualReduction.* It is also possible to provide an additional real/complex parameter (say alpha) : the diagonal coefficient of the pseudo-eliminated part or the penalization coefficient.

```
ReductionMethodType method;  //type of reduction method
complex_t alpha;            //diagonal or penalization coefficient
ReductionMethod(ReductionMethodType= _noReduction, const complex_t& = 1.);
void print(ostream& out) const;
friend  :ostream& operator << (ostream&, const ReductionMethod&);
```

When reduction method is not specified, the pseudo reduction with 1 as diagonal coefficient is used. **Only the pseudo reduction method is available!**

When TermMatrix is constructed, it is automatically computed except if it has been set not to be computed, using the `TermOption` *_notCompute* in its construction.

Developers may used other construction/destruction stuff:

```
void initFromBlf(const BilinearForm &, const String& na ="",
                 bool noass = false);
void initTermVector(TermVector&, ValueType, bool col=true);
template<typename T>
void initTermVectorT(TermVector&,const T&, bool col=true);
void insert(const SuTermMatrix &);
void insert(SuTermMatrix *);
void copy(const TermMatrix&);
void clear();
virtual ~TermMatrix();
```

This class provides a lot of accessors and properties (shorcuts to other class accessors):

```
bool isSingleUnknown() const;
set<const Unknown*> rowUnknowns() const;
set<const Unknown*> colUnknowns() const;
Number nbTerms() const;
ValueType valueType() const;
AccessType storageAccess() const;
void setStorage(StorageType, AccessType);
StorageType storageType() const
bool hasConstraints() const;
FactorizationType factorization() const;
SymType globalSymmetry() const;
TermMatrix operator()(const Unknown&,const Unknown&) const;

//stuff reserved to developers
cit_mustm begin() const;
it_mustm begin();
cit_mustm end() const;
it_mustm end();
map<uvPair, SuTermMatrix*>& suTerms();
MatrixEntry*& scalar_entries();
const MatrixEntry* scalar_entries() const;
MatrixEntry*& rhs_matrix();
const MatrixEntry* rhs_matrix() const;
const vector<DofComponent>& cdofsr() const;
const vector<DofComponent>& cdofsc() const;
vector<DofComponent>& cdofsr();
vector<DofComponent>& cdofsc();
SuTermMatrix& subMatrix(const Unknown*,const Unknown*);
const SuTermMatrix& subMatrix(const Unknown*,const Unknown*) const;
SuTermMatrix* subMatrix_p(const Unknown*,const Unknown*);
const SuTermMatrix* subMatrix_p(const Unknown*,const Unknown*) const;

TermVector& getRowCol(number_t, AccessType, TermVector&) const;
TermVector row(number_t) const;
TermVector column(number_t) const;
template <typename T>
LargeMatrix<T>& getLargeMatrix(StrucType =_undefStrucType) const;
template <typename T>
HMatrix<T,FeDof>& getHMatrix(StrucType =_undefStrucType) const;
```

The access operator() returns a SuTermMatrix as a TermMatrix (obviously a single unknown one). Note that it is a full copy. To avoid copy, use subMatrix member functions.

it_mustm and cit_mustm are iterator aliases:

```
typedef map<uvPair, SuTermMatrix*>::iterator it_mustm;
typedef map<uvPair, SuTermMatrix*>::const_iterator cit_mustm;
```

It is also possible to get row or column (index starts from 1) of the TermMatrix if it is a single unknown one and to access to the LargeMatrix or the HMatrix object that really stores the matrix values:

```
TermVector& getRowCol(number_t, AccessType, TermVector&) const;
TermVector row(number_t) const;
TermVector column(number_t) const;
template <typename T>
LargeMatrix<T>& getLargeMatrix(StrucType =_undefStrucType) const;
template <typename T>
HMatrix<T,FeDof>& getHMatrix(StrucType =_undefStrucType) const;
```

The setStorage function allows the user to impose the matrix storage.

The class proposes to users interfaces to computation algorithms (FE computation and algebraic operations):

```
void compute();
void compute(const LcTerm&,const String& na="");

template<typename T> TermMatrix& operator*=(const T&);
template<typename T> TermMatrix& operator/=(const T&);
TermMatrix& operator+=(const TermMatrix&);
TermMatrix& operator-=(const TermMatrix&);
friend TermVector& multMatrixVector(const TermMatrix&,const TermVector&, TermVector&);
friend TermVector& multVectorMatrix(const TermMatrix&, const TermVector&, TermVector&);
friend TermVector operator*(const TermMatrix&,const TermVector&);
friend TermVector operator*(const TermVector&, const TermMatrix&);
friend TermMatrix operator*(const TermMatrix&, const TermMatrix&);
```

The computation of TermMatrix is a quite intricate process in case of essential conditions to apply to bilinear form. The implementation of compute() looks like (some details are omitted):

```
void TermMatrix::compute()
{
  //compute suterms
  for(it_mustm it = suTerms_.begin(); it != suTerms_.end(); it++)
      it->second->compute();
  if(constraints_u_p==0 && constraints_v_p==0) {computed() = true; return;}
  //deal with essential conditions
  bool global=false;
  if(constraints_u_p!=0) global=constraints_u_p->isGlobal();
  if(constraints_v_p!=0 && !global) global=constraints_u_p->isGlobal();
  if(global) toGlobal(_noStorage, _noAccess, _noSymmetry, false);
  else toScalar();
  switch(computingInfo_.elimination)
    {
      case _noElimination              :  break;
      case _pseudoElimination          :  pseudoElimination(); break;
    }
  computed() = true;
}
```

The principle of pseudo-elimination consists in combining some rows and columns, and "eliminating" some rows and columns (in fact set to 0 except diagonal coefficient). Two cases are to be considered:

- case of essential conditions which do not couple unknowns
- case of essential conditions which couples unknowns (global constraints)

In the first case, the pseudo-elimination process may be performed on each matrix of `SuTermMatrix` involving unknowns concerned by essential conditions whereas in the second case, the process must be performed and the whole matrix of `TermMatrix`. If no such representation exists, we have to create it (`toGlobal` function). See the `pseudoElimination()` function.

This class offers many interfaces to factorization tools and direct solvers :

```
//developers stuff
void initTermVector(TermVector&, ValueType, bool col=true);
template<typename T>
void initTermVectorT(TermVector&, const T&, bool col=true);

void toScalar(bool keepEntries=false);
void toGlobal(StorageType, AccessType, SymType=_noSymmetry, bool keepSuTerms=false);
void toSkyline();
void mergeNumbering(map<const Unknown*, list<SuTermMatrix* >&, map<SuTermMatrix*, vector<Number
     > >&, vector<DofComponent>&, AccessType);
void addIndices(vector<set<Number> >&, MatrixStorage*, const vector<Number>&, const
     vector<Number>&);
void mergeBlocks();
friend TermVector prepareLinearSystem(TermMatrix&, TermVector&, MatrixEntry*&, VectorEntry*&,
     bool toScal=false);
void pseudoElimination();

//direct solver member functions
void ldltSolve(const TermVector&, TermVector&);
void ldlstarSolve(const TermVector&,TermVector&);
void luSolve(const TermVector&,TermVector&);
void umfpackSolve(const TermVector&,TermVector&);
void sorSolve(const TermVector& V, TermVector& R, const Real w, SorSolverType sType );
void sorUpperSolve(const TermVector& V, TermVector& R, const Real w );
void sorDiagonalMatrixVector(const TermVector& V, TermVector& R, const Real w );
void sorLowerSolve(const TermVector& V, TermVector& R, const Real w );
void sorDiagonalSolve(const TermVector& V, TermVector& R, const Real w );
```

End users have to use the following external functions:

```
//factorization tool
void ldltFactorize(TermMatrix&, TermMatrix&);
void ldlstarFactorize(TermMatrix&, TermMatrix&);
void luFactorize(TermMatrix&, TermMatrix&);
void umfpackFactorize(TermMatrix&, TermMatrix&);
void factorize(TermMatrix&, TermMatrix&, FactorizationType ft=_noFactorization);

//direct solver (one right hand side)
TermVector factSolve(TermMatrix&, const TermVector&);
TermVector ldltSolve(TermMatrix&, const TermVector&);
TermVector ldlstarSolve(TermMatrix&, const TermVector&);
TermVector luSolve(TermMatrix&, const TermVector&);
TermVector gaussSolve(TermMatrix&, const TermVector&, bool keepA = false);
TermVector umfpackSolve(TermMatrix&, const TermVector&, bool keepA = false);
TermVector magmaSolve(TermMatrix& A, const TermVector& B, bool useGPU=false,
                      bool keepA=false);
TermVector lapackSolve(TermMatrix& A, const TermVector& B, bool keepA=false);
TermVector directSolve(TermMatrix&, const TermVector&, bool keepA = false);
TermVector schurSolve(TermMatrix&, const TermVector&, const Unknown&, const Unknown&,
                      bool keepA = false);

//direct solver (few right hand sides)
TermVectors factSolve(TermMatrix&, const vector<TermVector>&);
TermVectors ldltSolve(TermMatrix&, const vector<TermVector>&, TermMatrix&);
TermVectors ldlstarSolve(TermMatrix&, const vector<TermVector>&, TermMatrix&);
TermVectors luSolve(TermMatrix&, const vector<TermVector>&, TermMatrix&);
TermVectors gaussSolve(TermMatrix&, const vector<TermVector>&,bool keepA = false);
TermVectors umfpackSolve(TermMatrix&, const vector<TermVector>&,bool keepA = false);
TermVectors directSolve(TermMatrix&, const vector<TermVector>&,bool keepA = false);

// direct solver (TermMatrix right hand side)
TermMatrix factSolve(TermMatrix&, TermMatrix&);
TermMatrix directSolve(TermMatrix&, TermMatrix&, KeepStatus=_keep);
TermMatrix inverse(TermMatrix&);
```

factorize(), factSolve() and directSolve functions are general functions that determine automatically the adapted methods to apply.

To use umfpackSolve, magmaSolve or lapackSolve, libraries UMFPACK, MAGMA, LAPACK-BLAS have to be installed and activated. directSolve chooses UMFPACK solver when matrix is sparse and UMFPACK available, and LAPACK solver when matrix is dense and LAPACK available. UMFPACK solver is always faster than XLIFE++ solvers but LAPACK solver may be slower than the XLIFE++ gauss solver if non optimized LAPACK-BLAS libraries are used

Note that the factSolve and directSolve functions can use a TermMatrix as right hand side. In that case, they compute $\mathbb{A}^{-1}\mathbb{B}$ using a factorization of $\mathbb{A}$. The inverse() function computes the inverse of a TermMatrix using the directSolve function with the identity matrix as right hand side. These functions provide some TermMatrix that are stored as column dense storage. So be care with memory usage!

Up to now, the usage of factSolve, directSolve functions with a TermMatrix as right hand side and inverse() is restricted to single unknown TermMatrix.

In a same way, interfaces to various iterative solvers are provided :

```
//! general iterative solver
TermVector iterativeSolveGen(IterativeSolverType isType, TermMatrix& A,
        TermVector& B, const TermVector& X0, const PreconditionerTerm& P,
        const real_t tol, const number_t iterMax, const real_t omega,
        const number_t krylovDim, const number_t verboseLevel);
//! general front end for iterativeSolve
TermVector iterativeSolve(TermMatrix& A, TermVector& B, const TermVector& X0,
       const PreconditionerTerm& P, const vector<Parameter>& ps);

//! user front-end for iterative solver
inline TermVector iterativeSolve(TermMatrix& A, TermVector& B, const TermVector& X0, const
     PreconditionerTerm& P, 0 to 5 Parameter);
inline TermVector iterativeSolve(TermMatrix& A, TermVector& B, const PreconditionerTerm& P, 0 to
     6 Parameter);
inline TermVector iterativeSolve(TermMatrix& A, TermVector& B, const TermVector& X0, 0 to 6
     Parameter);
inline TermVector iterativeSolve(TermMatrix& A, TermVector& B, 0 to 6 Parameter);

//! user front-end for BiCG solver
inline TermVector bicgSolve(TermMatrix& A, TermVector& B, const TermVector& X0, const
    PreconditionerTerm& P, 0 to 4 Parameter);
inline TermVector bicgSolve(TermMatrix& A, TermVector& B, const PreconditionerTerm& P, 0 to 4
    Parameter);
inline TermVector bicgSolve(TermMatrix& A, TermVector& B, const TermVector& X0, 0 to 4 Parameter);
inline TermVector bicgSolve(TermMatrix& A, TermVector& B, 0 to 4 Parameter);

//! user front-end for BiCGStab solver
inline TermVector bicgStabSolve(TermMatrix& A, TermVector& B, const TermVector& X0, const
    PreconditionerTerm& P, 0 to 4 Parameter);
inline TermVector bicgStabSolve(TermMatrix& A, TermVector& B, const PreconditionerTerm& P, 0 to 4
    Parameter);
inline TermVector bicgStabSolve(TermMatrix& A, TermVector& B, const TermVector& X0, 0 to 4
    Parameter);
inline TermVector bicgStabSolve(TermMatrix& A, TermVector& B, 0 to 4 Parameter);

//! user front-end for CG solver
inline TermVector cgSolve(TermMatrix& A, TermVector& B, const TermVector& X0, const
    PreconditionerTerm& P, 0 to 4 Parameter);
inline TermVector cgSolve(TermMatrix& A, TermVector& B, const PreconditionerTerm& P, 0 to 4
    Parameter);
inline TermVector cgSolve(TermMatrix& A, TermVector& B, const TermVector& X0, 0 to 4 Parameter);
inline TermVector cgSolve(TermMatrix& A, TermVector& B, 0 to 4 Parameter);

//! user front-end for CGS solver
inline TermVector cgsSolve(TermMatrix& A, TermVector& B, const TermVector& X0, const
    PreconditionerTerm& P, 0 to 4 Parameter);
inline TermVector cgsSolve(TermMatrix& A, TermVector& B, const PreconditionerTerm& P, 0 to 4
    Parameter);
inline TermVector cgsSolve(TermMatrix& A, TermVector& B, const TermVector& X0, 0 to 4 Parameter);
inline TermVector cgsSolve(TermMatrix& A, TermVector& B, 0 to 4 Parameter);

//! user front-end for GMRes solver
inline TermVector gmresSolve(TermMatrix& A, TermVector& B, const TermVector& X0, const
    PreconditionerTerm& P, 0 to 4 Parameter);
inline TermVector gmresSolve(TermMatrix& A, TermVector& B, const PreconditionerTerm& P, 0 to 4
    Parameter);
inline TermVector gmresSolve(TermMatrix& A, TermVector& B, const TermVector& X0, 0 to 4
    Parameter);
inline TermVector gmresSolve(TermMatrix& A, TermVector& B, 0 to 4 Parameter);

//! user front-end for QMR solver
inline TermVector qmrSolve(TermMatrix& A, TermVector& B, const TermVector& X0, const
    PreconditionerTerm& P, 0 to 4 Parameter);
inline TermVector qmrSolve(TermMatrix& A, TermVector& B, const PreconditionerTerm& P, 0 to 4
    Parameter);
inline TermVector qmrSolve(TermMatrix& A, TermVector& B, const TermVector& X0, 0 to 4 Parameter);
inline TermVector qmrSolve(TermMatrix& A, TermVector& B, 0 to 4 Parameter);
```

`iterativeSolve(...)` are the front end of all other iterative methods.
`iterativeSolveGen(...)` are the front end of all iterative methods.

To compute eigenvalues, internal solvers or interface to arpack solvers are available:

```
//! general eigen solver
EigenElements eigenSolveGen(TermMatrix* pA, TermMatrix* pB, number_t nev, string_t which, real_t
    tol, EigenComputationalMode eigCompMode,
                              complex_t sigma, const char mode, EigenSolverType solver);
//! general eigen solver
EigenElements eigenInternGen(TermMatrix* pA, TermMatrix* pB, number_t nev, string_t which, real_t
    tol, EigenComputationalMode eigCompMode,
                              complex_t sigma, bool isShift);

//! general front-end for generalized eigen solver
```

```
EigenElements eigenSolve(TermMatrix& A, TermMatrix& B, vector<Parameter> ps);

//! user front-end for eigen solver
EigenElements eigenSolve(TermMatrix& A, TermMatrix& B, 0 to 10 Parameter);
EigenElements eigenSolve(TermMatrix& A, 0 to 10 Parameter);

//! user front-end for internal eigen solver
inline EigenElements eigenInternSolve(TermMatrix& A, TermMatrix& B, 0 to 9 Parameter);
inline EigenElements eigenInternSolve(TermMatrix& A, 0 to 9 Parameter);

//! user front-end for external Arpack eigen solver
inline EigenElements arpackSolve(TermMatrix& A, TermMatrix& B, 0 to 9 Parameter);
inline EigenElements arpackSolve(TermMatrix& A, 0 to 9 Parameter);
```

The `EigenElements` class handles the list of eigenvalues and the list of eigenvectors. See the `TermVector` section.

⚠ ARPACK solver are available only if ARPACK library is installed.

When addressing integral representations, say

$$r(x) = \int_{\Sigma} op(K)(x,y) * op(u)(y)\, dy$$

one can be interested in the matrix with coefficients

$$r_{ij} = \int_{\Sigma} op(K)(x_i,y) * op(w_j)(y)\, dy$$

where $(x_i)_i$ are some points and $(w_j)_j$ some shape functions related to the unknown $u$. Special functions, named `integralFunction` will produce such matrices embedded in a `TermMatrix` object:

```
TermMatrix integralRepresentation(const Unknown&, const GeomDomain&,
                                  const LinearForm&);
TermMatrix integralRepresentation(const GeomDomain&, const LinearForm&);
TermMatrix integralRepresentation(const vector<Point>&, const LinearForm&);
```

When no domain is explicitly passed, one shadow `PointsDomain` object will be created from the list of points given. When no unknown is explicitly passed, one (minimal) space and related shadow unknown will be created to represent the row unknown.
These functions call the fundamental computation function:

```
template<typename T, typename K>
void SuTermMatrix::computeIR(const SuLinearForm&f, T*, K&, const vector<Point>& xs);
```

Once a `TermMatrix` is computed, it is possible to access to one of its coefficient and to change its value. Because, `TermMatrix` is a block matrix indexed by unknowns, a pair of unknowns has to be specified except if it is a single unknown matrix. Row index and col index of the sub-matrix coefficient may be specified either by numbers or by dofs:

```
Value getValue(number_t,number_t) const;
Value getValue(const Unknown&,const Unknown&,number_t,number_t) const;
void  setValue(number_t, number_t, const Value&);
void  setValue(const Unknown&,const Unknown&,number_t,number_t,const Value&);
Value getValue(const Dof& du,const Dof& dv) const;
void  setValue(const Dof& du,const Dof& dv,const Value& val);
Value getValue(const Unknown& u,const Unknown& v,const Dof& du,const Dof& dv) const;
void  setValue(const Unknown& u,const Unknown& v, const Dof& du, const Dof& dv, const Value& val);
```

These functions use some Value objects that have to be real/complex scalars or real/complex matrices according to the matrix coefficient type!

There exists also functions that addresses scalar representation when matrix is related to vector unknown:

```
Value  getScalarValue(const Unknown&,const Unknown&,number_t,number_t,dimen_t=0, dimen_t=0) const;
void   setScalarValue(const Unknown&,const Unknown&,number_t,number_t,const
       Value&,dimen_t=0,dimen_t=0);
Value  getScalarValue(number_t,number_t,dimen_t=0,dimen_t=0) const;
void   setScalarValue(number_t,number_t,const Value&,dimen_t=0,dimen_t=0);
```

The following function can assign a same value to rows or columns:

```
void  setRow(const Value&,number_t r1,number_t r2);
void  setCol(const Value&,number_t c1,number_t c2);
void  setRow(const Unknown&,const Unknown&,const Value&,number_t r1,number_t r2);
void  setCol(const Unknown&,const Unknown&,const Value&,number_t c1,number_t c2);
void  setRow(const Value& val,const Dof& d);
void  setCol(const Value& val,const Dof& d);
void  setRow(const Unknown& u,const Unknown& v,const Value& val,const Dof& d);
void  setCol(const Unknown& u,const Unknown& v,const Value& val,const Dof& d);
```

The link between dof and row/col index is given by the following functions:

```
number_t rowRank(const Dof&) const;
number_t colRank(const Dof&) const;
number_t rowRank(const Unknown&, const Unknown&, const Dof&) const;
number_t colRank(const Unknown&, const Unknown&, const Dof&) const;
```

The setValue, setRow, setCol functions never modify the matrix storage!

These functions are no longer available if the matrix has moved to its global representation and lost its block representation!

Finally some print and export functions are provided:

```
//as member function
void print(ostream&) const;
void viewStorage(ostream&) const;
void saveToFile(const String&, StorageType, bool=false) const;
//as non member function
void saveToFile(const String&, const TermMatrix&, StorageType,
                bool enc = false);
```

| | |
|---|---|
| library : | **term** |
| header : | **TermMatrix.hpp** |
| implementation : | **TermMatrix.cpp** |
| unitary tests : | **test_TermMatrix.cpp** |
| header dependences : | **SuTermMatrix.hpp, termUtils.hpp, Term.hpp, form.h, config.h, utils.h** |

## 11.7 The SuTermMatrix class

The SuTermMatrix class carries numerical representation of a single unknown pair bilinear form and more generally any matrix attached to a pair of unknowns (row unknown and row column).

By convention, 'u' refers to column (unknown of bilinear form) and 'v' to row (test function in bilinear form).

```
class SuTermMatrix : public Term
{protected :
 SuBilinearForm* sublf_p;          //bilinear form through pointer
 const Unknown* u_p;               //column unknown
 const TestFunction* v_p;          //row unknown
 mutable Space* space_u_p;         //pointer to u-space
 mutable Space* space_v_p;         //pointer to v-space
 vector<Space *> subspaces_u;   //u-subspaces involved
 vector<Space *> subspaces_v;   //v-subspaces involved
 MatrixEntry* entries_p;           //matrix as LargeMatrix
 MatrixEntry* scalar_entries_p;    //scalar matrix as LargeMatrix
 vector<DofComponent> cdofs_u;  //component u-dof list
 vector<DofComponent> cdofs_v;  //component v-dof list
 MatrixEntry* rhs_matrix_p;        //correction matrix when essential cond.
}
```

The sublf_p contains a pointer to a SuBiLinearForm (single unknown pair bilinear form). It may be null, that means there is no explicit bilinear form attached to the SuTermMatrix.
The space_u_p (resp. space_u_p) pointer points to the largest subspace involved in SuTermMatrix columns (resp. rows). These pointer should never be null because they carry the rom and column dofs numbering. For this reason too, the largest subspaces have to be correctly updated during any operation on SuTermMatrix.
The Space* vector subspaces_u (resp. subspaces_v) contains the subspaces (as subspace of largest space) attached to basic bilinear forms defined in the SuBiLinearForm pointer (if defined), see buildSubspaces function.

Do not confuse the space_u_p pointer and u_p->space_p pointer that specifies the whole space. They may be the same!

The numerical representation of matrix is defined in the entries_p MatrixEntry pointer as a real/complex matrix or a real/complex matrix of matrices, regarding the value type (real or complex) and the structure of the unknowns (scalar or vector). If required, matrix of matrices representation may be expanded to a matrix of scalars stored in the scalar_entries_p MatrixEntry pointer. In that case, the cdofs_u and cdofs_v vectors of DofComponent give the row and column numbering (in DofComponent ) of entries. Note that if SuTermMatrix is of scalar type, scalar_entries_p = entries_p.
In case of essential conditions applied to, rhs_matrix_p MatrixEntry pointer may be allocated to store the eliminated part of SuTermMatrix. Note that, SuTermMatrix class does not manage SetOfConstraints objects, the treatment of essential condition being driven by TermMatrix!

The SuTermMatrix class also handles HMatrix (hierarchical matrix):

```
HMatrixEntry<FeDof>* hm_entries_p; //hierarchical matrix
HMatrixEntry<FeDof>* hm_scalar_entries_p; //scalar hierarchical matrix
ClusterTree<FeDof>*  cluster_u;    //column cluster tree
ClusterTree<FeDof>*  cluster_v;    //row cluster tree
```

HMatrix stuff is described in chapter 10. Let's remember that the hierarchical matrix are built from the clustering of row and column indices (cluster_u, cluster_v). There are two HMatrixEntry pointers, one to handle any matrix (scalar or matrix), the other one to handle the scalar representation of a matrix of matrices if it is required. When HMatrix is a scalar one, both the pointers are the same.

The SuTermMatrix class provides some constructors from bilinear form, a constructor from SuTermVector (diagonal matrix), a constructor from row dense matrix, a constructor from linear combination and a copy constructor:

```
// basic constructor
SuTermMatrix(const Unknown*, Space*, const Unknown*, Space*, MatrixEntry*, const String& na="");
//constructor from bilinear form
SuTermMatrix(SuBilinearForm* sublf = 0, const String& na="", bool noass=false);
SuTermMatrix(SuBilinearForm* sublf = 0, const String& na="",
             ComputingInfo cp= ComputingInfo());
SuTermMatrix(SuBilinearForm*, const Unknown*, const Unknown*, Space*, Space*,
             const vector<Space *>&, const vector<Space *>&,
             const String&, MatrixEntry* =0);
//constructor of diagonal matrix
SuTermMatrix(SuTermVector &, const String& na="");
SuTermMatrix(const Unknown*, Space*, const Unknown*, Space*, SuTermVector&,
              StorageType=_noStorage, AccessType=_noAccess, const String& na="");
void diagFromSuTermVector(const Unknown*, Space*, const Unknown*,Space*, SuTermVector&,
                          StorageType=_noStorage, AccessType=_noAccess,
                          const String& na="");
// constructor from a row dense matrix
SuTermMatrix(const Unknown*, Space*, const Unknown*, Space*, const vector<T>&, number_t,
    number_t, const string_t& ="");
//constructor from linear combination
SuTermMatrix(const LcTerm&,const String& na="");
//copy constructor and assign operator
SuTermMatrix(const SuTermMatrix&,const String& na="");
void copy(const SuTermMatrix&);
SuTermMatrix& operator=(const SuTermMatrix&);
//destructor, clear
virtual ~SuTermMatrix();
void clear();
```

There is no specific constructor for SuTermMatrix of type Hmatrix. It is induced by some properties of the bilinear form; more precisely by a particular choice of integration method.

It provides a lot of accessors and property functions:

```
TermType termType() const;
ValueType valueType() const;
StrucType strucType() const;
Space& space_u() const;
Space& space_v() const;
Space* space_up() const;
Space* space_vp() const;
Space*& space_up();
Space*& space_vp();
const Unknown* up() const;
const Unknown* vp() const;
const Unknown*& up();
const Unknown*& vp();
MatrixEntry*& entries();
const MatrixEntry* entries() cons;
MatrixEntry*& scalar_entries();
const MatrixEntry* scalar_entries() const;
MatrixEntry*& rhs_matrix();
const MatrixEntry* rhs_matrix() const;
const vector<DofComponent>& cdofsu() const;
const vector<DofComponent>& cdofsv() cons;
vector<DofComponent>& cdofsu();
vector<DofComponent>& cdofsv();
SymType symmetry() const;
```

```
StorageType storageType() const;
MatrixStorage* storagep() const;
void setStorage(StorageType, AccessType);
void toStorage(StorageType, AccessType);
```

The main computation functions and related stuff follow:

```
void compute();
void compute(const LcTerm&,const String& na="");
template<unsigned int CM>
void compute(const vector<SuBilinearForm>&, ValueType, StrucType);
template<typename T, typename K>
void computeIR(const SuLinearForm&f, T*, K&, const vector<Point>&);

void buildSubspaces();
void setStorage(StorageType, AccessType);
void toStorage(StorageType, AccessType);
void addDenseToStorage(const vector<SuBilinearForm>&,MatrixStorage*) const;
void toScalar(bool keepEntries=false);
vector<SuBilinearForm> getSublfs(ComputationType, ValueType&) const;
void updateStorageType(const vector<SuBilinearForm>&,set<Number>&,
                       set<Number>&,StorageType&) const;
```

`SuTermMatrix` may be modified by the following algebraic operators:

```
template<typename T>
SuTermMatrix& operator*=(const T&);
template<typename T>
SuTermMatrix& operator/=(const T&);
SuTermMatrix& operator+=(const SuTermMatrix&);
SuTermMatrix& operator-=(const SuTermMatrix&);
friend SuTermVector operator*(const SuTermMatrix&, const SuTermVector&);
friend SuTermMatrix operator*(const SuTermMatrix&, const SuTermMatrix&);
```

It is also possible to access to one matrix coefficient, to change it, to assign a given value to a row or a column:

```
Value getValue(number_t, number_t) const;
Value getScalarValue(number_t, number_t, dimen_t=0, dimen_t=0) const;
void  setValue(number_t, number_t, const Value&);
void  setScalarValue(number_t, number_t, const Value&, dimen_t=0, dimen_t=0);
void  setRow(const Value&, number_t r1, number_t r2);
void  setCol(const Value&, number_t r1, number_t r2);
number_t rowRank(const Dof&) const;
number_t rowRank(const DofComponent&) const;
number_t colRank(const Dof&) const;
number_t colRank(const DofComponent&) const;
```

The row/col index may be either numbers or dofs; the link between dof and index number is get using `rowRank`, `colRank` functions.

The `setValue`, `setRow`, `setCol` functions never modify the matrix storage!

Finally, there are some print and export stuff:

```
void print(ostream&) const;
void print(ostream&, bool) const;
void viewStorage(ostream&) const;
void saveToFile(const String&, StorageType, bool=false) const;
```

Most of the previous functions works when SuTermMatrix handles a HMatrix, but some not. As there is no check, be cautious! Besides, there are some specific functions related to Hmatrix representation:

```
bool hasHierarchicalMatrix() const;
HMatrix<T,FeDof>& getHMatrix(StrucType str=_undefStrucType) const;
```

| | |
|---|---|
| library : | **term** |
| header : | **SuTermMatrix.hpp** |
| implementation : | **SuTermMatrix.cpp** |
| unitary tests : | **test_TermMatrix.cpp** |
| header dependences : | **Term.hpp, LcTerm.hpp, termUtils.hpp, form.h, config.h, utils.h** |

## 11.8 The `LcTerm` class

The `LcTerm` class is a template class handling a linear combination of terms of type `TermVector`, `TermMatrix`, `SuTermVector` or `SuTermMatrix`. It is automatically involved as a result whenever any linear combination of `Term`'s is handled:

```
TermVector tv1, tv2;
...
out<<norm2(tv1-tv2);
```

In this example `tv1-tv2` produces a `LcTerm<TermVector>` that is cast implicitly to a `TermVector` because the definition of a constructor of `TermVector` from a `LcTerm<TermVector>`. Then any functions defined on `TermVector` may be applied, the `norm2` function in this example.

The `LcTerm` class inherits from `vector<pair<const TT *, complex_t >>`

```
template <typename TT>
class LcTerm : public vector<pair<const TT *, complex_t> >
{
public:
 string_t nametype;
 typedef typename vector<pair<const TT *, complex_t> >::iterator iterator;
 typedef typename vector<pair<const TT *, complex_t> >::const_iterator const_iterator;
```

It has template constructors and insertion functions (`push_back`):

```
template<typename T>
  LcTerm(const TT*,const T&);
  LcTerm(const TT*,const T&, const TT*, const T&);
  LcTerm(const TT&,const T&);
  LcTerm(const TT&,const T&, const TT&, const T&);
  LcTerm(const vector<const TT *>&, const vector<T>&);
  void push_back(const Term*,const T&);
  void push_back(const Term&,const T&);
```

and to avoid some `std::vector` member functions are overloaded:

```
number_t size() const ;
const_iterator begin();
const_iterator end();
iterator begin();
iterator end();
```

It supports the following algebraic operations:

```
template<typename T>
  LcTerm<TT>& operator*=(const T&);
  LcTerm<TT>& operator/=(const T&);
LcTerm<TT>& operator+=(const LcTerm<TT>&);
LcTerm<TT>& operator-=(const LcTerm<TT>&);
```

and provides the following utilities

```
ValueType coefType() const;
void print(ostream &) const;
template <typename TX>
friend ostream& operator<<(ostream &,const LcTerm<TX>&)
```

Note that `TermVector` and `TermMatrix` classes have functions that creates some `LcTerm` objects.

| | |
|---|---|
| library : | **term** |
| header : | **LcTerm.hpp** |
| implementation : | |
| unitary tests : | |
| header dependences : | **Term.hpp, config.h, utils.h** |

## 11.9 The `SymbolicTermMatrix` class

Sometimes, numerical methods involve more complex combinations of `TermMatrix` than linear combinations, for instance $\mathbb{A} = \mathbb{M} + \mathbb{K}\mathbb{M}^{-1}\mathbb{K}^t$ where $\mathbb{M}$ and $\mathbb{K}$ are sparse matrices. Generally, it is not a good idea to compute $\mathbb{A}$ because the result is a dense matrix. The purpose of the `SymbolicTermMatrix` class is to describe as symbolic this matrix, not to compute it but to compute $\mathbb{A}X$ with $X$ a `TermVector`.
A `SymbolicTermMatrix` object is a node of the binary tree with the following data

- a symbolic operation (one of id, +, -,*, /, inv, tran, conj, adj )
- a TermMatrix object (pointer to), may be 0
- up to two SymbolicTermMatrix objects (pointer to)
- a coefficient (complex scalar) applied to the operation

Using these data, the symbolic form of the $\mathbb{A}$ matrix is presented on figure 11.1. On a node, there is either a `TermMatrix` (leaves) or a pair of `SymbolicTermMatrix`.

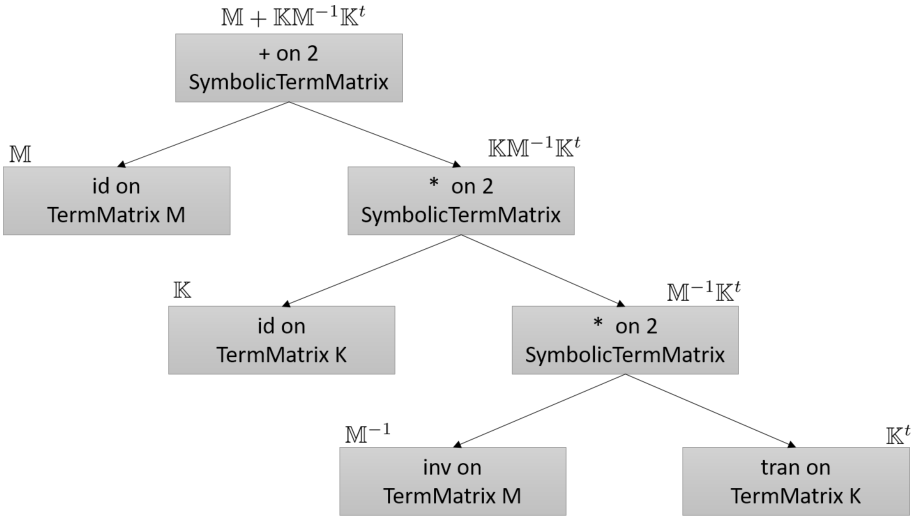


Figure 11.1: Tree representation of matrix $\mathbb{M}+\mathbb{K}\mathbb{M}^{-1}\mathbb{K}^t$

So the SymbolicTermMatrix class has the following data members

```
class SymbolicTermMatrix
{public:
  SymbolicTermMatrix* st1_, *st2_;
  const TermMatrix* tm_;
  complex_t coef_;
  SymbolicOperation op_;
  bool delMat_;
```

the following constructors and destructor stuff

```
SymbolicTermMatrix();
SymbolicTermMatrix(const TermMatrix&, const complex_t& =complex_t(1.,0.));
SymbolicTermMatrix(SymbolicOperation, SymbolicTermMatrix*, SymbolicTermMatrix*=0);
SymbolicTermMatrix(LcTerm<TermMatrix>& lc);
~SymbolicTermMatrix();
void add(LcTerm<TermMatrix>&, std::vector<std::pair<const TermMatrix*, complex_t> >::iterator);
SymbolicTermMatrix(const SymbolicTermMatrix&);
SymbolicTermMatrix& operator=(const SymbolicTermMatrix&);
```

The delMat variable is a flag telling the TermMatrix can be deleted because one of the constructors creates a copy of the original one.

```
SymbolicTermMatrix();
SymbolicTermMatrix(const TermMatrix&, const complex_t& =complex_t(1.,0.));
SymbolicTermMatrix(SymbolicOperation, SymbolicTermMatrix*, SymbolicTermMatrix*=0);
SymbolicTermMatrix(LcTerm<TermMatrix>& lc);
~SymbolicTermMatrix();
void add(LcTerm<TermMatrix>&, std::vector<std::pair<const TermMatrix*, complex_t> >::iterator);
SymbolicTermMatrix(const SymbolicTermMatrix&);
SymbolicTermMatrix& operator=(const SymbolicTermMatrix&);
```

The class offers classic print stuff :

```
string_t asString() const;
void print(std::ostream&) const;
void print(PrintStream& os) const {print(os.currentStream());}
friend std::ostream& operator<<(std::ostream& ,const SymbolicTermMatrix&)
```

Besides a lot of operator are provided :

```
SymbolicTermMatrix& operator *(const TermMatrix&,SymbolicTermMatrix&);
SymbolicTermMatrix& operator *(SymbolicTermMatrix&, const TermMatrix&);
SymbolicTermMatrix& operator +(const TermMatrix&,SymbolicTermMatrix&);
SymbolicTermMatrix& operator +(SymbolicTermMatrix&, const TermMatrix&);
SymbolicTermMatrix& operator -(const TermMatrix&,SymbolicTermMatrix&);
SymbolicTermMatrix& operator -(SymbolicTermMatrix&, const TermMatrix&);
SymbolicTermMatrix& operator +(LcTerm<TermMatrix>&,SymbolicTermMatrix&);
SymbolicTermMatrix& operator +(SymbolicTermMatrix&, LcTerm<TermMatrix>&);
SymbolicTermMatrix& operator -(LcTerm<TermMatrix>&,SymbolicTermMatrix&);
SymbolicTermMatrix& operator -(SymbolicTermMatrix&, LcTerm<TermMatrix>&);
SymbolicTermMatrix& operator *(LcTerm<TermMatrix>&,SymbolicTermMatrix&);
SymbolicTermMatrix& operator *(SymbolicTermMatrix&, LcTerm<TermMatrix>&);
SymbolicTermMatrix& operator *(SymbolicTermMatrix&, SymbolicTermMatrix&);
SymbolicTermMatrix& operator +(SymbolicTermMatrix&, SymbolicTermMatrix&);
SymbolicTermMatrix& operator -(SymbolicTermMatrix&, SymbolicTermMatrix&);
SymbolicTermMatrix& conj(SymbolicTermMatrix&);
SymbolicTermMatrix& adj(SymbolicTermMatrix&);
SymbolicTermMatrix& tran(SymbolicTermMatrix&);
SymbolicTermMatrix& operator *(SymbolicTermMatrix&, const complex_t&);
SymbolicTermMatrix& operator *(const complex_t&, SymbolicTermMatrix&);
SymbolicTermMatrix& operator /(SymbolicTermMatrix&, const complex_t&);
SymbolicTermMatrix& inv(const TermMatrix&);
SymbolicTermMatrix& inv(SymbolicTermMatrix&);
```

Because some syntaxes may be ambiguous,the operator ˜ is overloaded in order to move a `TermMatrix` to a `SymbolicTermMatrix`:

```
SymbolicTermMatrix& operator~(const TermMatrix&):
```

The most important functions are function that compute recursively the matrix vector product $\mathbb{A}X$ :

```
TermVector operator*(const SymbolicTermMatrix&, const TermVector&);
TermVector multMatrixVector(const SymbolicTermMatrix&, const TermVector&);
TermVector operator*(const TermVector&, const SymbolicTermMatrix&);
TermVector multVectorMatrix(const TermVector&, const SymbolicTermMatrix&);
```

| | |
|---:|---|
| library : | **term** |
| header : | **SymbolicTermMatrix.hpp** |
| implementation : | **SymbolicTermMatrix.cpp** |
| unitary tests : | **unit_TermMatrix.cpp** |
| header dependences : | **TermMatrix.hpp, config.h, utils.h** |

## 11.10 The computation algorithms

### 11.10.1 Matrix computation

In this section, we explain how the computation of matrix from bilinear form works. This computation depends on the type of the bilinear form (single integral term, double integral term, ...) and the types of unknown and test function. This section addresses only the computation of `SuTermMatrix`.

The principle of computation, implemented in `SuTermMatrix::compute()`, consists in 4 steps:

- collect basic bilinear forms along their domain and their computation type (see `SuTermMatrix::getSuBlfs()` function.):

| | | |
|---|---|---|
| _FEComputation | single integral on a domain | u,v in FE spaces |
| _FEextComputation | single integral on a boundary domain with non tangential derivatives | u,v in FE spaces |
| _DGComputation | single integral on a sides domain involving mean-jump operators | u,v in FE spaces (discontinuous) |
| _IEComputation | double integral on a domains pair | u,v in FE space, standard Kernel |
| _SPComputation | single integral on a domain | u,v in SP spaces |
| _FESPComputation | single integral on a domain | one in SP space, other in FE space |
| _IESPComputation | double integral on a domains pair | u,v in FE space, TensorKernel |
| _IEHMComputation | double integral on a domains pair | u,v in FE space, HMatrix |

- construct a storage consistent with all collections to compute (imposed by user or chosen between compressed sparse storage or dense storage)
- create `MatrixEntry` with the right structure and value types
- for each collection, call the computation function regarding its computation type

This last step looks like in `SuTermMatrix::compute()`:

```
if(FEsublfs.size()>0)    compute<_FEComputation>(FEsublfs, vt, str);
if(FEextsublfs.size()>0) compute<_FEextComputation>(FEextsublfs, vt, str);
if(SPsublfs.size()>0)    compute<_SPComputation>(SPsublfs, vt, str);
if(FESPsublfs.size()>0)  compute<_FESPComputation>(FESPsublfs, vt, str);
if(IEsublfs.size()>0)    compute<_IEComputation>(IEsublfs, vt, str);
if(IEextsublfs.size()>0) compute<_IEComputation>(IEextsublfs, vt, str);
if(IESPsublfs.size()>0)  compute<_IESPComputation>(IESPsublfs, vt, str);
if(DGsublfs.size()>0)    compute<_DGComputation>(DGsublfs, vt, str);
```

where all specializations of `compute<unsigned int CM>` are implemented in the *XXMatrixComputation.hpp* files included add the end of the *SuTermMatrix.hpp* file. All the computation algorithms mainly work as follows:

```
retry general data (spaces, subspaces, domains, ...)
loop on element on domain 1
  retry element data (local to global numbering)
  (loop on element on domain 2)     only for IE and IESP computation
    (retry element data)
     compute shapevalues
     loop on basic bilinear form
        loop on quadrature points
           compute operator on unknowns
          add in elementary matrix using tensorial operations
        assembly in global matrix
```

For sake of simplicity, evaluation of operators returns always a **scalar vector**, even if the unknowns are vector ones. So this vector has to be correctly reinterpreted when it is added in elementary block matrix.

When there is a HMatrix computation that requires a specific representation (HMatrixEntry), this one is achieved after all the computations requiring a MatrixEntry. Then the MatrixEntry (if it exists one) is merged in the HMatrixEntry. Obviously, anything cannot be merged to HMatrixEntry!

For IE computation, some specialized function are devoted to particular integration method adapted to singular kernels (Sauter-Schwab method for instance). They are implemented in particular files (*SauterSchwabbIM.hpp*, *LenoirSallesM.hpp,DuffyIM.hpp*), see the *src/term/computation* directory.

Up to now, most of the computation functions have been parallelized (multi-threading with omp).

### 11.10.2 Understanding TermMatrix operations

The following figure sketchs out how the operations are processed in the class hierarchy from `TermMatrix` to storage classes that implement the compution algorithms:

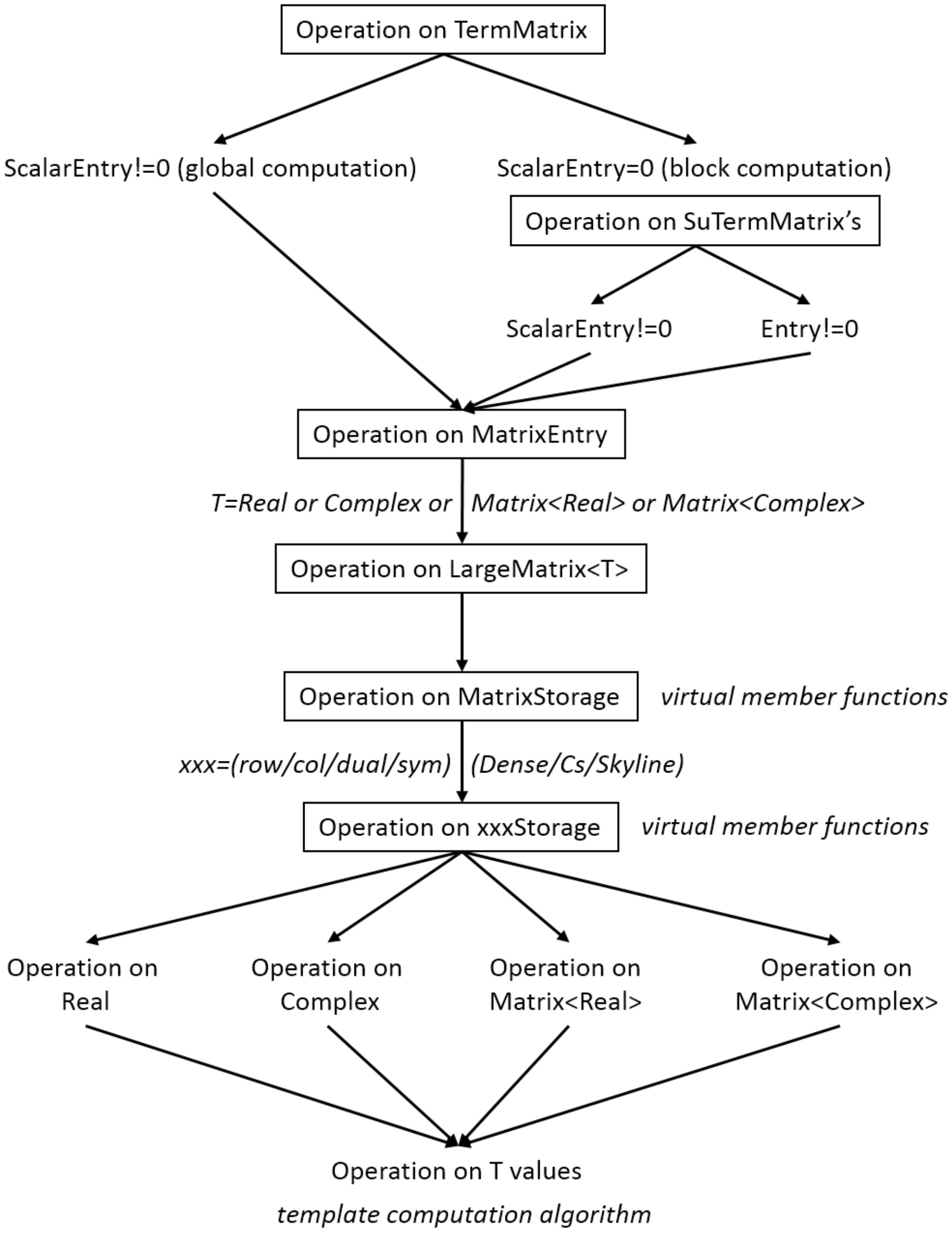

Operation on TermMatrix
ScalarEntry!=0 (global computation)
ScalarEntry=0 (block computation)
Operation on SuTermMatrix's
ScalarEntry!=0
Entry!=0
Operation on MatrixEntry
T=Real or Complex or
Matrix<Real> or Matrix<Complex>
Operation on LargeMatrix<T>
Operation on MatrixStorage
virtual member functions
xxx=(row/col/dual/sym)
(Dense/Cs/Skyline)
Operation on xxxStorage
virtual member functions
Operation on Real
Operation on Complex
Operation on Matrix<Real>
Operation on Matrix<Complex>
Operation on T values
template computation algorithm

Figure 11.2: The process of a TermMatrix operation

### 11.10.3 Vector computation

For the moment, the SuTermVector class provides

- the computeFE function that computes single integral on a FE space
- the computeIR function that computes integral representation

These functions are implemented in the *FeVectorComputation.hpp* file included by the *SuTermVector.hpp* file. It works as matrix computation but it is simpler.

## 11.11 The Projector class

The Projector class is intended to handle projection from one FE space, say $V$ to an other FE space, say $W$. The projection $w \in W$ of a $v \in V$ is based on a bilinear form, say $a(.,.)$, defined on both spaces :

$$a(w,\tilde{w}) = a(v,\tilde{w})\ \ \forall \tilde{w} \in W.$$

Let $(w_i)_{i=1,n}$ a basis of $W$ and $(v_i)_{i=1,m}$ a basis of $V$, the above problem is equivalent to the matrix problem:

$$\mathbb{A}\,W = \mathbb{B}\,V$$

where $\mathbb{A}_{ij} = a(w_j, w_i)$, $\mathbb{B}_{ij} = a(v_j, w_i)$, $v = \sum_{i=1,m} V_i\, v_i$ and $w = \sum_{i=1,n} W_i\, w_i$. The bilinear form should be symmetric and positive on the space $W$ in order to the matrix $\mathbb{A}$ be invertible. The most simple example is the $L^2$ projection related to the bilinear form:

$$a(w,\tilde{w}) = \int_\Omega w\,\tilde{w}\,d\Omega.$$

As a consequence, the Projector class manages the following data:

```
class Projector
{
public:
ProjectorType projectorType;  //!< type of projection
string_t name;                //!< name of projection
protected:
Space* V_, *W_;               //!< spaces involved
Unknown* u_V, *u_W;           //!< internal unknowns
const GeomDomain* domain_;    //!< domain  involved in bilinear forms
BilinearForm* a_V, *a_W;      //!< bilinear forms used by projector
mutable TermMatrix* A_, *B_;  //!< matrix a(W,W) and a(W,V)
mutable TermMatrix* invA_B;   //!< matrix inv(A)*B if allocated
}
```

where the projector type is one of the following:

```
enum ProjectorType {_noProjectorType=0, _userProjector, _L2Projector, _H1Projector,
     _H10Projector};
```

Because, bilinear forms in XLiFE++ are linked to unknowns/spaces, the class manages two bilinear forms and their matrix representation. The unknowns used by the Projector are not some user unknowns but are specific to the class. Finally, it can allocate a TermMatrix object representing the matrix $\mathbb{A}^{-1}\mathbb{B}$.

Besides, in order to save time and memory, all the projectors that have been handled (explicitely or implicitely) are listed in a static vector:

```
static std::vector<Projector*> theProjectors;
```

Projector are constructed from spaces, a projector type or a bilinear form and an optional name. When dealing with the restriction of a space to a domain, the domain has to be given. When dealing with projection of vector unknown, the sizes have to be specified.

```
Projector(Space& V, Space& W, ProjectorType pt=_L2Projector,
          const string_t& na="");
Projector(Space& V, Space& W, const GeomDomain&, ProjectorType pt=_L2Projector,
          const string_t& na="");
Projector(Space& V, Space& W, BilinearForm& a, const string_t& na="");
Projector(Space& V, dimen_t nbcV, Space& W, dimen_t nbcW,
          ProjectorType pt=_L2Projector, const string_t& na="");
Projector(Space& V, dimen_t nbcV, Space& W, dimen_t nbcW, const GeomDomain&,
          ProjectorType pt=_L2Projector, const string_t& na="");
Projector(Space& V, dimen_t nbcV, Space& W, dimen_t nbcW, BilinearForm& a,
          const string_t& na="");
~Projector();
void init(dimen_t nbc_V, dimen_t nbc_W);
```

The `init()` function do really the job of construction. In particular, it computes the matrix `A_` and `B_` and do a factorization of `A_`.

Note that the `TermMatrix` is not allocated at the construction. To allocate it, one has to call the member function:

```
TermMatrix& asTermMatrix(const Unknown&, const Unknown&,
                         const string_t& = "invA_B");
```

that returns a reference to the `TermMatrix` `invA_B` and deletes the `TermMatrix` `A_` and `B_`.

Once constructed, projectors can process `TermVector`'s by using one of the three operator functions:

```
TermVector operator()(TermVector& V,const Unknown& u) const;
TermVector operator()(const TermVector& V) const;
TermVector& operator()(TermVector& V, TermVector& PV) const;
```

Because an unknown is always linked to any `TermVector`, the user can pass the unknown either in a explicit way or in a implicit way when the `TermVector` result is passed to the operator. When no unknown is passed to, the unknown of the projection will be the first unknown linked to the space $W$. If the `TermMatrix` `invA_B` is allocated, the projection does the product `invA_B * V`, if not the projection does the product `B_ * V` and solve the linear system `A_ * X = B_ * V` using the `factSolve` functions.

Projection can also be processed by using the operator *:

```
friend TermVector operator*(const Projector& P, const TermVector& V);
```

that only calls `P(V)`.

Users can compute the projection of a `TermVector` without instanciating a `Projector` object:

```
TermVector projection(const TermVector& V, Space& W, ProjectorType pt=_L2Projector);
```

In that case, a `Projector` object is created in the back.

Two functions deal with the list of all projectors:

```
friend Projector& findProjector(Space& V, Space& W,
                               ProjectorType pt=_L2Projector);
static void clearGlobalVector();
```

The `findProjector` creates a new projector if projector has not been found.

Finally, there are some print stuff:

```
void print(ostream&) const;
friend ostream& operator<<(ostream&, const Projector&);
```

| | |
|---:|:---|
| library : | **term** |
| header : | **Projector.hpp** |
| implementation : | **Projector.cpp** |
| unitary tests : | **unit_Projector.cpp** |
| header dependences : | **Term.hpp, config.h, utils.h** |

# 12 The *essentialConditions* library

To take into account linear essential conditions (conditions acting on unknown or test function spaces), XLiFE++ proposes a general approach based on an abstract algebraic representation of essential conditions, say

$$\mathbb{C}U = G$$

where $U$ represents the vector of components of a function $u$ in space $\mathcal{U} = \left\{\sum_{i=1,n} U_i\, w_i\right\}$, $(w_i)_{i=1,n}$ the basis of discrete space, $\mathbb{C}$ a $p \times n$ matrix and $G$ a $p$ vector. In other words, we consider the discrete constrained space :

$$\widetilde{\mathcal{U}} = \left\{\sum_{i=1,n} U_i\, w_i,\ \mathbb{C}U = G\right\}. \tag{12.1}$$

Such representation may be also used for constraints on test function :

$$\widetilde{\mathcal{V}} = \left\{\sum_{i=1,m} V_i \tau_i,\ \mathbb{D}V = 0\right\}. \tag{12.2}$$

Both may exist in the same time and may be different. Nevertheless, constraints on test functions are always homogeneous ones! In usual cases, the test function constraints are the linear part of unknown constraints ($\mathbb{C} = \mathbb{D}$).

## 12.1 A general process

The first step consists in writing essential conditions given in a symbolic form (see documentation of EssentialConditions class) as a constraints system, details being exposed in documentation of Constraints class). As constraints may be redundant, the constraints system has to be reduced to a minimal system, eliminating redundant conditions or identifying conflicts in constraints. This is achieved using QR factorization. Once the constraints systems are reduced, the main work consists to use them in matrix problems we deal with. As we will see, it is possible to consider different techniques : *real reduction* (some rows and columns of system are deleted), *pseudo reduction* (some rows and columns of system are replaced), *penalization* (some rows and columns of system are penalized) and *duality* (constraints system and new dual unknowns are introduced in the problem).

### Reinterpretation of a linear system with constraints

We consider a general discrete variational problem :

$$\text{find } u \in \widetilde{\mathcal{U}} \text{ such that } a(u,v) = l(v) \quad \forall v \in \widetilde{\mathcal{V}}, \tag{12.3}$$

where the spaces $\widetilde{\mathcal{U}}$ and $\widetilde{\mathcal{V}}$ are given by (12.1-12.2), $a(.,.)$ a bilinear form on $\mathcal{U} \times \mathcal{V}$ and $l(.)$ a linear form on $\mathcal{V}$. We assume in the following, that the constraints systems $\mathbb{C}U = G$ and $\mathbb{D}V = 0$ are reduced, so the $m \times n$ matrix $\mathbb{C}$ and the $p \times q$ matrix $\mathbb{D}$ have the following representation :

$$\mathbb{C} = [\mathbb{E}\ \mathbb{R}] \text{ and } \mathbb{D} = [\mathbb{F}\ \mathbb{S}] \tag{12.4}$$

where $\mathbb{E}$ is a $m \times m$ upper triangular matrix (invertible), $\mathbb{R}$ a $m \times n - m$ matrix (may be null, $n \geq m$), $\mathbb{F}$ a $p \times p$ upper triangular matrix (invertible) and $\mathbb{S}$ a $p \times q - p$ matrix (may be null, $q \geq p$). The column indices $\mathscr{E}$ (resp.$\mathscr{F}$) of $\mathbb{E}$ (resp. $\mathbb{F}$) correspond to the eliminated unknowns (resp. test functions) and the column indices $\mathscr{R}$ (resp. $\mathscr{S}$) of $\mathbb{R}$ (resp. $\mathbb{S}$) correspond to reduced unknowns (resp. test functions).

Introducing $\mathbb{X} = \mathbb{E}^{-1}\,\mathbb{R}$ and $\mathbb{Y} = \mathbb{F}^{-1}\,\mathbb{S}$, the constraints read :

$$U_{\mathscr{E}} + \mathbb{X}\,U_{\mathscr{R}} = \mathbb{E}^{-1}G \text{ and } V_{\mathscr{F}} + \mathbb{Y}\,V_{\mathscr{S}} = 0 \tag{12.5}$$

where $U_{\mathscr{E}}$ (resp. $U_{\mathscr{R}}$) denotes the unknown components restricted to indices $\mathscr{E}$ (resp. $\mathscr{R}$) and $V_{\mathscr{F}}$ (resp. $V_{\mathscr{S}}$) denotes the test function components restricted to indices $\mathscr{F}$ (resp. $\mathscr{S}$).
The space $\widetilde{\mathscr{U}}$ may be reinterpreted by eliminating the components $U_{\mathscr{E}}$ :

$$\begin{aligned}
\sum_{i=1,n} U_i\,w_i &= \sum_{i\in\mathscr{E}} U_i\,w_i + \sum_{i\notin\mathscr{E}} U_i\,w_i \\
&= -\sum_{i\in\mathscr{E}}\sum_{j\in\mathscr{R}} \mathbb{X}_{ij}U_j\,w_i + \sum_{j\notin\mathscr{E}} U_j\,w_j + \sum_{i\in\mathscr{E}} (\mathbb{E}^{-1}G)_i\,w_i \\
&= \sum_{j\notin\mathscr{E}} u_j\left(w_j - \sum_{i\in\mathscr{E}} \mathbb{X}_{ij}\,w_i\right) + \sum_{i\in\mathscr{E}} (\mathbb{E}^{-1}G)_i\,w_i \ \text{ (setting } \mathbb{X}_{ij} = 0\ \forall i,\ \forall j \notin \mathscr{E}).
\end{aligned}$$

Considering the functions

$$\widetilde{w}_j = w_j - \sum_{i\in\mathscr{E}} \mathbb{X}_{ij}\,w_i \quad j \notin \mathscr{E}, \tag{12.6}$$

the vector space $\widetilde{\mathscr{U}}_0$ associated to $\widetilde{\mathscr{U}}$ is generated by the functions $\widetilde{w}_j$ :

$$\widetilde{\mathscr{U}_0} = \left\{\sum_{i\notin\mathscr{E}} U_i\,\widetilde{w}_i\right\}.$$

In a same way, the vector space $\widetilde{\mathscr{V}}$ is generated by the functions :

$$\widetilde{\tau}_j = \tau_j - \sum_{i\in\mathscr{F}} \mathbb{Y}_{ij}\,w_i \quad j \notin \mathscr{F}, \tag{12.7}$$

and

$$\widetilde{\mathscr{V}} = \left\{\sum_{i\notin\mathscr{F}} U_i\widetilde{\tau}_i\right\}.$$

Setting $g = \sum_{i\in\mathscr{E}} (\mathbb{E}^{-1}G)_i\,w_i$, the problem (12.3) is equivalent to

$$\text{find } \widetilde{u} \in \widetilde{\mathscr{U}_0} \text{ such that } a(\widetilde{u}, \overline{\widetilde{v}}) = l(\overline{\widetilde{v}}) - a(g, \overline{\widetilde{v}}) \ \ \forall v \in \widetilde{\mathscr{V}} \tag{12.8}$$

equivalent to

$$\text{find } \widetilde{u} = \sum_{j\notin\mathscr{E}} \widetilde{U}_j\,\widetilde{w}_j \text{ such that } \sum_{j\notin\mathscr{E}} \widetilde{U}_j\,a(\widetilde{w}_j, \overline{\widetilde{\tau}}_i) = l(\overline{\widetilde{\tau}}_i) - a(g, \overline{\widetilde{\tau}}_i) \ \ \forall i \notin \mathscr{F}. \tag{12.9}$$

The system (12.9) may be explicited by using (assuming $\tau_i$ is a real function) :

$$a(\widetilde{w}_j, \overline{\widetilde{\tau}}_i) = a(w_j, \tau_i) - \sum_{k\in\mathscr{E}} \mathbb{X}_{kj}\,a(w_k, \tau_i) - \sum_{k\in\mathscr{F}} \overline{\mathbb{Y}}_{ki}\,a(w_j, \tau_k) + \sum_{k\in\mathscr{E}}\sum_{l\in\mathscr{F}} \mathbb{X}_{kj}\overline{\mathbb{Y}}_{li}\,a(w_k, \tau_l) \tag{12.10}$$

and

$$l(\overline{\widetilde{\tau}}_i) = l(\tau_i) - \sum_{k\in\mathscr{F}} \overline{\mathbb{Y}}_{ki}\,l(\tau_k). \tag{12.11}$$

Finally, from the knowledge of all $a(w_j, \tau_i)$ and $l(\tau_i)$ corresponding to the computation without essential conditions, it is possible to construct the system (12.9). In terms of matrix, the different operations are mainly row or column combinations. XLIFE++ implements this general scheme. In a simple case, the Dirichlet problem for instance, the previous expression are trivial because $\mathbb{X} = \mathbb{Y} = 0$, $\widetilde{w}_j = w_j$, $\forall j \notin \mathscr{E}$ and $\tau_j = w_j$.
When condition is not homogeneous ($g \neq 0$), there is a contribution from $g$ and a part of matrix representing $a(.,.)$ (columns with index in $\mathscr{E}$). In order to avoid additional reduction process when an other data $g$ is considered, it is possible to keep in memory this part of matrix.

### Overview of classes involved

To describe essential conditions, XLIFE++ uses :

- some classes used to describe (bi)linearform : Unknown DifferentialOperator OperatorOnUnknown
- the class LcOperatorOnUnknown which handles linear combination of OperatorOnUnknown and allow to associate geometric domains (GeomDomain). The general syntaxes look like ($\diamond$ represent any algebraic operation consistant with objects involved) :

  $$a_1 * op_1(f_1 \diamond u_1 \diamond g_1)|dom_1 + a_2 * op_2(f_2 \diamond u_2 \diamond g_2)|dom_2 + ...$$

  $$(a_1 * op_1(f_1 \diamond u_1 \diamond g_1) + a_2 * op_2(f_2 \diamond u_2 \diamond g_2) + ...)|dom$$

  This class supports a lot of expressions but just a few ones could be used as essential condition ! This class belongs to the *operator* library.
- To transform a previous expression as an essential condition, it is required to give a right hand side :

  LcOperatorOnUnknown = constant or LcOperatorOnUnknown = function

  it produces an object of EssentialCondition class.
- Concatanating EssentialCondition objects using the operator & produces a set of essential conditions managed by EssentialConditions class.

All these classes are user classes!

Constraints is the core class implementing most of the algorithms : transformation of symbolic conditions into constraints system, reduction of constraints system, reduction or pseudo-reduction of matrix, right hand side correction.

## 12.2 The EssentialCondition class

The EssentialCondition class handles the symbolic representation of an essential condition in the form $expression(u_1|dom_1, u_2|dom_2, ...) = f$ where $expression(...)$ is a LcOperatorOnUnknown object and $f$ is a Function object.

```
class EssentialCondition
{
  protected :
  LcOperatorOnUnknown ecTerms_;  // combination of operator on unknown
  Function *fun_p;               // function defining data of EC
                                 // (=0 when EC is homogeneous)
  EcType type_;                  // type of essential condition
}
```

The type of essential condition are listed in the *EcType* enumeration:

```
enum EcType {_undefEcType,        //undefined type
             _DirichletEc,        //one unknown, one domain
             _transmissionEc,     //two unknowns, one domain
             _periodicEc,         //one unknown, two domains
             _crackEc,            //two unknowns, two domains
             _meanEc              //intg_D(opu)=f
            };
```

The class proposes basic constructors which do full copy of LcOperatorOnUnknown and Function objects:

```
EssentialCondition()
EssentialCondition(const LcOperatorOnUnknown&);
EssentialCondition(const LcOperatorOnUnknown&, const Function&);
EssentialCondition(Domain&, const LcOperatorOnUnknown&);
EssentialCondition(Domain&, const LcOperatorOnUnknown&, const Function&);
EssentialCondition(const EssentialCondition&);
EssentialCondition& operator=(const EssentialCondition&);
```

some accessors or shotrcuts :

```
const std::vector<OpuValPair>& bcTerms() const;
const Function& fun() const;
Function*& funp();
it_opuval begin();
cit_opuval begin() const;
it_opuval end();
cit_opuval end() const;
Number size() const;
EcType type() const;
```

some function giving properties

```
bool isSingleUnknown() const;
Dimen nbOfUnknowns() const;
const Unknown* unknown() const;
std::set<const Unknown*> unknowns() const;
bool isSingleDomain() const;
Domain* domain() const;
std::set<Domain*> domains() const;
Dimen nbOfDomains() const;
Number nbTerms() const;
Complex coefficient() const;
std::vector<Complex> coefficients() const;
std::set<DiffOpType> diffOperators() const;
bool nbOfDifOp() const;
DiffOpType diffOperator() const;
bool isHomogeneous() const;
String name() const;
```

some functions to set type and domain:

```
EcType setType();                //set the type of the Essential condition
void setDomain(Domain& dom)      //affect domain to EC
EssentialCondition& operator |(Domain&)     //affect domain of EC
```

When affect the domain using *setDomain* function or | operator, all the domains defined in EcTerms are reset to the new domain. This domain affectation is also done by the non member function:

```
EssentialCondition on(const Domain&, const EssentialCondition&);
```

and printing facilities:

```
void print(std::ostream&) const;
friend std::ostream& operator<<(std::ostream&, const EssentialCondition&);
```

To construct essential condition on the fly, the = operator of classes Unknown, OperatorOnUnknown and LcOperatorOnUnknown are overloaded:

```
EssentialCondition LcOperatorOnUnknown::operator = (const Real &):
EssentialCondition LcOperatorOnUnknown::operator = (const Complex &);
EssentialCondition LcOperatorOnUnknown::operator = (const Function &);
EssentialCondition OperatorOnUnknown::operator = (const Real &);
EssentialCondition OperatorOnUnknown::operator = (const Complex &);
EssentialCondition OperatorOnUnknown::operator = (const Function &);
EssentialCondition Unknown::operator = (const Real &);
EssentialCondition Unknown::operator = (const Complex &);
EssentialCondition Unknown::operator = (const Function &);
```

All these member functions are implemented in the file *EssentialCondition.cpp*.

| | |
|---|---|
| library : | **essentialCondition** |
| header : | **EssentialCondition.hpp** |
| implementation : | **EssentialCondition.cpp** |
| unitary tests : | **test_EssentialCondition.cpp** |
| header dependences : | **Operator.h, config.h, utils.h** |

## 12.3 The `EssentialConditions` class

The `EssentialConditions` class manages a list of `EssentialCondition`. It inherits from `list<EssentialConditions>` with no additional member data:

```
class EssentialConditions : public std::list<EssentialCondition>
```

As it is a user class, it mainly interfaces function of `list` class

```
//constructors and assign
EssentialConditions() {}
EssentialConditions(const EssentialCondition&);
EssentialConditions(const EssentialCondition&, const EssentialCondition&);
EssentialConditions(const EssentialConditions&);
EssentialConditions& operator = (const EssentialConditions&);
//utilities
bool coupledUnknowns() const;
std::set<const Unknown*> unknowns() const;
const Unknown* unknown() const;
void print(std::ostream&) const;
friend std::ostream& operator << (std::ostream&, const EssentialConditions &);
```

It overloads the & operator to concatenate `EssentialCondition`:

```
EssentialConditions operator & (const EssentialCondition&, const EssentialCondition&);
EssentialConditions operator & (const EssentialCondition&, const EssentialConditions&);
EssentialConditions operator & (const EssentialConditions&, const EssentialCondition&);
EssentialConditions operator & (const EssentialConditions&, const EssentialConditions&);
```

| | |
|---|---|
| library : | **essentialCondition** |
| header : | **EssentialConditions.hpp** |
| implementation : | **EssentialConditions.cpp** |
| unitary tests : | **test_EssentialCondition.cpp** |
| header dependences : | **EssentialCondition.hpp, Operator.h, config.h, utils.h** |

## 12.4 The Constraints class

The Constraints class handles the algebraic representation $\mathbb{C}U = G$ of a set of essential conditions (EssentialConditions
:

```
class Constraints
{
 protected :
 MatrixEntry* matrix_p;                       //constraints matrix
 VectorEntry* rhs_p;                          //constraints right hand side
 public :
 EssentialConditions conditions_;             //list of essential conditions
 std::vector<DofComponent> cdofsr_;           //row DofComponent's of matrix_p
 std::vector<DofComponent> cdofsc_;           //col DofComponent's of matrix_p
 std::map<DofComponent, Number> elcdofs_;     //map of eliminated cdofs
 std::map<DofComponent, Number> recdofs_;     //map of reduced cdofs
 bool reduced;                                //true if reduced system
 bool local;                                  //true if local conditions
 bool symmetric;                              //true if keep symmetry
 bool isId;                                   //true if Id matrix
}
```

Even if unknowns involved in constraints system are vector unknowns, the representation uses scalar unknown numbering (*cdofsc_* vector). The *cdofsr_* handles row numbering, each row corresponding to one constraint equation linked to an "artificial" test function. The *elcdofs_* map carries the eliminated index set $\mathscr{E}$ and *recdofs_* map carries the reduced index set $\mathscr{R}$ . Constraints is processed in two steps :

- construction of the constraint system from the list of essential conditions : each condition are translated in its matrix representation, then all the matrix representations are merged in a large one
- reduction of the large constraints system using QR algorithm with removing the redundant constraints and identifying the conflicting constraints

A constraint is local (*local* = *true*) if it involves only one dof. Dirichlet conditions are local and transmission or periodic conditions are not. The class proposes mainly the constructor from a list of essential conditions and usual copy and delete stuff (full copy):

```
Constraints(MatrixEntry* =0, VectorEntry* =0);
Constraints(const EssentialCondition&);
Constraints(const Constraints&);
Constraints& operator=(const Constraints&);
void copy(const Constraints&);
~Constraints();
void clear();
```

some accessors and property functions :

```
const MatrixEntry* matrixp() const;
const VectorEntry* rhsp() const;
bool coupledUnknowns() const;
const Unknown* unknown() const;
std::set<const Unknown*> unknowns() const;
```

The fundamental functions are the building functions

```
bool createDirichlet(const EssentialCondition&); //create from Dirichlet cond.
void createLf(const EssentialCondition&);         //create from linear form cond.
void createNodal(const EssentialCondition&);      //create general condition
MatrixEntry* constraintsMatrix(const OperatorOnUnknown&, const GeomDomain*,
       Space*, const complex_t&, vector<Point>&, const Function*,
       vector<DofComponent>&);                    //create submatrix of a constraint
```

```
void concatenateMatrix(MatrixEntry&, std::vector<DofComponent>&, const MatrixEntry&,
       const std::vector<DofComponent>&);  //concatenate 2 constraints matrices
void reduceConstraints(real_t aszero);      //reduce constraints matrix
template <typename T>
void buildRhs(const Function*, vector<Point>&, const T&);  //tool building rhs
```

Functions *createXXX(const EssentialCondition&)* build the matrix representation for *XXX* condition. Now, there exist Dirichlet, transmission and periodic type. It is quite easy to add new translation functions to take into account new ones. The *reduceConstraints* function processes the reduction of any constraints sytem using QR algorithm. The *asZero* variable is used to round to zero very small values induced by rounding errors in QR algorithm. This function modifies the current matrix and right hand side vector. So the original representation is lost after reduction!

To build the matrix representation of a set of essential conditions, two cases have to be considered:

- no condition that couples two unknowns (independent conditions); in that case one constraints system is built for each unknown
- there exists one coupling condition (coupled conditions); in that case a unique constraints system for all unknowns is built

For instance, the conditions ($u_1$, $u_2$ two unknowns):

$$u_1 = 0|\Sigma \quad u_1 = 0|\Gamma \quad u_2 = 0|\Gamma$$

gives two constraints system, one merging $u_1$ conditions and an other one for $u_2$. While the conditions :

$$u_1 = 0|\Sigma \quad u_1 = 0|\Gamma \quad u_2 - u_1 = g|\Gamma$$

gives a global constraints system merging all conditions.

The merging and building process is done by an external functions that return a list of Constraints indexed by unknown (Unknown pointer). In case of coupled conditions, the list contains only one Constraints indexed by 0.

```
map<const Unknown*, Constraints*> mergeConstraints(vector<Constraints*>&);
map<const Unknown*, Constraints*> buildConstraints(const EssentialConditions&);
```

The *buildConstraints* function looks like (iterator declaration omitted):

```
map<const Unknown*, Constraints*> buildConstraints(const EssentialConditions& ecs){
map<const Unknown*, Constraints*> mconstraints
vector<Constraints *> constraints(ecs.size());
itc=constraints.begin();
//translate conditions into constraints
for(ite=ecs.begin(); ite!=ecs.end(); ite++, itc++)
          *itc=new Constraints(*ite);
//merge constraints
mconstraints =  mergeConstraints(constraints);
//reduce constraints
for(itm=mconstraints.begin(); itm!=mconstraints.end(); itm++)
          itm->second->reduceConstraints();
return mconstraints;}
```

The Constraints class provides important tools that take into account essential conditions in linear systems:

```
void pseudoColReduction(MatrixEntry*, vector<DofComponent>&,
                        vector<DofComponent>&, MatrixEntry*&);
void pseudoRowReduction(MatrixEntry*, vector<DofComponent>&,
                        vector<DofComponent>&);
friend void extendStorage(MatrixEntry*, vector<DofComponent>&,
            vector<DofComponent>&, const Constraints*, const Constraints*);
void extractCdofs(const vector<DofComponent>&, map<DofComponent, Number>&,
                  map<DofComponent, Number>&, bool useDual=false) const;
friend void appliedRhsCorrectorTo(VectorEntry*, vector<DofComponent>&,
             MatrixEntry*, const Constraints*, const Constraints*,
             ReductionMethod);
```

The functions *pseudoColReduction* and *pseudoRowReduction* performs the reduction of system matrix according to relation 12.10. The *pseudoColReduction* also stores the part of matrix system to be memorized to process right hand side correction. If case of non homogeneous constraints, the function *appliedRhsCorrectorTo* modifies the system right hand side according to relation 12.11. Regarding unknown and test function constraints, *extendStorage* function extends the storage of a matrix. This extension occurs when constraints are not local. *extractCdofs* function is a facility to localized eliminated or reduced rows/columns in matrix. All of these functions are called by compute functions of `TermMatrix` class.

In order to deal with constraints acting on different matrix blocs, the `SetOfConstraints` class is provided. It manages mainly a map relating unknown and constraint:

```
class SetOfConstraints : public map<const Unknown*, Constraints*>
{
public:
SetOfConstraints(const Unknown*, Constraints*);   //from a constraints pointer
SetOfConstraints(const map<const Unknown*, Constraints*>& mc);    //from pointers
SetOfConstraints(const EssentialConditions&);     //from EssentialConditions
SetOfConstraints(const SetOfConstraints&); //copy constructor with full copy
SetOfConstraints& operator = (const SetOfConstraints&);//assignment with copy
~SetOfConstraints();    //destructor deallocating constraints pointers
void clear();           //deallocate constraints pointer and reset the map

Constraints* operator()(const Unknown*) const; //acces operator from unknown
bool isGlobal() const;              //true if a unique global constraint
bool isReduced() const;             //true if  all constraints have been reduced
void print(std::ostream&) const;    //print utility
friend std::ostream& operator<<(std::ostream&, const SetOfConstraints&);
};
```

The `SetOfConstraints` objects are very important because they are used by the `TermMatrix` objects when they have to deal with essential conditions!

| | |
|---:|:---|
| library : | **essentialCondition** |
| header : | **Constraints.hpp** |
| implementation : | **Constraints.cpp** |
| unitary tests : | **test_Constraints.cpp** |
| header dependences : | **EssentialCondition.hpp, EssentialConditions.hpp, LargeMatrix.h, config.h, utils.h** |

# 13 The *solvers* library

The *solvers* library comes with some iterative solver methods which target a linear system. These solvers can be divided into two kinds of group. One is for symmetric linear system and another is for a non-symmetric system. Each solver uses *largeMatrix* and *Vector* as inputs and returns the result in a *Vector*. The type of problem, real or complex, needs specified also as another input of a solver. In some cases, a solver can take advantage of a `Preconditioner` as an extra input to decrease the conditioner number of the system. A `Preconditioner`, which is also a *LargeMatrix* involved with matrix factorization, is only available in the type of `SkylineStorage` and `CsStorage`.
All solvers in the library are based on the class `IterativeSolver`, which provides some basic properties and methods. Specific iterative algorithms are implemented in the inherited class for two cases: with and without a preconditioner.

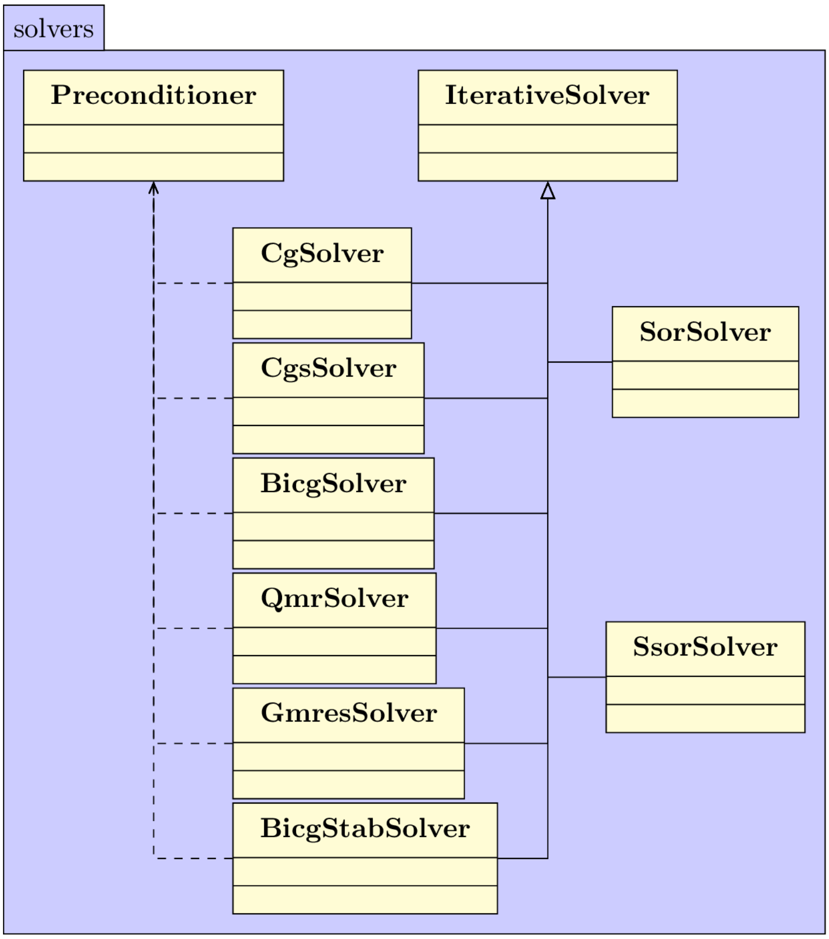


Figure 13.1: The *solvers* library main class diagram

## 13.1 The `IterativeSolver` class

As the base class of all other solver classes, the `IterativeSolver` provides some basic properties and methods for all descendants.

```
class IterativeSolver
{
  public:
    //! Constructor by name
    IterativeSolver(const string_t& name, number_t vb = 0);
    //! Constructor by type
    IterativeSolver(IterativeSolverType ist, number_t vb = 0);
    //! Full constructor without type
    IterativeSolver(const string_t& name, number_t maxOfIt, real_t eps, number_t vb = 0, bool
        prec = true);
    //! Full constructor without name
    IterativeSolver(IterativeSolverType ist, number_t maxOfIt, real_t eps, number_t vb = 0, bool
        prec = true);
    //! Full constructor
    IterativeSolver(const string_t& name, IterativeSolverType ist, number_t maxOfIt, real_t eps,
        number_t vb = 0, bool prec = true);

    //! Destructor
    virtual ~IterativeSolver();

    //! Iterative solver name for documentation purposes
    string_t name() { return name_; }
    //! Reset Solver
    void resetSolver();

  protected:
    //! Define a default value for the maximum number of iterations
    number_t maximumOfIterations(const size_t nbRows);
    ...
```

A solver object can be constructed in several ways: With default values or with user-input values. Information of solver can be printed out with some auxiliary functions.

```
    void printHeader(const size_t) const;
    void printHeader(const size_t, const String&) const;
    void printHeader(const size_t, const Real) const;
    void printHeader(const size_t, const Number) const;
    void printHeader(const size_t, const Number, const String&) const;
    void printOutput() const;
    void printIteration() const;
```

In order to avoid invalid cast from complex to real and vice versa, some inline functions are provided.

```
inline void assign(Real& x, const Real& y) { x = y; }
inline void assign(Complex& x, const Real& y) { x = y; }
inline void assign(Complex& x, const Complex& y) { x = y; }
inline void assign(Real& x, const Complex& y) { x = y.real(); }
```

| | |
|---|---|
| library : | **solvers** |
| header : | **IterativeSolver.hpp** |
| implementation : | **IterativeSolver.cpp** |
| unitary tests : | **test_BicgSolver.hpp, test_BicgStabSolver.hpp, test_CgSolver.hpp, test_CgsSolver.hpp, test_GmresSolver.hpp, test_QmrSolver.hpp, test_SorSolver.hpp, test_SsorSolver.hpp** |
| header dependences : | **Preconditioner.hpp, config.h, utils.h** |

## 13.2 The Preconditioner class

In some cases, the rate of convergence of an iterative solver can increase as a result of preconditioning. A precondtioner is basically a special matrix which can be factorized. There exist several types of matrix-factorization for Preconditioner: LU, LDLt, LDL*, Diag and SOR. Because of constraints of factorizing, only matrices of SkylineStorage and CsStorage can be used as a preconditioner.
In detail, a preconditioner is based on a template class Mat, on which all the preconditioned-solver are processed.

```
template<class Mat>
class Preconditioner
{
  public:
    Mat* precondMatrix_p; // pointer to precondition matrix
  private:
    //! Type of preconditioner
    PreconditionerType type_;
    //! Relaxation parameter for SSOR preconditioners
    Real omega_;
  public:
    Preconditioner()
      : precondMatrix_p(0), type_(_noPreconditioner), omega_(0.)  { }

    Preconditioner(PreconditionerType pt, Mat& A, const Real w = 1.)
     : precondMatrix_p(&A), type_(pt), omega_(w)  { }

    Preconditioner(Mat& A, PreconditionerType pt, const Real w = 1.)
      : precondMatrix_p(&A), type_(pt), omega_(w)  {  }
    ~Preconditioner() {};
    //! Return type of precondionner
    static String name(PreconditionerType pt)
    {
      String s("");
      switch ( pt )
      {
        case _lu:        s = "LU"; break;
        case _ldlt:      s = "LDLt"; break;
        case _ldlStar:   s = "LDL*"; break;
        case _ssor:      s = "SSOR"; break;
        case _diag:      s = "Diagonal"; break;
          //case myPreconditioner: s = "User Supplied"; break;
        default: break;
      }
      return s;
    }
    ...
```

A preconditioner can only templated with a specific kind of matrix that can be decomposed. There are only two types of storage, with which matrix can be factorized: SkylineStorage with LU, LDLt, LDL* factorization; CsStorage with SOR and DIAG factorization.

There are several constructors:

```
Preconditioner()
: precondMatrix_p(0), type_(_noPreconditioner), omega_(0.)  { }

Preconditioner(PreconditionerType pt, Mat& A, const Real w = 1.)
: precondMatrix_p(&A), type_(pt), omega_(w)  {  }

Preconditioner(Mat& A, PreconditionerType pt, const Real w = 1.)
```

```
: precondMatrix_p(&A), type_(pt), omega_(w)   {   }
```

The PreconditionerType is an enumeration.

```
enum PreconditionerType {_noPreconditioner, _lu, _ldlt, _ldlStar, _ssor, _diag,
    _myPreconditioner};
```

| | |
|---|---|
| library : | **solvers** |
| header : | **Preconditioner.hpp** |
| implementation : | **Preconditioner.hpp** |
| unitary tests : | **test_LargeMatrixSkylineStorage.cpp, test_LargeMatrixCsStorage.cpp** |
| header dependences : | **config.h, utils.h** |

## 13.3 Solvers

Each solver class in the *solvers* library implements a specific iterative method to solve a linear system: A*X=B in two cases: Real or Complex. The algorithm of all solvers except Sor and Sor can work with and without a Preconditioner. Each solver takes largeMatrix $matA$ and Vector $vecB$ as inputs and a Vector $vecX$ as output whose value is initialized with the input Vector $vecX0$.
A solver without a preconditioner is invoked with the overloading operator():

```
template<class Mat, class VecB, class VecX>
VecX operator()(Mat& matA, VecB& vecB, VecX& vecX0, ValueType solType)
```

Meanwhile, solver with a preconditioner $pc$ can be used with the call

```
template<class Mat, class VecB, class VecX, class Prec>
VecX operator()(Mat& matA, VecB& vecB, VecX& vecX0, Prec& pc, ValueType solType)
```

User must specify the type of solver solType, which can be _real or _complex.
The algorithm corresponds to without-preconditioner solver

```
template<typename K, class Mat, class VecB, class VecX>
void algorithm(Mat& matA, VecB& vecB, VecX& vecX, VecX& vecR)
```

and to a preconditioned one

```
template<typename K, class Mat, class VecB, class VecX, class Prec>
void algorithm(Mat& matA, VecB& vecB, VecX& vecX, VecX& vecR, Prec& pc)
```

### 13.3.1 The BicgSolver class

This class implements the Biconjugate Gradient method to solve a linear system. There are several basic constructors calling IterativeSolver constructors

```
class BicgSolver : public IterativeSolver
{
  public:
    //! Default Constructor
    BicgSolver() : IterativeSolver(_bicg) {}
    //! Full constructor
    BicgSolver(real_t eps, number_t maxOfIt = defaultMaxIterations, number_t vb = 0)
    : IterativeSolver(_bicg, maxOfIt, eps, vb) {}

    //! contructors with key-value system
    BicgSolver(const Parameter& p1) : IterativeSolver(_bicg)
    {
      std::vector<Parameter> ps(1, p1);
      real_t omega=1.; number_t krylovDim=defaultKrylovDimension;
      IterativeSolverType ist=_bicg;
      buildSolverParams(ps, epsilon_, maxOfIterations_, omega, krylovDim, verboseLevel_, name_,
          ist);
    }
    BicgSolver(const Parameter& p1, const Parameter& p2) : IterativeSolver(_bicg)
    {
      std::vector<Parameter> ps(2);
      ps[0]=p1; ps[1]=p2;
      real_t omega=1.; number_t krylovDim=defaultKrylovDimension;
      IterativeSolverType ist=_bicg;
      buildSolverParams(ps, epsilon_, maxOfIterations_, omega, krylovDim, verboseLevel_, name_,
          ist);
    }
    BicgSolver(const Parameter& p1, const Parameter& p2, const Parameter& p3) :
        IterativeSolver(_bicg)
    {
      std::vector<Parameter> ps(3);
      ps[0]=p1; ps[1]=p2; ps[2]=p3;
      real_t omega=1.; number_t krylovDim=defaultKrylovDimension;
      IterativeSolverType ist=_bicg;
      buildSolverParams(ps, epsilon_, maxOfIterations_, omega, krylovDim, verboseLevel_, name_,
          ist);
    }
    ...
```

| | |
|---|---|
| library : | **solvers** |
| header : | |
| implementation : | |
| unitary tests : | **test_BicgSolver.hpp** |
| header dependences : | **IterativeSolver.hpp, Preconditioner.hpp** |

### 13.3.2 The BicgStabSolver class

This class implements the Biconjugate Gradient Stabilized method to solve a linear system. There are several basic constructors calling IterativeSolver constructors

```
class BicgStabSolver : public IterativeSolver
{
  public:
    //! Default Constructor
    BicgStabSolver() : IterativeSolver(_bicgstab) {}
    //! Full Constructor
    BicgStabSolver(real_t eps, number_t maxOfIt = defaultMaxIterations, number_t vb = 0)
    : IterativeSolver(_bicgstab, maxOfIt, eps, vb) {}

    //! contructors with key-value system
    BicgStabSolver(const Parameter& p1) : IterativeSolver(_bicgstab)
    {
      std::vector<Parameter> ps(1, p1);
      real_t omega=1.; number_t krylovDim=defaultKrylovDimension;
      IterativeSolverType ist=_bicgstab;
      buildSolverParams(ps, epsilon_, maxOfIterations_, omega, krylovDim, verboseLevel_, name_,
          ist);
    }
    BicgStabSolver(const Parameter& p1, const Parameter& p2) : IterativeSolver(_bicgstab)
    {
```

```
    std::vector<Parameter> ps(2);
    ps[0]=p1; ps[1]=p2;
    real_t omega=1.; number_t krylovDim=defaultKrylovDimension;
    IterativeSolverType ist=_bicgstab;
    buildSolverParams(ps, epsilon_, maxOfIterations_, omega, krylovDim, verboseLevel_, name_,
        ist);
  }
  BicgStabSolver(const Parameter& p1, const Parameter& p2, const Parameter& p3) :
      IterativeSolver(_bicgstab)
  {
    std::vector<Parameter> ps(3);
    ps[0]=p1; ps[1]=p2; ps[2]=p3;
    real_t omega=1.; number_t krylovDim=defaultKrylovDimension;
    IterativeSolverType ist=_bicgstab;
    buildSolverParams(ps, epsilon_, maxOfIterations_, omega, krylovDim, verboseLevel_, name_,
        ist);
  }
  ...
```

| | |
|---|---|
| library : | **solvers** |
| header : | |
| implementation : | |
| unitary tests : | **test_BicgStabSolver.hpp** |
| header dependences : | **IterativeSolver.hpp, Preconditioner.hpp** |

### 13.3.3 The `CgSolver` class

This class implements the Conjugate Gradient method to solve a linear system. There are several basic constructors calling `IterativeSolver` constructors

```
class CgSolver : public IterativeSolver
{
  public:
  //! Default constructor
  CgSolver(): IterativeSolver(_cg) {}
  //! Full constructor
  CgSolver(real_t eps, number_t maxOfIt = defaultMaxIterations, number_t vb = 0)
  : IterativeSolver(_cg, maxOfIt, eps, vb) {}

  //! contructors with key-value system
  CgSolver(const Parameter& p1) : IterativeSolver(_cg)
  {
    std::vector<Parameter> ps(1, p1);
    real_t omega=1.; number_t krylovDim=defaultKrylovDimension;
    IterativeSolverType ist=_cg;
    buildSolverParams(ps, epsilon_, maxOfIterations_, omega, krylovDim, verboseLevel_, name_,
        ist);
  }
  CgSolver(const Parameter& p1, const Parameter& p2) : IterativeSolver(_cg)
  {
    std::vector<Parameter> ps(2);
    ps[0]=p1; ps[1]=p2;
    real_t omega=1.; number_t krylovDim=defaultKrylovDimension;
    IterativeSolverType ist=_cg;
    buildSolverParams(ps, epsilon_, maxOfIterations_, omega, krylovDim, verboseLevel_, name_,
        ist);
  }
  CgSolver(const Parameter& p1, const Parameter& p2, const Parameter& p3) : IterativeSolver(_cg)
  {
    std::vector<Parameter> ps(3);
    ps[0]=p1; ps[1]=p2; ps[2]=p3;
    real_t omega=1.; number_t krylovDim=defaultKrylovDimension;
    IterativeSolverType ist=_cg;
    buildSolverParams(ps, epsilon_, maxOfIterations_, omega, krylovDim, verboseLevel_, name_,
        ist);
  }
  ...
```

| | |
|---:|---|
| library : | **solvers** |
| header : | |
| implementation : | |
| unitary tests : | **test_CgSolver.hpp** |
| header dependences : | **IterativeSolver.hpp, Preconditioner.hpp** |

### 13.3.4 The CgsSolver class

This class implements the Conjugate Gradient Squared method to solve a linear system. There are several basic constructors calling IterativeSolver constructors

```
class CgsSolver : public IterativeSolver
{
  public:
    //! Default constructor
    CgsSolver()
      : IterativeSolver(_cgs) {}
    //! Full constructor
    CgsSolver(real_t eps, number_t maxOfIt = defaultMaxIterations, number_t vb = 0)
      : IterativeSolver(_cgs, maxOfIt, eps, vb) {}

    //! contructors with key-value system
    CgsSolver(const Parameter& p1) : IterativeSolver(_cgs)
    {
      std::vector<Parameter> ps(1, p1);
      real_t omega=1.; number_t krylovDim=defaultKrylovDimension;
      IterativeSolverType ist=_cgs;
      buildSolverParams(ps, epsilon_, maxOfIterations_, omega, krylovDim, verboseLevel_, name_,
          ist);
    }
    CgsSolver(const Parameter& p1, const Parameter& p2) : IterativeSolver(_cgs)
    {
      std::vector<Parameter> ps(2);
      ps[0]=p1; ps[1]=p2;
      real_t omega=1.; number_t krylovDim=defaultKrylovDimension;
      IterativeSolverType ist=_cgs;
      buildSolverParams(ps, epsilon_, maxOfIterations_, omega, krylovDim, verboseLevel_, name_,
          ist);
    }
    CgsSolver(const Parameter& p1, const Parameter& p2, const Parameter& p3) :
        IterativeSolver(_cgs)
    {
      std::vector<Parameter> ps(3);
      ps[0]=p1; ps[1]=p2; ps[2]=p3;
      real_t omega=1.; number_t krylovDim=defaultKrylovDimension;
      IterativeSolverType ist=_cgs;
      buildSolverParams(ps, epsilon_, maxOfIterations_, omega, krylovDim, verboseLevel_, name_,
          ist);
    }
    ...
```

| | |
|---|---|
| library : | **solvers** |
| header : | |
| implementation : | |
| unitary tests : | **test_CgsSolver.hpp** |
| header dependences : | **IterativeSolver.hpp, Preconditioner.hpp** |

### 13.3.5 The `GmresSolver` class

This class implements the Generalized Minimal Residual method to solve a linear system. Different from other solvers, the `GmresSolver` has more constructors: user can specify the Krylov dimension in the constructor.

```
class GmresSolver : public IterativeSolver
{
  private:
    number_t krylovDim_;  //!< Dimension of Krylov space

  public:
    //! Constructor with Krylov dimension
    GmresSolver(number_t kd=defaultKrylovDimension)
      : IterativeSolver(_gmres, defaultMaxIterations, theDefaultConvergenceThreshold),
        krylovDim_(kd) {}
    //! Full constructor
    GmresSolver(number_t kd, real_t eps, number_t maxOfIt = defaultMaxIterations, number_t vb = 0)
    : IterativeSolver(_gmres, maxOfIt, eps, vb), krylovDim_(kd) {}

    //! contructors with key-value system
    GmresSolver(const Parameter& p1) : IterativeSolver(_gmres)
    {
      std::vector<Parameter> ps(1, p1);
      real_t omega=1.;
      IterativeSolverType ist=_gmres;
      buildSolverParams(ps, epsilon_, maxOfIterations_, omega, krylovDim_, verboseLevel_, name_,
          ist);
    }
    GmresSolver(const Parameter& p1, const Parameter& p2) : IterativeSolver(_gmres)
    {
      std::vector<Parameter> ps(2);
      ps[0]=p1; ps[1]=p2;
      real_t omega=1.;
      IterativeSolverType ist=_gmres;
      buildSolverParams(ps, epsilon_, maxOfIterations_, omega, krylovDim_, verboseLevel_, name_,
          ist);
    }
    GmresSolver(const Parameter& p1, const Parameter& p2, const Parameter& p3) :
        IterativeSolver(_gmres)
    {
      std::vector<Parameter> ps(3);
      ps[0]=p1; ps[1]=p2; ps[2]=p3;
      real_t omega=1.;
      IterativeSolverType ist=_gmres;
      buildSolverParams(ps, epsilon_, maxOfIterations_, omega, krylovDim_, verboseLevel_, name_,
          ist);
    }
    GmresSolver(const Parameter& p1, const Parameter& p2, const Parameter& p3, const Parameter&
        p4) : IterativeSolver(_gmres)
    {
      std::vector<Parameter> ps(4);
      ps[0]=p1; ps[1]=p2; ps[2]=p3; ps[3]=p4;
      real_t omega=1.;
      IterativeSolverType ist=_gmres;
      buildSolverParams(ps, epsilon_, maxOfIterations_, omega, krylovDim_, verboseLevel_, name_,
          ist);
    }
    ...
```

| | |
|---|---|
| library : | **solvers** |
| header : | |
| implementation : | |
| unitary tests : | **test_GmresSolver.hpp** |
| header dependences : | **IterativeSolver.hpp, Preconditioner.hpp** |

### 13.3.6 The QmrSolver class

This class implements the Quasi-Minimal Residual method to solve a linear system. There are several basic constructors calling IterativeSolver constructors

```
class QmrSolver : public IterativeSolver
{
  public:
    //! Constructor
    QmrSolver()
      : IterativeSolver(_qmr) {}
    //! Full Constructor
    QmrSolver(real_t eps, number_t maxOfIt = defaultMaxIterations, number_t vb = 0)
    : IterativeSolver(_qmr, maxOfIt, eps, vb) {}

    //! contructors with key-value system
    QmrSolver(const Parameter& p1) : IterativeSolver(_qmr)
    {
      std::vector<Parameter> ps(1, p1);
      real_t omega=1.; number_t krylovDim=defaultKrylovDimension;
      IterativeSolverType ist=_qmr;
      buildSolverParams(ps, epsilon_, maxOfIterations_, omega, krylovDim, verboseLevel_, name_,
          ist);
    }
    QmrSolver(const Parameter& p1, const Parameter& p2) : IterativeSolver(_qmr)
    {
      std::vector<Parameter> ps(2);
      ps[0]=p1; ps[1]=p2;
      real_t omega=1.; number_t krylovDim=defaultKrylovDimension;
      IterativeSolverType ist=_qmr;
      buildSolverParams(ps, epsilon_, maxOfIterations_, omega, krylovDim, verboseLevel_, name_,
          ist);
    }
    QmrSolver(const Parameter& p1, const Parameter& p2, const Parameter& p3) :
        IterativeSolver(_qmr)
    {
      std::vector<Parameter> ps(3);
      ps[0]=p1; ps[1]=p2; ps[2]=p3;
      real_t omega=1.; number_t krylovDim=defaultKrylovDimension;
      IterativeSolverType ist=_qmr;
      buildSolverParams(ps, epsilon_, maxOfIterations_, omega, krylovDim, verboseLevel_, name_,
          ist);
    }
    ...
```

| | |
|---|---|
| library : | **solvers** |
| header : | |
| implementation : | |
| unitary tests : | **test_QmrSolver.hpp** |
| header dependences : | **IterativeSolver.hpp, Preconditioner.hpp** |

### 13.3.7 The `SorSolver` class

This class implements the Successive Over Relaxation method to solve a linear system. For this solver, user can have more choices to specify the relaxation factor *omega* in the constructor. Different from other solvers above, `SorSolver` doesn't work with a preconditioner.

```
class SorSolver : public IterativeSolver
{
  private:
    real_t omega_;   //!< relaxation factor of SOR method

  public:
    //! Constructor with omega
    SorSolver(real_t w=1.) : IterativeSolver(_sor), omega_(w) {}
    //! Full constructor
    SorSolver(real_t w, real_t eps, number_t maxOfIt = defaultMaxIterations, number_t vb = 0)
    : IterativeSolver(_sor, maxOfIt, eps, vb), omega_(w) {}

    //! contructors with key-value system
    SorSolver(const Parameter& p1) : IterativeSolver(_sor)
    {
      std::vector<Parameter> ps(1, p1);
      number_t krylovDim=defaultKrylovDimension;
      IterativeSolverType ist=_sor;
      buildSolverParams(ps, epsilon_, maxOfIterations_, omega_, krylovDim, verboseLevel_, name_,
          ist);
    }
    SorSolver(const Parameter& p1, const Parameter& p2) : IterativeSolver(_sor)
    {
      std::vector<Parameter> ps(2);
      ps[0]=p1; ps[1]=p2;
      number_t krylovDim=defaultKrylovDimension;
      IterativeSolverType ist=_sor;
      buildSolverParams(ps, epsilon_, maxOfIterations_, omega_, krylovDim, verboseLevel_, name_,
          ist);
    }
    SorSolver(const Parameter& p1, const Parameter& p2, const Parameter& p3) :
        IterativeSolver(_sor)
    {
      std::vector<Parameter> ps(3);
      ps[0]=p1; ps[1]=p2; ps[2]=p3;
      number_t krylovDim=defaultKrylovDimension;
      IterativeSolverType ist=_sor;
      buildSolverParams(ps, epsilon_, maxOfIterations_, omega_, krylovDim, verboseLevel_, name_,
          ist);
    }
    SorSolver(const Parameter& p1, const Parameter& p2, const Parameter& p3, const Parameter& p4)
        : IterativeSolver(_sor)
    {
      std::vector<Parameter> ps(4);
      ps[0]=p1; ps[1]=p2; ps[2]=p3; ps[3]=p4;
      number_t krylovDim=defaultKrylovDimension;
      IterativeSolverType ist=_sor;
      buildSolverParams(ps, epsilon_, maxOfIterations_, omega_, krylovDim, verboseLevel_, name_,
          ist);
    }
    ...
```

| | |
|---|---|
| library : | **solvers** |
| header : | |
| implementation : | |
| unitary tests : | **test_SorSolver.hpp** |
| header dependences : | **IterativeSolver.hpp, Preconditioner.hpp** |

### 13.3.8 The SsorSolver class

This class implements the Symmetric Successive Over Relaxation method to solve a linear system. Like SorSolver, the SsorSolver only works without a preconditioner and user can specify the relaxation factor *omega* in the constructor.

```
class SsorSolver : public IterativeSolver
{
  private:
    real_t omega_;  //!< relaxation factor of SOR method

  public:
    //! Constructor with omega
    SsorSolver(real_t w=1.) : IterativeSolver(_ssor), omega_(w) {}
    //! Full constructor
    SsorSolver(real_t w, real_t eps, number_t maxOfIt = defaultMaxIterations, number_t vb = 0)
    : IterativeSolver(_ssor, maxOfIt, eps, vb), omega_(w) {}

    //! contructors with key-value system
    SsorSolver(const Parameter& p1) : IterativeSolver(_ssor)
    {
      std::vector<Parameter> ps(1, p1);
      number_t krylovDim=defaultKrylovDimension;
      IterativeSolverType ist=_ssor;
      buildSolverParams(ps, epsilon_, maxOfIterations_, omega_, krylovDim, verboseLevel_, name_,
          ist);
    }
    SsorSolver(const Parameter& p1, const Parameter& p2) : IterativeSolver(_ssor)
    {
      std::vector<Parameter> ps(2);
      ps[0]=p1; ps[1]=p2;
      number_t krylovDim=defaultKrylovDimension;
      IterativeSolverType ist=_ssor;
      buildSolverParams(ps, epsilon_, maxOfIterations_, omega_, krylovDim, verboseLevel_, name_,
          ist);
    }
    SsorSolver(const Parameter& p1, const Parameter& p2, const Parameter& p3) :
        IterativeSolver(_ssor)
    {
      std::vector<Parameter> ps(3);
      ps[0]=p1; ps[1]=p2; ps[2]=p3;
      number_t krylovDim=defaultKrylovDimension;
      IterativeSolverType ist=_ssor;
      buildSolverParams(ps, epsilon_, maxOfIterations_, omega_, krylovDim, verboseLevel_, name_,
          ist);
    }
    SsorSolver(const Parameter& p1, const Parameter& p2, const Parameter& p3, const Parameter&
        p4) : IterativeSolver(_ssor)
    {
      std::vector<Parameter> ps(4);
      ps[0]=p1; ps[1]=p2; ps[2]=p3; ps[3]=p4;
      number_t krylovDim=defaultKrylovDimension;
      IterativeSolverType ist=_ssor;
      buildSolverParams(ps, epsilon_, maxOfIterations_, omega_, krylovDim, verboseLevel_, name_,
          ist);
    }
    ...
```

| | |
|---:|:---|
| library : | **solvers** |
| header : | |
| implementation : | |
| unitary tests : | **test_SsorSolver.hpp** |
| header dependences : | **IterativeSolver.hpp, Preconditioner.hpp** |

# 14 The *umfpackSupport* library

Besides some built-in direct solvers for sparse linear system, XLIFE++ provides an interface to UMFPACK, a set of routines for solving non symmetric sparse linear systems, $Ax = b$, using the Unsymmetric MultiFrontal method. More information can be found at http://www.cise.ufl.edu/research/sparse/umfpack/.

The aim of *umfpackSupport* is to make ease of the UMFPACK for XLIFE++'s users, allowing them to solve the linear system $Ax = b$ with a simple call. Instead of invoking "multi-argument" UMFPACK solver, user can make call of them as any built-in iterative solver in the context of XLIFE++.

## 14.1 The UMFPACK wrappers

Written in ANSI/ISO C, UMFPACK library consists of 32 user-callable routines. Nearly all these routines come in four versions, with different sizes of integers and for real or complex floating-point numbers:

- real double precision, **int** integers
- complex double precision, **int** integers
- real double precision, **SuiteSparse_long** integers
- complex double precision, **SuiteSparse_long** integers

Only the interfaces to the first two versions are implemented in XLIFE++. However, more versions can be easily added in the need of user.
Because callable UMFPACK routines are written in C, so as to call them correctly from the C++ environment of XLIFE++, we must make these routines "extern C". And it's the role of UmfPackWrappers. Only some primary routines of UMFPACK are made interface; however, it's not difficult to include others.

```
#ifdef __cplusplus
extern "C" {
#endif

int DISYMBOLIC(int n_row, int n_col, const int Ap[], const int Ai[], const double Ax[], void**
    Symbolic, const double Control[UMFPACK_CONTROL], double Info[UMFPACK_INFO]);
int DINUMERIC(const int Ap[], const int Ai[], const double Ax[], void* Symbolic, void** Numeric,
    const double Control[UMFPACK_CONTROL], double Info[UMFPACK_INFO]);
int DISOLVE(int sys, const int Ap[], const int Ai[], const double Ax[], double X[], const double
    B[], void* Numeric, const double Control[UMFPACK_CONTROL], double Info[UMFPACK_INFO]);
void DIFREESYMBOLIC(void** Symbolic);
void DIFREENUMERIC(void** Numeric);
    ...

int ZISYMBOLIC(int n_row, int n_col, const int Ap[], const int Ai[], const double Ax[], const
    double Az[], void** Symbolic, const double Control[UMFPACK_CONTROL], double
    Info[UMFPACK_INFO]);
int ZINUMERIC(const int Ap[], const int Ai[], const double Ax[], const double Az[], void*
    Symbolic, void** Numeric, const double Control[UMFPACK_CONTROL], double Info[UMFPACK_INFO]);
int ZISOLVE(int sys, const int Ap[], const int Ai[], const double Ax[], const double Az[], double
    Xx[], double Xz[], const double Bx[], const double Bz[], void* Numeric, const double
    Control[UMFPACK_CONTROL], double Info[UMFPACK_INFO]);
void ZIFREESYMBOLIC(void** Symbolic);
void ZIFREENUMERIC(void** Numeric);
```

```
    ...
```

Routine names beginning with DI correspond to the version of real double precision, **int** integers, the ones with ZI imply the versions of complex double precision, **int** integers.

## 14.2 The `UMFPACK` class

The `UMFPACK` class plays a role of high-level wrapper of routines provided by UmfPackWrappers:

- *SYMBOLIC: performing a symbolic decomposition on the sparcity of a matrix
- *NUMERIC: performing a numeric decomposition of a matrix
- *FREESYMBOLIC: freeing symbolic object created by *SYMBOLIC
- *FREENUMERIC: freeing numeric object created by *NUMERIC
- *GETLUNZ: returning the number of non-zeros in lower matrix L and upper matrix U in LU decomposition
- *GETNUMERIC: retrieving lower matrix L, upper matrix U, permutation P,Q, and scale factor R
- *GETDET: returning determinant of original matrix

The "*" corresponds to DI-real double precision, or ZI-complex double precision.
All these routines are organized under templated "class-like" interface.

```
template<typename OrdinalType, typename ScalarType>
class UMFPACK
{
  public:
    typedef typename NumTraits<ScalarType>::magnitudeType MagnitudeType;


    //! Default Constructor.
    inline UMFPACK(void) {}

    //! Destructor.
    inline ~UMFPACK(void) {}

    OrdinalType symbolic(OrdinalType nRow, OrdinalType nCol, const OrdinalType Ap[], const
        OrdinalType Ai[], const ScalarType Ax[], void** Symbolic, const MagnitudeType
        Control[UMFPACK\_CONTROL], MagnitudeType Info[UMFPACK\_INFO]);

    OrdinalType numeric(const OrdinalType Ap[], const OrdinalType Ai[], const ScalarType Ax[],
        void* Symbolic, void** Numeric, const MagnitudeType Control[UMFPACK\_CONTROL],
        MagnitudeType Info[UMFPACK\_INFO]);

    void freeSymbolic(void** Symbolic);
    void freeNumeric(void** Numeric);

    OrdinalType solve(OrdinalType sys, const OrdinalType Ap[], const OrdinalType Ai[], const
        ScalarType Ax[], ScalarType X[], const ScalarType B[], void* Numeric, const
        MagnitudeType Control[UMFPACK\_CONTROL], MagnitudeType Info[UMFPACK\_INFO]);

    OrdinalType getLunz(OrdinalType* lnz, OrdinalType* unz, OrdinalType* nRow, OrdinalType* nCol,
        OrdinalType* nzUdiag, void* Numeric);

    OrdinalType getNumeric(OrdinalType Lp[], OrdinalType Lj[], ScalarType Lx[], OrdinalType Up[],
        OrdinalType Ui[], ScalarType Ux[], OrdinalType P[], OrdinalType Q[], ScalarType Dx[],
        OrdinalType* doRecip, ScalarType Rs[], void* Numeric);
    OrdinalType getDeterminant(ScalarType* Mx, ScalarType* Ex, void* NumericHandle, ScalarType
        UserInfo[UMFPACK\_INFO]);
    ...
```

One advantage of this orgnization is to allow the specialization of code corresponding to the two versions: real double precision and complex double precision with **int** integer.

```
template<>
class UMFPACK<int, double>
{
  public:
    inline UMFPACK(void) {}
    inline ~UMFPACK(void) {}

    int symbolic(int nRow, int nCol, const int Ap[], const int Ai[], const double Ax[], void**
        Symbolic, const double Control[UMFPACK_CONTROL], double Info[UMFPACK_INFO]);

    int numeric(const int Ap[], const int Ai[], const double Ax[], void* Symbolic, void**
        Numeric, const double Control[UMFPACK_CONTROL], double Info[UMFPACK_INFO]);

    void freeSymbolic(void** Symbolic);

    void freeNumeric(void** Numeric);

    int solve(int sys, const int Ap[], const int Ai[], const double Ax[], double X[], const
        double B[], void* Numeric, const double Control[UMFPACK_CONTROL], double
        Info[UMFPACK_INFO]);
    ...
```

The specialization of complex version comes with an extra method for the linear system $Ax = b$ with $A$ complex double precision and $b$ real double precision.

```
template<>
class UMFPACK<int, std::complex<double> >
{
  public:
    inline UMFPACK(void) {}
    inline ~UMFPACK(void) {}

    int symbolic(int nRow, int nCol, const int Ap[], const int Ai[], const std::complex<double>
        Ax[], void** Symbolic, const double Control[UMFPACK_CONTROL], double Info[UMFPACK_INFO]);

    int numeric(const int Ap[], const int Ai[], const std::complex<double> Ax[], void* Symbolic,
        void** Numeric, const double Control[UMFPACK_CONTROL], double Info[UMFPACK_INFO]);

    void freeSymbolic(void** Symbolic);

    void freeNumeric(void** Numeric);

    int solve(int sys, const int Ap[], const int Ai[], const std::complex<double> Ax[],
        std::complex<double> X[], const std::complex<double> B[], void* Numeric, const double
        Control[UMFPACK_CONTROL], double Info[UMFPACK_INFO]);

    // Solve in case AX=B with A complex, B real
    int solveCR(int sys, const int Ap[], const int Ai[], const std::complex<double> Ax[],
        std::complex<double> X[], const double Bx[], const double Bz[], void* Numeric, const
        double Control[UMFPACK_CONTROL], double Info[UMFPACK_INFO]);
    ...
```

| | |
|---|---|
| library : | **umfpackSupport** |
| header : | **UmfPack.hpp** |
| implementation : | **UmfPack.cpp** |
| unitary tests : | **test_UmfPackSolver.cpp** |
| header dependences : | **utils.h** |

## 14.3 The UmfPackSolver class

The class, as its name, serves for solving the sparse linear system $Ax = b$. Being similar to other solvers of XLiFE++, this solver can be provoked with a call of operator(). For example:

```
UmfPackSolver umfpackSolver;
// With A largeMatrix; b and x are std::vector
umfpackSolver(A,b,x);
```

By calling the solver in this way, the storage and values of the largeMatrix $A$ are extracted and these extractions are converted to the format of UMFPACK including: column pointer, row index and values. These three are inputs to underlying UMFPACK routines. Because extraction and conversion between largeMatrix of XLiFE++ and UMFPACK format are expensive, in some cases, it's better to directly make use of the conversion and it can be easily done by calling operator() with more inputs

```
// Solve AX=B with UmfPack
// \param[in] colPointer column pointer of CSC-like Umfpack format (after calling function
    extract2UmfPack of largeMatrix)
// \param[in] rowIdx row index of CSC-like Umfpack format (after calling function extract2UmfPack
    of largeMatrix)
// \param[in] values values of CSC-like Umfpack format (after calling function extract2UmfPack of
    largeMatrix)
// \param[in] vecB vector B (vector B should be std::vector)
// \param[in] vecX vector X (vector X should be std::vector)
template<class ScalarTypeMat, class VecB, class VecX>
void operator()(int size, const std::vector<int>& colPointer, const std::vector<int>& rowIdx,
    const std::vector<ScalarTypeMat>& values, const VecB& vecB, VecX& vecX,
    UmfPackComputationMode sys=_A)
```

One of a technical issue on working with different types of scalar value, in this case, there are Real and Complex values, is the static dispatching. For dispatching at runtime, we can use simple *if-else* statements or the switch statement. However, the *if-else* statement requires both branches to compile successfully, even when the condition tested by if is known at compile time. To overcome this problem, we use a simple technique that is intially described in Alexandrescu, mapping integral Constants to Types:

```
template <int v>
struct Int2Type
{
enum { value = v };
};
```

Int2Type generates a distinct type for each distinct constant integral value passed. This is because different template instantiations are distinct types; thus, Int2Type<0> is different from Int2Type<1>, and so on. In addition, the value that generates the type is "saved" in the enum member value.
For a linear system $Ax = b$, we can divide into four cases depending to the scalar type of $A$ and $b$, and corresponding to each case, there is a Int2Type:

- $A$ real and $b$ real; Int2Type<0>
- $A$ real and $b$ complex; Int2Type<1>

- $A$ complex and $b$ real; `Int2Type<2>`
- $A$ complex and $b$ complex; `Int2Type<3>`

Because each case above needs processing in a different way, we define an internal class of `UmfPackSolver` to take care of it.

```
// Auxiliary internal class to process 4 cases of equation AX = B:
//      + A:real, B: real
//      + A:real, B:complex
//      + A:complex, B: real
//      + A:complex, B:complex
template<typename ScalarTypeMat, typename VecB, typename VecX>
class SolverIntern
{
  public:
    typedef typename NumTraits<ScalarTypeMat>::magnitudeType MagType;
    typedef typename Conditional<NumTraits<ScalarTypeMat>::IsComplex, ScalarTypeMat, typename
        VectorTrait<VecB>::Type>::type ScalarType;

    SolverIntern() {}
   ...
```

For example, the case of $A$ real and $b$ real.

```
// Solve AX=B in case A Real, B Real
void solve(int sys, int nRows, int nCols, const std::vector<int>& colPointer, const
     std::vector<int>& rowIdx, const std::vector<ScalarTypeMat>& values, const VecB& vecB, VecX&
     vecX, Int2Type<0>)
{
  void* symbolic;
  void* numeric;
  double* null = (double*) NULL;

  UMFPACK<int, ScalarType> umfPack;

  (void)umfPack.symbolic(nRows, nCols, &(colPointer[0]),
      &(rowIdx[0]),&(values[0]),&symbolic,null,null);
  (void)umfPack.numeric(&(colPointer[0]), &(rowIdx[0]), &(values[0]), symbolic, &numeric,
      null,null);
  (void)umfPack.solve((int)sys, &(colPointer[0]), &(rowIdx[0]),&(values[0]), &vecX[0], &vecB[0],
      numeric, null, null);
  umfPack.freeSymbolic(&symbolic);
  umfPack.freeNumeric(&numeric);
}
```

| | |
|---|---|
| library : | **umfpackSupport** |
| header : | **UmfPackSolver.hpp** |
| implementation : | |
| unitary tests : | **test_UmfPackSolver.cpp** |
| header dependences : | **utils.h, UmfPack.hpp** |

## 14.4 The `UmfPackLU` class

UMFPACK library allows not only to solve the linear system $Ax = b$ but also to retrieve more information. There are cases where users may wish to do more with the LU factorization of a matrix rather than solve a linear system. And the `UmfPackLU` class is for this purpose. Not like to the "non-templated" `UmfPackSolver` class, the `UmfPackLU` depends on the type of input matrix.

```
template<typename MatrixType>
class UmfPackLU
{
  public:
    typedef typename MatrixType::ScalarType ScalarType;

    struct LUMatrixType {
      std::vector<int> outerIdx;
      std::vector<int> innerIdx;
      std::vector<ScalarType> values;
    };

  public:
    UmfPackLU() { init();}
    UmfPackLU(const MatrixType& matrix)
    {
      init();
      compute(matrix);
    }
...
```

Apart from solving the linear system $Ax = b$, this class provides some methods to work with LU factorization.

```
inline const LUMatrixType& matrixL() const
{
  if (extractedDataAreDirty_) extractData();
  return (lMatrix_);
}

inline const LUMatrixType& matrixU() const
{
  if (extractedDataAreDirty_) extractData();
  return (uMatrix_);
}

inline const std::vector<int>& permutationP() const
{
  if (extractedDataAreDirty_) extractData();
  return (pPerm_);
}

inline const std::vector<int>& permutationQ() const
{
  if (extractedDataAreDirty_) extractData();
  return (qPerm_);
}

inline const std::vector<Real>& scaleFactorR() const
{
  if (extractedDataAreDirty_) extractData();
  return (rScaleFact_);
}
```

All these methods above return the result of LU factorization. $PAQ = LU$. The matrix **U** is returned in compressed column form (with sorted columns). The matrix **L** is returned in compressed row form (with sorted rows). One remarkable thing is that the compressed column (row) form is similar to CSC (CSR) of XLiFE++. These two matrix are returned in form of struct `LUMatrixType`

```
struct LUMatrixType
{
  std::vector<int> outerIdx;
  std::vector<int> innerIdx;
  std::vector<ScalarType> values;
};
```

The *outerIdx* corresponds to the *colPointer* of CSC and *rowPointer* of CSR, while the *innerIdx* corresponds to the *rowIndex* of CSC and *colIndex* of CSR. Remember that, not like CSC or CSR, the *values* of `LUMatrixType` struct doesn't contain the "first-position" zero (0).
The permutations P and Q are represented as permutation vectors, where $P[k] = i$ means that row i of the original matrix is the the k-th row of $PAQ$, and where $Q[k] = \mathrm{j}$ means that column j of the original matrix is the k-th column of PAQ.
The vector R is the scale factor in the LU factorization. The first value of *scaleFactorR* defines how the scale factors Rs are to be interpreted. If it's one(1), then the scale factors *scaleFactorR[i+1]* are to be used by multiplying row i of matrix A by *scaleFactorR[i]*. Otherwise, the entries in row i are to be divided by *scaleFactorR[i+1]*.
Before retrieving all these above values, a matrix at least needs factorizing. It can be done in two ways, by constructor

```
UmfPackLU(const MatrixType& matrix)
{
  init();
  compute(matrix);
}
```

or by the method **compute**

```
/*! Computes the sparse Cholesky decomposition of \a largeMatrix
 */
void compute(const MatrixType& matrix)
{
  analyzePattern(matrix);
  factorize(matrix);
}
```

In this function, a symbolic decomposition on the sparsity of a matrix is performed by **analyzePattern** then a numeric decomposition performed by **factorize**.
After the matrix is factorized, its factorization can be used to solve the linear system $Ax = b$ with :

```
template<typename VectorScalarType>
void solve(const std::vector<VectorScalarType>& b, std::vector<typename
    Conditional<NumTraits<ScalarType>::IsComplex, ScalarType, VectorScalarType>::type >& x)
    const;
```

One advantage of `UmfPackLU` over `UmfPackSolver` is that for a same matrix A, it only needs to do factorization once then all these factorizations can be used over and over again to solve the linear system $Ax = b$. Of course, it doesn't have the flexibility of "non-templated" `UmfPackSolver`, it needs template arguments in order to define type of matrix. Depending on a specific demand, one can be a better choice than another!!!

| | |
|---:|:---|
| library : | **umfpackSupport** |
| header : | **UmfPackLU.hpp** |
| implementation : | |
| unitary tests : | **test_UmfPackSolver.cpp** |
| header dependences : | **utils.h, UmfPack.hpp** |

# 15 The *eigenSolvers* library

The *eigenSolvers* library comes with built-in solvers of eigen problem which deal with sparse matrices. The user interface of eigen solvers is similar to the *solvers*: all solvers are invoked with operator().
To calculate eigenvalues and eigenvector, at the moment, nearly all finite-element libraries rely on a well-known large scale eigen solver ARPACK. Although this library is efficient and robust in computing varieties of eigen problem, it relies largely on other libraries: BLAS and LAPACK. The fact that in order to use ARPACK, users must already have these two installed, as well as all these libs are in Fortran, can make programming an efficient-C++ finite-element application a harsh work.
So as to ease user out of the complexities and dependencies, XLIFE++ supplies an intern eigensolver which is capable of solving large scale eigen problems with several algorithms. Two goals motivated the development of this intern eigensolver: independence and simplicity. The intention of *independence*, as mentioned above, is to free XLIFE++ from other Fortran libraries. The concept of *simplicity* drives the development of this part to allow users to call this eigen solver like other solvers (e.x: GmResSolver, ...) in XLIFE++. This is encouraged by promoting code modularization and multiple level of access to solvers and data. In the following, we outline the intern eigen solver structure. In particular, we present

***eigenCore*** the eigen solver of *dense* matrix

***eigenSparse*** the eigen solver of *sparse* matrix based on *eigenCore*

## 15.1 *eigenCore* sub-library

Most of the standard eigenvalue algorithms exploit projection processes in order to extract approximate eigenvectors from a given subspace. The basic idea of a projection method is to extract an approximate eigenvector from a specified low-dimensional subspace. If these approximation can be extracted, a small matrix eigenvalue problem is obtained. The numerical solution of the small $m \times m$ eigenvalue problem will be treated by the *eigenCore* library. The *eigenCore* library is organized in multi-level, each of which utilizes subroutines provided by the lower one.

- *utils* : the lowest level provides various basic operations
- *decomposition* : the second level implements several decomposition algorithms
- *eigenSolver* : the highest level solves different eigen problem

### 15.1.1 *utils* part

This part contains several classes which work on different basic operations.

**The `VectorEigenDense` class**

Class `VectorEigenDense` is derived directly from `Vector`. Besides taking advantages of all funtionalities of `Vector`, this class supplements some particular functions to calculate Householder transformation.

```
template<typename K>
class VectorEigenDense : public Vector<K>
{
public:
    typedef typename VectorEigenDense::type_t Scalar;
    typedef typename NumTraits<Scalar >::RealScalar RealScalar;
    typedef typename VectorEigenDense::it_vk it_vk;
    typedef typename VectorEigenDense::cit_vk cit_vk;

    VectorEigenDense() : Vector<K>(), acType_(_col) {}
    VectorEigenDense(const Dimen l) : Vector<K>(l, K()), acType_(_col) {}
    ...
```

This class offers some additional functions to calculate House holder values.

```
void makeHouseHolderInPlace(K& tau, Real& beta);
void makeHouseHolderInPlace(K& tau, Real& beta, Number tail);
void makeHouseHolder(VectorEigenDense<K>& essential, K& tau, Real& beta) const;
```

Note that the in the future, we may improve calculation performance of eigensolver for *dense* matrix by changing this class `VectorEigenDense`. By using the same block of allocated data, we can gain more efficiencies. However, for the moment, it's sufficient to have this class inherited from class `Vector`

| | |
|---|---|
| library : | **eigenSolvers** |
| header : | |
| implementation : | |
| unitary tests : | **test_EigenSolverUtils.cpp** |
| header dependences : | **Traits.hpp** |

### The `MatrixEigenDense` class

Class `MatrixEigenDense` inherits from the fundamental class `Matrix`. Basically, this class reuses all functionalities of its father in addition to some methods to support computing House holder, Cholesky composition and Jacobian rotation.

```
template<typename K>
class MatrixEigenDense : public Matrix<K>
{
public:
    typedef typename MatrixEigenDense<K>::type_t Scalar;
    typedef typename NumTraits<Scalar >::RealScalar RealScalar;
    typedef typename std::vector<K>::iterator it_vk;
    typedef typename std::vector<K>::const_iterator cit_vk;

    MatrixEigenDense() : Matrix<K>(), col_(1) {}
    MatrixEigenDense(const Dimen r) : Matrix<K>(r,r), col_(r) {}
    ...
```

Householder computation can be invoked with

```
void applyHouseholderOnTheLeft(const VectorEigenDense<K>& essential, const K& tau);
void applyHouseholderOnTheRight(const VectorEigenDense<K>& essential, const K& tau);
```

Cholesky decomposition can be calculated by

```
MatrixEigenDense<K> cholesky() const;
```

or one can call Jacobian rotation with

```
template<typename OtherScalar>
inline void applyOnTheLeft(Index p, Index q, const JacobiRotation<OtherScalar>& j);
template<typename OtherScalar>
inline void applyOnTheRight(Index p, Index q, const JacobiRotation<OtherScalar>& j);
```

Similar to class `VectorEigenDense`, in the future, this class may be improved to make *eigenCore* more efficient.

| | |
|---|---|
| library : | **eigenSolvers** |
| header : | |
| implementation : | |
| unitary tests : | **test_EigenSolverUtils.cpp** |
| header dependences : | **Traits.hpp** |

### The `JacobiRotation` class

Class `JacobiRotation` represents a *Jacobian* or *Givens* rotation, 2D rotation in a plane defined by its cosine and sine.

```
template<typename Scalar>
class JacobiRotation
{
  public:
    typedef typename NumTraits<Scalar>::RealScalar RealScalar;

    /** Default constructor without any initialization. */
    JacobiRotation() {}

    /** Construct a planar rotation from a cosine-sine pair (\a c, \c s). */
    JacobiRotation(const Scalar& c, const Scalar& s) : c_(c), s_(s) {}

    Scalar& c() { return c_; }
    Scalar c() const { return c_; }
    Scalar& s() { return s_; }
    Scalar s() const { return s_; }
    ...
```

The class provide two basic operations: making a Jacobi rotation and applying this rotation on both the right and left side of a selfadjoint 2 × 2 matrix; making a Givens rotation and applying this rotation on the left side of a vector.

```
template<typename Scalar>
bool JacobiRotation<Scalar>::makeJacobi(RealScalar x, Scalar y, RealScalar z);
template<typename Scalar>
void JacobiRotation<Scalar>::makeGivens(const Scalar& p, const Scalar& q, Scalar* z);
```

| | |
|---|---|
| library : | **eigenSolvers** |
| header : | |
| implementation : | |
| unitary tests : | **test_EigenSolverUtils.cpp** |
| header dependences : | **Traits.hpp** |

### The `NumTraits` class

`NumTraits` greatly facilitate the management of the sort of extra parameters that come up during the implementation of eigensolver algorithm.

```
template<typename K>
struct NumTraits {};

template<>
struct NumTraits<Real> {
    enum {
      IsComplex = 0
    };
    static inline bool isReal() { return true;}
    static inline bool isComplex() { return false;}
    static inline Real zero() { return Real(0.0);}
    static inline Real one() { return Real(1.0);}
    static inline Real imag(const Real& v) { return v;}
    static inline Real real(const Real& v) { return v;}
    static inline Real value(const Real& v) { return v;}
    static inline Real abs2(const Real& v) { return v*v;}
    static inline Real epsilon() { return std::numeric_limits<Real>::epsilon(); }
    typedef Real RealScalar;
    typedef Complex ComplexScalar;
};

template<>
struct NumTraits<Complex> {
    enum {
      IsComplex = 1
    };
    static inline bool isReal() {return false;}
    static inline bool isComplex() { return true;}
    static inline Complex zero() { return Complex(0.0,0.0);}
    static inline Complex one() { return Complex(1.0,0.0);}
    static inline Real imag(const Complex& v) { return v.imag();}
    static inline Real real(const Complex& v) { return v.real();}
    static inline Complex value(const Complex& v) { return v;}
    static inline Real abs2(const Complex& v) { return v.real()*v.real() + v.imag()*v.imag();}
    typedef Real RealScalar;
    typedef Complex ComplexScalar;
};
```

| | |
|---|---|
| library : | **eigenSolvers** |
| header : | |
| implementation : | |
| unitary tests : | **test_EigenSolverUtils.cpp** |
| header dependences : | **utils.h** |

### 15.1.2 *decomposition* part

All classes of this section utilize functions provided from the lower level - `utils` - to implement various decomposition algorithms, which play an important role in solving different eigen problems.

#### The `Tridiagonalization` class

Class `Tridiagonalization` performs a tridiagonal decomposition of a self-adjoint matrix $A$ such that: $A = QTQ^*$ where $Q$ is unitary and $T$ a real symmetric tridiagonal matrix. A tridiagonal matrix is a matrix which has non-zero elements only on the main diagonal and the first diagonal below and above it. This class is used in SelfAdjointEigenSolver to compute the eigenvalues and eigenvectors of a selfadjoint matrix.

```
template<typename _MatrixType>
class Tridiagonalization
{
  public:

    /** \brief Synonym for the template parameter \p _MatrixType. */
    typedef _MatrixType MatrixType;
    typedef typename MatrixType::type_t Scalar;
    typedef typename NumTraits<Scalar>::RealScalar RealScalar;
    typedef VectorEigenDense<Scalar> CoeffVectorType;
    typedef VectorEigenDense<RealScalar> DiagonalType;
    ...
    Tridiagonalization(Dimen size);
    Tridiagonalization(const MatrixType& matrix);
    ...
```

This class comes with default constructor with size of the matrix whose tridiagonal decomposition will be computed. In fact, this parameter is just a hint. After being created, object of this class can be used to calculate any square *dense* matrix with

```
Tridiagonalization& compute(const MatrixType& matrix);
```

The unitary matrix $Q$ can only be invoked after calling the *compute*:

```
MatrixType matrixQ();
```

"Householder coefficients" can be retrieved by

```
inline CoeffVectorType householderCoefficients() const;
```

We don't need the full-form of matrix $T$ in computation of eigenvalues; however its real diagonal and its real sub-diagonal are essential in calculating eigenvalues of the matrix. These two values can be retrieved with:

```
DiagonalReturnType diagonal() const;
SubDiagonalReturnType subDiagonal() const;
```

For example, the following 5 × 5 real symmetric matrix

$$A = \begin{bmatrix} 1.36 & -0.816 & 0.521 & 1.43 & -0.144 \\ -0.816 & -0.659 & 0.794 & -0.173 & -0.406 \\ 0.521 & 0.794 & -0.541 & 0.461 & 0.179 \\ 1.43 & -0.173 & 0.461 & -1.43 & 0.822 \\ -0.144 & -0.406 & 0.179 & 0.822 & -1.37 \end{bmatrix}$$

after being tridiagonalized, has diagonal and sub-diagonal vectors
diagonal = ( 1.36 -0.659 -0.541 -1.43 -1.37 )
sub-diagonal = ( -0.816 0.794 0.461 0.822 )

| | |
|---:|---|
| library : | **eigenSolvers** |
| header : | |
| implementation : | |
| unitary tests : | **test_EigenSolverDecomposition.cpp** |
| header dependences : | **Traits.hpp, VectorEigenDense.hpp, HouseHolderSequence.hpp** |

### The `HessenbergDecomposition` class

Class `HessenbergDecomposition` performs an Hessenberg decomposition of a matrix $A$. In the real case, the Hessenberg decomposition consists of an orthogonal matrix $Q$ and a Hessenberg matrix $H$ such that $A = QHQ^T$. An orthogonal matrix is a matrix whose inverse equals its transpose ($Q^{-1} = Q^T$). A Hessenberg matrix has zeros below the subdiagonal, so it is almost upper triangular. The Hessenberg decomposition of a complex matrix is $A = QHQ^*$ with $Q$ unitary (that is, $Q^{-1} = Q^*$).

```
template<typename _MatrixType>
class HessenbergDecomposition
{
  public:

    /** \brief Synonym for the template parameter \p _MatrixType. */
    typedef _MatrixType MatrixType;

    /** \brief Scalar type for matrices of type #MatrixType. */
    typedef typename MatrixType::type_t Scalar;

    /** \brief Type for vector of Householder coefficients.
      *
      * This is column vector with entries of type #Scalar. The length of the
      * vector is one less than the size of #MatrixType,
      */
    typedef VectorEigenDense<Scalar> CoeffVectorType;

    /** \brief Return type of matrixQ() */
    typedef typename HouseholderSequence<MatrixType,CoeffVectorType>::ConjugateReturnType
        HouseholderSequenceType;

    /** \brief Default constructor; the decomposition will be computed later.
      *
      * \param [in] size  The size of the matrix whose Hessenberg decomposition will be computed.
      *
      * The default constructor is useful in cases in which the user intends to
      * perform decompositions via compute().  The \p size parameter is only
      * used as a hint. It is not an error to give a wrong \p size, but it may
      * impair performance.
      *
      * \sa compute() for an example.
      */
    HessenbergDecomposition(Number size)
      : matrix_(size,size),
        isInitialized_(false)
    {
      if(size>1)
        hCoeffs_.resize(size-1);
    }
    ...
```

We can use the constructor which computes the Hessenberg decomposition at construction time.

```
HessenbergDecomposition(const MatrixType&);
```

Once the decomposition is computed, we can use the `matrixH()` and `matrixQ()` functions to construct the matrices $H$ and $Q$ in the decomposition.

```
MatrixType matrixQ();
MatrixType matrixH() const;
```

Alternatively, calling the function `compute()` to compute the Hessenberg decomposition of a given matrix. then we can use these two functions above

```
HessenbergDecomposition& compute(const MatrixType& matrix);
```

For instance, the following 5 × 5 real symmetric matrix

$$A = \begin{bmatrix} 1.36 & -0.816 & 0.521 & 1.43 & -0.144 \\ -0.816 & -0.659 & 0.794 & -0.173 & -0.406 \\ 0.521 & 0.794 & -0.541 & 0.461 & 0.179 \\ 1.43 & -0.173 & 0.461 & -1.43 & 0.822 \\ -0.144 & -0.406 & 0.179 & 0.822 & -1.37 \end{bmatrix}$$

has Hessenberg decomposition

$$H = \begin{bmatrix} 1.36 & 1.7328972849 & 0 & 0 & 0 \\ 1.7328972849 & -1.1933420269 & -0.96533126903 & -9.1846580094e-17 & 2.021583842e-16 \\ 0 & -0.96533126903 & -1.2812029745 & 0.21380585197 & 1.9428902931e-16 \\ 0 & 0 & 0.21380585197 & -1.6885671008 & 0.34719629211 \\ 0 & 0 & 0 & 0.34719629211 & 0.16311210222 \end{bmatrix}$$

and unitary matrix

$$Q = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & -0.47088769029 & 0.12629876626 & -0.67227759101 & -0.55709626223 \\ 0 & 0.30065255716 & -0.19453390601 & 0.43672469898 & -0.82524913607 \\ 0 & 0.82520759451 & 0.045097442878 & -0.56297063107 & -0.0079192904815 \\ 0 & -0.083097827699 & -0.97168482632 & -0.20094388887 & 0.092438643767 \end{bmatrix}$$

| | |
|---:|:---|
| library : | **eigenSolvers** |
| header : | |
| implementation : | |
| unitary tests : | **test_EigenSolverDecomposition.cpp** |
| header dependences : | **Traits.hpp, VectorEigenDense.hpp** |

### The `RealSchur` class

Class `RealSchur` performs a real Schur decomposition of a square matrix. Given a real square matrix $A$, this class computes the real Schur decomposition: $A = UTU^T$ where $U$ is a real orthogonal matrix and $T$ is a real quasi-triangular matrix. An orthogonal matrix is a matrix whose inverse is equal to its transpose, $U^{-1} = U^T$. A quasi-triangular matrix is a block-triangular matrix whose diagonal consists of 1-by-1 blocks and 2-by-2 blocks with complex eigenvalues. The eigenvalues of the blocks on the diagonal of $T$ are the same as the eigenvalues of the matrix $A$, and thus the real Schur decomposition is used in `RealEigenSolver` to compute the eigendecomposition of a matrix.

```
template<typename _MatrixType>
class RealSchur
{
  public:
    typedef _MatrixType MatrixType;
    typedef typename MatrixType::type_t Scalar;
    typedef typename NumTraits<Scalar>::ComplexScalar ComplexScalar;

    typedef VectorEigenDense<ComplexScalar> EigenvalueType;
    typedef VectorEigenDense<Scalar> ColumnVectorType;

    /** \brief Default constructor.
      *
      * \param [in] size  Positive integer, size of the matrix whose Schur decomposition will be
          computed.
      *
      * The default constructor is useful in cases in which the user intends to
      * perform decompositions via compute().  The \p size parameter is only
      * used as a hint. It is not an error to give a wrong \p size, but it may
      * impair performance.
      *
      * \sa compute() for an example.
      */
    RealSchur(Index size)
            : matT_(size, size),
              matU_(size, size),
              hess_(size),
              maxIterations_(40),
              isInitialized_(false),
              matUisUptodate_(false),
              info_(_noConvergence)
    { }
    ...
```

We can use the constructor which computes the real Schur decomposition at construction time.

```
RealSchur(const MatrixType& matrix, bool computeU = true);
```

Once the decomposition is computed, we can use the `matrixU()` and `matrixT()` functions to retrieve the matrices $U$ and $T$ in the decomposition.

```
MatrixType matrixU() const;
MatrixType matrixT() const;
```

Alternatively calling the function `compute()` to compute the real Schur decomposition of a given matrix, after that we are able to use these two functions above.
The implementation of Schur decomposition of real square matrix is adapted from `http://math.nist.gov/javanumerics/jama/`, whose code is based on EISPACK. The Schur decomposition is computed by first reducing the matrix to $Hessenberg$ form using the class `HessenbergDecomposition`. The $Hessenberg$ matrix is then reduced to triangular form by performing $FrancisQR$ iterations with implicit double shift.
There are several auxiliary functions in order to implement this algorithm :

```
Scalar computeNormOfT();
Index findSmallSubdiagEntry(Index iu, Scalar norm);
void splitOffTwoRows(Index iu, bool computeU, Scalar exshift);
void computeShift(Index iu, Index iter, Scalar& exshift, Vector3s& shiftInfo);
void initFrancisQRStep(Index il, Index iu, const Vector3s& shiftInfo, Index& im, Vector3s&
     firstHouseholderVector);
void performFrancisQRStep(Index il, Index im, Index iu, bool computeU, const Vector3s&
     firstHouseholderVector);
```

For instance, the following 5 × 5 non symmetric matrix

$$A = \begin{bmatrix} 1.8779 & -0.5583 & -0.2099 & 0.2696 & 0.1097 \\ 0.9407 & -0.3114 & -1.6989 & 0.4943 & 1.1287 \\ 0.7873 & -0.57 & 0.6076 & -1.4831 & -0.29 \\ -0.8759 & -1.0257 & -0.1178 & -1.0203 & 1.2616 \\ 0.3199 & -0.9087 & 0.6992 & -0.447 & 0.4754 \end{bmatrix}$$

has the quasi-triangular matrix in the Schur decomposition

$$H = \begin{bmatrix} 1.6552531332 & -0.30767059895 & -0.45435806468 & 1.5602779282 & 0.68358491675 \\ 0 & 1.1891303949 & 1.9306398993 & 0.96785347442 & 0.57970343469 \\ 0 & -1.3969331077 & 0.22387492903 & -0.78380738142 & 1.27402357 \\ 0 & 0 & 0 & 0.092450608769 & -0.5563858236 \\ 0 & 0 & 0 & 0 & -1.5315090659 \end{bmatrix}$$

and the orthogonal matrix in the Schur decomposition.

$$Q = \begin{bmatrix} 0.72665944996 & 0.28908942548 & -0.090578168382 & 0.61658006012 & 0.0042394246225 \\ 0.13365823926 & 0.75252664471 & -0.11720311204 & -0.52512343394 & -0.35545454525 \\ 0.50462706182 & -0.59105620177 & -0.20754951129 & -0.34476029525 & -0.4838053679 \\ -0.1068784212 & 0.010284495663 & 0.747282602 & 0.23512571367 & -0.61217305049 \\ 0.43362431945 & -0.026033604674 & 0.61363746549 & -0.41222645012 & 0.51459752796 \end{bmatrix}$$

| | |
|---|---|
| library : | **eigenSolvers** |
| header : | |
| implementation : | |
| unitary tests : | **test_EigenSolverDecomposition.cpp** |
| header dependences : | **Jacobi.hpp, VectorEigenDense.hpp, HessenbergDecomposition.hpp** |

### 15.1.3 *eigenSolver* main part

In this section, there are solvers for three kinds of eigen problem :

- Hermitian eigenproblem
- Generalized Hermitian eigenproblem
- Non-Hermitian (real) eigenproblem

The following presents eigen solver classes corresponding to each kind of eigen problem.

**The `SelfAdjointEigenSolver` class**

Class `SelfAdjointEigenSolver` computes eigenvalues and eigenvectors of self-adjoint matrices. A matrix $A$ is selfadjoint if it equals its adjoint. For real matrices, this means that the matrix is symmetric: it equals its transpose.
This class computes the eigenvalues and eigenvectors of a self-adjoint matrix. These are the scalars $\lambda$ and vectors $v$ such that $Av = \lambda v$. The eigenvalues of a self-adjoint matrix are always real. If $D$ is a diagonal matrix with the eigenvalues on the diagonal, and $V$ is a matrix with the eigenvectors as its columns, then $A = VDV^{-1}$ (for self-adjoint matrices, the matrix $V$ is always invertible). This is called the eigendecomposition. The implemented algorithm exploits the fact that the matrix is self-adjoint, making it faster and more accurate than the general purpose eigenvalue algorithms implemented in RealEigenSolver.

```
template<typename _MatrixType>
class SelfAdjointEigenSolver
{
  public:

    typedef _MatrixType MatrixType;

    /** \brief Scalar type for matrices of type \p _MatrixType. */
    typedef typename MatrixType::type_t Scalar;

    /** \brief Real scalar type for \p _MatrixType.
      *
      * This is just \c Scalar if #Scalar is real (e.g., \c float or
      * \c double), and the type of the real part of \c Scalar if #Scalar is
      * complex.
      */
    typedef typename NumTraits<Scalar>::RealScalar RealScalar;
    /** \brief Type for vector of eigenvalues as returned by eigenvalues().
      *
      * This is a column vector with entries of type #RealScalar.
      * The length of the vector is the size of \p _MatrixType.
      */
    typedef VectorEigenDense<RealScalar> RealVectorType;
    typedef Tridiagonalization<MatrixType> TridiagonalizationType;

    /** \brief Default constructor for fixed-size matrices.
      *
      * The default constructor is useful in cases in which the user intends to
      * perform decompositions via compute().
      *
      */
    SelfAdjointEigenSolver()
        : eivec_(),
          eivalues_(),
          subdiag_(),
          maxIterations_(30),
          isInitialized_(false)
    { }
    ...
```

We can use the constructor which computes the eigenvalues and eigenvectors at construction time.

```
SelfAdjointEigenSolver(const MatrixType& matrix, Int options = _computeEigenVector);
```

Once the eigenvalue and eigenvectors are computed, they can be retrieved with

```
const RealVectorType& eigenvalues() const;
const MatrixType& eigenvectors() const;
```

Alternatively, we can call the function `compute()` to compute the eigenvalues and eigenvectors of a given matrix.

```
SelfAdjointEigenSolver& compute(const MatrixType& matrix, Int options = _computeEigenVector);
```

This implementation uses a symmetric QR algorithm. The matrix is first reduced to tridiagonal form using the `Tridiagonalization` class. The tridiagonal matrix is then brought to diagonal form with implicit symmetric QR steps with Wilkinson shift.

For instance, the following 5 × 5 real symmetric matrix

$$A = \begin{bmatrix} 1.36 & -0.816 & 0.521 & 1.43 & -0.144 \\ -0.816 & -0.659 & 0.794 & -0.173 & -0.406 \\ 0.521 & 0.794 & -0.541 & 0.461 & 0.179 \\ 1.43 & -0.173 & 0.461 & -1.43 & 0.822 \\ -0.144 & -0.406 & 0.179 & 0.822 & -1.37 \end{bmatrix}$$

has eigenvalues and corresponding (column) eigenvector

eigenvalues = ( -2.64925 -1.76682 -0.742793 0.22723 2.29163 )

$$\text{eigenvectors} = \begin{bmatrix} -0.32648814917 & -0.098193931162 & 0.34709885718 & -0.010999922777 & 0.87359305479 \\ -0.20806598152 & -0.64229394812 & 0.22733262857 & 0.66233712946 & -0.23194058392 \\ 0.050094522003 & 0.62960023585 & -0.16376394055 & 0.73987891396 & 0.16387387324 \\ 0.72069515152 & -0.39678270513 & -0.40156098976 & 0.11452959441 & 0.38573789934 \\ -0.57289010572 & -0.15486595502 & -0.79985773898 & -0.025508690809 & 0.085967242812 \end{bmatrix}$$

| | |
|---|---|
| library : | **eigenSolvers** |
| header : | |
| implementation : | |
| unitary tests : | **test_EigenSolverInternCore.cpp** |
| header dependences : | **VectorEigenDense.hpp, Tridiagonalization.hpp** |

### The `GeneralizedSelfAdjointEigenSolver` class

Class `GeneralizedSelfAdjointEigenSolver` computes eigenvalues and eigenvectors of the generalized self-adjoint eigen problem.
This class solves the generalized eigenvalue problem $Av = \lambda Bv$. In this case, the matrix $A$ should be self-adjoint and the matrix $B$ should be positive definite.

```
template<typename _MatrixType>
class GeneralizedSelfAdjointEigenSolver : public SelfAdjointEigenSolver<_MatrixType>
{
    typedef SelfAdjointEigenSolver<_MatrixType> Base;
public:
    typedef _MatrixType MatrixType;

    /** \brief Default constructor for fixed-size matrices.
      *
      * The default constructor is useful in cases in which the user intends to
      * perform decompositions via compute().
      */
    GeneralizedSelfAdjointEigenSolver() : Base() {}

    /** \brief Constructor, pre-allocates memory for dynamic-size matrices.
      *
      * \param [in]  size  Positive integer, size of the matrix whose
      * eigenvalues and eigenvectors will be computed.
      *
      * \sa compute() for an example
      */
    GeneralizedSelfAdjointEigenSolver(Index size)
        : Base(size)
    {}
    ...
```

We can use the constructor which computes the eigenvalues and eigenvectors at construction time.

```
    GeneralizedSelfAdjointEigenSolver(const MatrixType& matA, const MatrixType& matB,
                                      int options = _computeEigenVector|_Ax_lBx)
      : Base(matA.numOfCols());
```

Alternatively, we can call the function *compute()* to compute the eigenvalues and eigenvectors of a given matrix.

```
    GeneralizedSelfAdjointEigenSolver& compute(const MatrixType& matA, const MatrixType& matB,
                                               int options = _computeEigenVector|_Ax_lBx);
```

Eigenvalues and eigenvectors can be retrieved with same functions of `SelfAdjointEigenSolver`

```
const RealVectorType& eigenvalues() const;
const MatrixType& eigenvectors() const;
```

For instance, the following 5 × 5 real symmetric matrix $A$ and positive definite matrix $B$

$$A = \begin{bmatrix} 1.36 & -0.816 & 0.521 & 1.43 & -0.144 \\ -0.816 & -0.659 & 0.794 & -0.173 & -0.406 \\ 0.521 & 0.794 & -0.541 & 0.461 & 0.179 \\ 1.43 & -0.173 & 0.461 & -1.43 & 0.822 \\ -0.144 & -0.406 & 0.179 & 0.822 & -1.37 \end{bmatrix}$$

$$B = \begin{bmatrix} 1.1981 & 1.4405 & 1.5367 & 1.0971 & 1.1276 \\ 1.4405 & 2.1207 & 1.9115 & 1.3836 & 1.642 \\ 1.5367 & 1.9115 & 2.4828 & 1.7702 & 1.7543 \\ 1.0971 & 1.3836 & 1.7702 & 1.4359 & 1.2428 \\ 1.1276 & 1.642 & 1.7543 & 1.2428 & 1.424 \end{bmatrix}$$

has eigenvalues and corresponding (column) eigenvector
eigenvalues = ( -40.0667 -12.6587 -3.08602 0.0522151 40.3448 )

$$\text{eigenvectors} = \begin{bmatrix} -2.5241477328 & -0.01326907506 & 0.83333293087 & -0.040348533316 & 4.3939678718 \\ 3.7607674197 & 0.3488243247 & 1.1073133113 & -0.3174355818 & -4.3303408407 \\ 3.0396247156 & 2.615639864 & -0.34676637691 & -0.36756457169 & -3.9258019948 \\ 0.45843793898 & -2.0051996759 & -0.65863554474 & -0.039469282032 & 1.4762595546 \\ -6.6376554636 & -1.9381010232 & -0.97022016252 & 0.070809133211 & 4.9718019236 \end{bmatrix}$$

| | |
|---|---|
| library : | **eigenSolvers** |
| header : | |
| implementation : | |
| unitary tests : | **test_EigenSolverInternCore.cpp** |
| header dependences : | **Tridiagonalization.hpp** |

### The `RealEigenSolver` class

Class `RealEigenSolver` computes eigenvalues and eigenvectors of general real matrices.
The eigenvalues and eigenvectors of a matrix $A$ are scalars $\lambda$ and vectors $v$ such that $Av = \lambda v$. If $D$ is a diagonal matrix with the eigenvalues on the diagonal, and $V$ is a matrix with the eigenvectors as its columns, then $AV = VD$. The matrix $V$ is almost always invertible, in which case we have $A = VDV^{-1}$.
The eigenvalues and eigenvectors of the matrix may be complex, even when the matrix is real. However, we can choose real matrices $V$ and $D$ satisfying $AV = VD$, just like the eigendecomposition, if the matrix $D$ is not required to be diagonal, but if it is allowed to have blocks of the form

$$\begin{bmatrix} u & v \\ -v & u \end{bmatrix}$$

(where $u$ and $v$ are real numbers) on the diagonal. These blocks correspond to complex eigenvalue pairs $u \pm iv$. We call this variant of the eigendecomposition the pseudo-eigendecomposition.

```
template<typename _MatrixType>
class RealEigenSolver
{
  public:

    /** \brief Synonym for the template parameter \p _MatrixType. */
    typedef _MatrixType MatrixType;

    /** \brief Scalar type for matrices of type #MatrixType. */
    typedef typename MatrixType::type_t Scalar;
    typedef typename NumTraits<Scalar>::RealScalar RealScalar;
    typedef VectorEigenDense<Scalar> ColumnVectorType;
    typedef VectorEigenDense<Scalar> VectorType;

    /** \brief Complex scalar type for #MatrixType.
      *
      * This is \c std::complex<Scalar> if #Scalar is real (e.g.,
      * \c float or \c double) and just \c Scalar if #Scalar is
      * complex.
      */
    typedef typename NumTraits<Scalar>::ComplexScalar ComplexScalar;
    typedef VectorEigenDense<ComplexScalar> ComplexVectorType;

    /** \brief Type for vector of eigenvalues as returned by eigenvalues().
      *
      * This is a column vector with entries of type #ComplexScalar.
      * The length of the vector is the size of #MatrixType.
      */
    typedef VectorEigenDense<ComplexScalar> EigenvalueType;

    /** \brief Type for matrix of eigenvectors as returned by eigenvectors().
      *
      * This is a square matrix with entries of type #ComplexScalar.
      * The size is the same as the size of #MatrixType.
      */
    typedef MatrixEigenDense<ComplexScalar> EigenvectorsType;

    /** \brief Default constructor.
      *
      * The default constructor is useful in cases in which the user intends to
      * perform decompositions via RealEigenSolver::compute(const MatrixType&, bool).
      *
      * \sa compute() for an example.
      */
 RealEigenSolver() : eivec_(), eivalues_(), isInitialized_(false), realSchur_(), matT_() {}

    /**
     * \brief Default constructor with memory preallocation
      *
      * Like the default constructor but with preallocation of the internal data
      * according to the specified problem \a size.
      * \sa RealEigenSolver()
      */
    RealEigenSolver(Index size)
      : eivec_(size, size),
        eivalues_(size),
        isInitialized_(false),
        eigenvectorsOk_(false),
        realSchur_(size),
        matT_(size, size)
    {}
    ...
```

Same as other two eigensolvers, we can use the constructor which computes the eigenvalues and eigenvectors at construction time.

```
RealEigenSolver(const MatrixType& matrix, bool computeEigenvectors = true);
```

Once the eigenvalue and eigenvectors are computed, they can be retrieved with

```
const EigenvalueType& eigenvalues() const;
EigenvectorsType eigenvectors() const;
```

Alternatively, we can call the function `compute()` to compute the eigenvalues and eigenvectors of a given matrix.

```
RealEigenSolver& compute(const MatrixType& matrix, bool computeEigenvectors = true);
```

This implementation first reduces the matrix to real Schur form using the `RealSchur` class. The Schur decomposition is then used to compute the eigenvalues and eigenvectors.
For instance, the following 5 × 5 non symmetric matrix

$$A = \begin{bmatrix} 1.8779 & -0.5583 & -0.2099 & 0.2696 & 0.1097 \\ 0.9407 & -0.3114 & -1.6989 & 0.4943 & 1.1287 \\ 0.7873 & -0.57 & 0.6076 & -1.4831 & -0.29 \\ -0.8759 & -1.0257 & -0.1178 & -1.0203 & 1.2616 \\ 0.3199 & -0.9087 & 0.6992 & -0.447 & 0.4754 \end{bmatrix}$$

has eigenvalues and corresponding (column) eigenvector
eigenvalues = ( (1.65525,0) (0.706503,1.56973) (0.706503,-1.56973) (0.0924506,0) (-1.53151,0) )

$$\text{eigenvectors} = \begin{bmatrix} (0.727,0) & (0.177,-0.001) & (0.177,0.001) & (-0.230,0) & (-0.041,0) \\ (0.133,0) & (0.534,-0.218) & (0.534,0.218) & (-0.664,0) & (-0.392,0) \\ (0.504,0) & (-0.444,0.0814) & (-0.444,-0.0814) & (-0.336,0) & (-0.587,0) \\ (-0.106,0) & (0.011,0.457) & (0.0118,-0.457) & (0.135,0) & (-0.695,0) \\ (0.433,0) & (-0.036,0.469) & (-0.036,-0.469) & (-0.611,0) & (-0.121,0) \end{bmatrix}$$

| | |
|---:|---|
| library : | **eigenSolvers** |
| header : | |
| implementation : | |
| unitary tests : | **test_EigenSolverInternCore.cpp** |
| header dependences : | **VectorEigenDense.hpp, MatrixEigenDense.hpp, RealSchur.hpp** |

## 15.2 *eigenSparse* sub-library

The *eigenSparse* provides tools that are useful for solving a wide variety of eigenvalue problems. The solvers currently implemented within *eigenSparse* compute a partial eigen-decomposition for the generalized eigenvalue problem

$$Ax = Bx\lambda$$

We assume that the matrices A and B are large, possibly sparse, and that only their application to a block of vectors is required.
This section outlines the eigenSparse. Three subsections describe the eigenSparse operator/multivector interface, the eigensolver, and the various implementations provided by the eigenSparse.
The lib *eigenSparse* is highly independent of other packages of XLiFE++ except for *eigenCore* which provides essential functions in performing the dense arithmetic for Rayleigh-Ritz methods.

### 15.2.1 The Operator/Multivector Interface

*eigenSparse* utilizes traits classes to define interfaces for the scalar field, multivectors, and matrix operators. This allows generic programming techniques to be used when developing numerical algorithms in the *eigenSparse*. *eigenSparse*'s eigensolver is comprised of abstract numerical interfaces that are all implemented using templates and the functionality of the template arguments is provided through their corresponding trait classes. Most classes in *eigenSparse* accept three template parameters:

- a scalar type, describing the field over which the vectors and operators are defined;
- a multivector type over the given scalar field, providing a data structure that denotes a collection of vectors; and
- an operator type over the given scalar field, providing linear operators used to define eigenproblems and preconditioners.

We note that the *eigenSparse* was designed to support block methods, defined as those that apply A or B to a collection of vectors (a multivector). Algorithms in *eigenSparse* are developed at a high-level, where the underlying linear algebra objects are opaque. The choice in linear algebra is made through templating, and access to the functionality of the underlying objects is provided via the traits classes `MultiVecTraits` and `OperatorTraits`.

These classes define opaque interfaces, specifying the operations that multivector and operator classes must support in order to be used in *eigenSparse* without exposing low-level details of the underlying data structures. The `MultiVecTraits` and `OperatorTraits` classes specify the operations that the multivector and operator type must support in order for them to be used by *eigenSparse*.

The `OperatorTraits` class only needs to provide one method, described in the Table, that applies an operator to a multivector. This interface defines the only interaction required from an operator, even though the underlying operator may be a matrix, spectral transformation, or preconditioner.

| **OperatorTraits<ST,MV,OP>** | |
|---|---|
| *Method name* | *Description* |
| `apply`(A,X,Y) | Applies the operator A to the multivector X, placing the result in the multivector Y |

The methods defined by the `MultiVecTraits` class, listed in following table, are the nesseary creational and arithmetic ones. The creational methods generate empty or populated multivectors from a previously created multivector. The populated multivectors can be a deep copy, where the object contains the storage for the multivector entries, or a shallow copy, where the object has a view of another multivector's storage. A shallow copy is useful when only a subset of the columns of a multivector is required for computation, which is a situation that commonly occurs during the generation of a subspace.

| **MultiVecTraits<ST,MV>** | |
|---|---|
| *Method name* | *Description* |
| `clone(X,numvecs)` | Creates a new multivector from X with *numvecs* vectors |
| `cloneCopy(X,index)` | Creates a new multivector with a copy of the contents of a subset of the multivector X (deep copy) |
| `cloneView(X,index)` | Creates a new multivector that shares the selected contents of a subset of the multivector X (shallow copy) |
| `getVecLength(X)` | Returns the vector length of the multivector X |
| `getNumberVecs(X)` | Returns the number of vectors in the multivector X |
| `mvTimesMatAddMv`(alpha,X, D,beta,Y) | Applies a dense matrix D to multivector X and accumulates the result into multivector Y: $Y \leftarrow \alpha X D + \beta Y$ |
| `mvAddMv`(alpha,X,beta,Y) | Performs multivector: $Y \leftarrow \alpha X + \beta Y$ |
| `mvTransMv`(alpha,X,Y,D) | Computes the dense matrix $D \leftarrow \alpha X^H Y$ |
| `mvDot`(X,Y,d) | Computes the corresponding dot products: $d[i] \leftarrow \bar{a}_i y_i$ |
| `mvScale`(X,d) | Scales the i-th column of a multivector X by $d[i]$ |
| `mvNorm`(X,d) | Computes the 2-norm of each vector of $X : d[i] \leftarrow \|\|x_i\|\|_2$ |
| `setBlock`(X,Y,index) | Copies the vectors in X to a subset of vectors in Y |
| `mvInit`(X,alpha) | Replaces each entry in the multivector X with a scalar $\alpha$ |
| `mvRandom`(X) | Replaces the entries in the multivector X by random scalars |
| `mvPrint`(X) | Print the multivector X |

The arithmetic methods defined by the multiVecTraits are essential to the computations required by the Rayleigh-Ritz method and the general eigen-iteration. The mvTimesMatAddMv and mvAddMv methods, for instance, are necessary for updating the approximate eigenpairs and their residuals. The mvDot and mvTransMv methods are required by the orthogonalization procedure of the eigen-iteration. The mvScale and mvNorm methods are necessary, at the very least, for the computation of approximate eigenpairs and for some termination criteria of the eigen-iteration. Deflation and locking of converged eigenvectors necessitates the setBlock method in many cases. Initialization of the bases for the eigen-iteration requires methods such as mvRandom and mvInit. The ability to perform error checking and debugging is supported by methods that give dimensional attributes (getVecLength, getNumberVecs) and allow the users to print out a multivector (mvPrint).
Calling methods of MultiVecTraits and OperatorTraits requires that specializations of these traits classes have been implemented for given template arguments. XLiFE++ provides the following classes that can be used with these traits classes:

- MultiVectorAdapter, an extended version of Vector, allowing the process on block of vector.
- LargeMatrixAdapter, a wrapper of LargeMatrix in order to take adavantage of multiplication matrix-vector of sparse matrix

### The MultiVectorAdapter class

This class provides the implementations of the interfaces along with abstract MultiVec class. By inheriting directly from MultiVec class, the implementaion works via run-time polymorphism. This option isn't optimal from performance point of view because of the dispatching cost during run-time. In the near future, we can improve it by implementing a specialization of MultiVecTraits class, which allows compile-time polymorphism.
By using the pointer to each vector, MultiVectorAdapter class allows to create different objects, which share a same view of memory (shallow copy). This feature is essential when we want only to work on specific column vectors of a multivector.

```
template <class ScalarType>
class MultiVecAdapter : public MultiVec<ScalarType>
{
  public:
    typedef std::vector<ScalarType>* VectorPointer;

  //! Constructor for a \c numberVecs vectors of length \c length.
  MultiVecAdapter(const Number length, const Dimen numberVecs) :
    length_(length),
    numberVecs_(numberVecs)
  {
    check();

    data_.resize(numberVecs);
    ownership_.resize(numberVecs);

    // Allocates memory to store the vectors.
    for (Dimen v = 0 ; v < numberVecs_ ; ++v)
    {
      data_[v] = new std::vector<ScalarType>(length);
      ownership_[v] = true;
    }

    // Initializes all elements to zero.
    mvInit(0.0);
  }
 ...
```

### The `LargeMatrixAdapter` class

This class is simply a wrapper of `LargeMatrix` class in order to take advantage of consuming-time matrix-vector multiplication provided by XLiFE++. The method `apply` implemnt multiplication of a LargeMatrix with a block of vector. Noting that it's only a way to implement application of an operator to vector. Depending on specific eigenproblem, we can create a new class with a different approach to apply operator; for example, operator in case of spectral transformation to find the not-well separated eigenvalues.

```
template<typename ScalarType>
class LargeMatrixAdapter : public Operator<ScalarType>
{
private:
    typedef LargeMatrix<ScalarType> LMatrix;
public:
    LargeMatrixAdapter() { lMatrix_p = NULL; }
    LargeMatrixAdapter(LMatrix* p) { lMatrix_p = p; }

    LargeMatrixAdapter& operator=(LMatrix matrix) { lMatrix_p = &matrix; return *this; }


    //! Destructor.
    virtual ~LargeMatrixAdapter() {};

    void apply(const MultiVec<ScalarType>& x, MultiVec<ScalarType>& y) const
    {
        for (int i = 0; i< x.getNumberVecs(); ++i) {
            multMatrixVector(*lMatrix_p, *(x[i]), *(y[i]));
        }
    }
private:
    LMatrix*  lMatrix_p;
};
```

### The `LargeMatrixAdapterInverse` class

Similar to `LargeMatrixAdapter`, this class is simply a wrapper of `LargeMatrix` in order to take advantage of consuming-time matrix-vector multiplication provided by XLiFE++. The class operates on an already factorized matrix to carry out the multiplication of its inverse (if invertible) with a vector. Instead of invoking the function `multMatrixVector`, the method `apply` calls the routine `multInverMatrixVector` of class `LargeMatrix` with the type of factorization.

```
  template<typename MatrixType, typename ScalarType>
  class LargeMatrixAdapterInverse : public Operator<ScalarType>
  {
  private:
      typedef const MatrixType LMatrix;
  public:
//        LargeMatrixAdapterInverse() : lMatrix_p(NULL), fac_(_noFactorization) {}
      LargeMatrixAdapterInverse(LMatrix* p, FactorizationType fac) : lMatrix_p(p), fac_(fac) {}

      LargeMatrixAdapterInverse& operator=(LMatrix matrix) { lMatrix_p = &matrix; fac_ =
          _noFactorization; return (*this); }


      //! Destructor.
      virtual ~LargeMatrixAdapterInverse() {};

      void apply(const MultiVec<ScalarType>& x, MultiVec<ScalarType>& y) const
      {
          for (int i = 0; i< x.getNumberVecs(); ++i) {
              multInverMatrixVector(*lMatrix_p, *(x[i]), *(y[i]), fac_);
```

```
        }
    }

private:
    LMatrix*  lMatrix_p;
    FactorizationType fac_;
};
```

### The `LargeMatrixAdapterInverseGeneralized` class

On some specific eigen problems, it is better to do spectral transformation, especially, to find not well-seperated eigenvalues. This class serves for this purpose. As indicated by its name, this class works mainly for the spectral transformation of generalized eigen problem. The first operation is multiplication of the one matrix with a vector. The vector result is multiplied by the inverse of the second matrix which is provided in a form of factorized one. Both operations are done in the routine `apply`.

```
template<typename MatrixType, typename ScalarType>
class LargeMatrixAdapterInverseGeneralized : public Operator<ScalarType>
{
private:
    typedef const MatrixType LMatrix;
public:
    LargeMatrixAdapterInverseGeneralized(LMatrix* pA, LMatrix* pB, FactorizationType fac) :
        lMatrixA_p(pA), lMatrixB_p(pB), fac_(fac) {}

//      LargeMatrixAdapterInverseGeneralized& operator=(LMatrix matrix) { lMatrix_p = &matrix;
    fac_ = _noFactorization; return (*this); }


    //! Destructor.
    virtual ~LargeMatrixAdapterInverseGeneralized() {};

    void apply(const MultiVec<ScalarType>& x, MultiVec<ScalarType>& y) const
    {
        Vector<ScalarType> vecTemp(x.getVecLength());
        for (int i = 0; i< x.getNumberVecs(); ++i) {
            multMatrixVector(*lMatrixB_p, *(x[i]), vecTemp);
            multInverMatrixVector(*lMatrixA_p, vecTemp, *(y[i]), fac_);
        }
    }

private:
    LMatrix*  lMatrixA_p;
    LMatrix*  lMatrixB_p;
    FactorizationType fac_;
};
```

## 15.2.2 *eigenSparse* framework

*eigenSparse* is organized with a multi-tiered access for eigensolver algorithms. Users have the choice of interfacing at one of two levels: either working at a high-level with a eigensolver manager or working at a low-level directly with an eigensolver.

Consider as an example the block Davidson iteration.

```
Block Davidson Algorithm
Require: Set an initial guess V and H = []
for $iter = 1$ to $iter_{max}$ do
  repeat
    Compute M-orthonormal basis V for [V,H]
    Project A onto V: $\hat{A} = V^H AV$
    Compute selected eigenpairs (Q,Γ) of $\hat{A}$: $\hat{A}Q = Q\Gamma$
    Compute Ritz vectors: $X = VQ$
    Compute residuals: $R = AX - MX\Gamma$
    Precondition the residuals: $H = NR$
    Check convergence and possibly terminate iteration
  until the matrix V is not expandable
  Restart V
end for
```

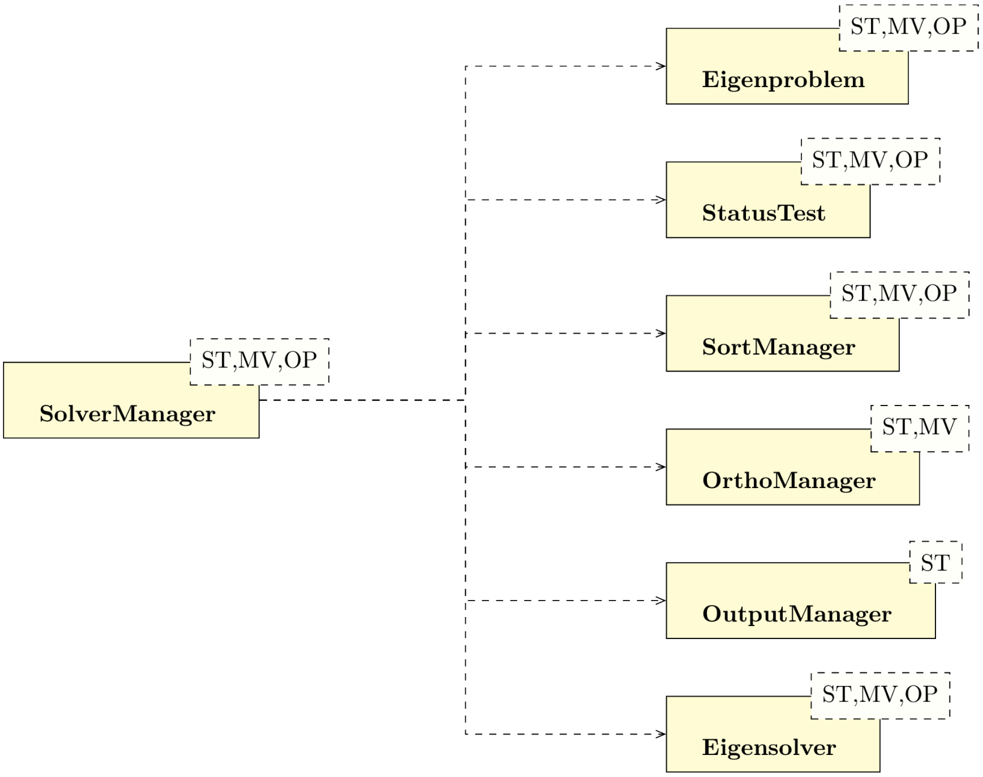


Figure 15.1: **SolverManager** class collaboration graph

The linear operators **A** and **M** define the eigenproblem to be solved. The linear operator **N** is a preconditioner for the problem, and its application to a block of vectors is required. Example preconditioners **N** include the inverse of the diagonal of **A** (Jacobi preconditioner), an algebraic multigrid preconditioner for **A**, or a preconditioned iteration that approximates the solution of a linear set of equations with **A**, e.g., the preconditioned conjugate gradient algorithm.

The *multivector* **V**, **X**, and **R** serve for some purpose. The column-vectors for matrix **V** form the basis for the Rayleigh-Ritz approximation conducted at Step 5-6. We make the specific choice that these vectors are orthonormal with respect to the inner product induced by the Hermitian positive-definite matrix **M**, but this is not a requirement.

The block Davidson eigensolver as described above is useful for examining some of the functionality provided by *eigenSparse*. The algorithm above highlights three levels of functionality. The first level is given by Steps 1-12 that constitute the eigensolver strategy to solve problem (2). The second level is given by Steps 2-10 that form the eigen-iteration. The third level consists of computational steps that can be implemented in a variety of manners, so encouraging modularization. Step 3 requires an orthonormalization method. The decisions involved in Step 5 require a determination of the eigenvalues and invariant subspace of interest, as well as a definition of accuracy. To check convergence in Step 9, several criteria are possible. For instance, a norm induced by a matrix other than **M** may be employed. The restarting of this eigensolver (Step 11) can be performed in a variety of ways and therefore need not be tightly coupled to the eigensolver. Each of these mechanisms provide opportunity for decoupling functionality that need not be implemented in a specific manner.

Looking deeper into the algorithm, the iteration repeats until the basis V is full (in which case it is time to restart) or some stopping criterion has been satisfied. Many valid stopping criteria exist, as well as many different methods for restarting the basis. Both of these, however, are distinct from the essential iteration as described above. A user wanting to perform block Davidson iterations could ask the solver to perform these iterations until a user-specified stopping criterion was satisfied or the basis was full, at which time the user would perform a restart. This allows the user complete control over the stopping criteria and the restarting mechanism, and leaves the eigensolver responsible for a relatively simple bit of state and behavior.

The eigensolvers (encapsulating an iteration and the associated state) are derived classes of the abstract base class `Eigensolver.` The goals of this class are three-fold:

- to define an interface used for checking the status of a solver by a status test;
- to contain the essential iteration associated with a particular eigensolver iteration;
- to contain the state associated with that iteration.

The status tests, assembled to describe a specific stopping criterion and queried by the eigensolver during the iteration, are represented as subclasses of `StatusTest`. The communication between status test and eigensolver occurs inside of the *iterate()* method provided by each `Eigensolver`. This code generally takes the form:

```
SomeEigensolver::iterate() {
while ( statustest.checkStatus(this) != _passed ) {
//
// perform eigensolver iterations
//
}
r
```

Each `StatusTest` provides a method, *checkStatus()*, which through queries to the methods provided by `Eigensolver`, determines whether the solver meets the criteria defined by that particular status test. After a solver returns from *iterate()*, the caller has the option of accessing the state associated with the solver and re-initializing the solver with a new state.

While this method of interfacing with the solver is powerful, it can be tedious. This method requires that user construct a number of support classes, in addition to managing call to *Eigensolver::iterate()*. The `SolverManager` class was developed to address this complaint. A solver manager is a class that wraps around an eigensolver, providing additional functionality while also handling lower-level interaction with the eigensolver that a user may not wish to handle. Solver managers are intended to be easy to use, while still providing the features and flexibility needed to solve real-world eigenvalue problems. For example, the `BlockDavidsonSolMgr` takes only two arguments in its constructor: an `Eigenproblem` specifying the eigenvalue problem to be solved and a `Parameters` of options specific to this solver manager. The solver manager instantiates an eigensolver, along with the status tests and other support classes needed by the eigensolver. To solve the eigenvalue problem, the user simply calls the *solve()* method of the solver manager. The solver manager performs repeated calls to the eigensolver *iterate()* method, performs restarts and locking, and places the final solution into the eigenproblem.

### 15.2.3 *eigenSparse* classes

The following lists and briefly describes the current classes of *eigenSparse*.

### The EigenProblem class

EigenProblem is a container for the components of an eigenvalue problem, as well as the solutions. By requiring eigen problems to derive from EigenProblem, *eigenSparse* defines a minimum interface that can be expected of all eigenvalue problems by the classes that will work with the problems (e.g., eigensolvers and status testers).

```
/*!
 * \class xlifepp::EigenProblem
  \brief This provides a basic implementation for defining standard or
  generalized eigenvalue problems.
*/
  template<class ScalarType, class MV, class OP>
  class EigenProblem
  {
  public:

    //! Empty constructor - allows xlifepp::EigenProblem to be described at a later time through
        "Set Methods".
    EigenProblem();

    //! Standard Eigenvalue Problem Constructor.
    EigenProblem(const SmartPtr<const OP>& Op, const SmartPtr<MV>& initVec);

    //! Generalized Eigenvalue Problem Constructor.
    EigenProblem(const SmartPtr<const OP>& Op, const SmartPtr<const OP>& B, const SmartPtr<MV>&
        initVec);

    //! Copy Constructor.
    EigenProblem(const Eigenproblem<ScalarType, MV, OP>& Problem);

    //! Destructor.
    ~EigenProblem() {};
    ...
```

Both the eigen problem and the eigensolver in *eigenSparse* are templated on the scalar type, the multivector type and the operator type. Before declaring an eigen problem, users must choose classes to represent these entities. Having done so, they can begin to specify the parameters of the eigen problem. The EigenProblem class defines set methods for the parameters of the eigen problem. These methods are:

- setOperator - set the operator for which the eigenvalues will be computed
- setA - set the A operator for the eigenvalue problem $Ax = Mx\lambda$
- setM - set the M operator for the eigenvalue problem $Ax = Mx\lambda$
- setPrec - set the preconditioner for the eigenvalue problem
- setInitVec - set the initial iterate
- setAuxVecs - set the auxiliary vectors, a subspace used to constrain the search space for the solution
- setNEV - set the number of eigenvalues to be computed
- setHermitian - specify whether the problem is Hermitian

In addition to these *set* methods, EigenProblem defines a method setProblem() that gives the class the opportunity to perform any initialization that may be necessary before the problem is handed off to an eigensolver, in addition to verifying that the problem has been adequately defined.

For each of the *set* methods listed above, there is a corresponding *get* function. These are the functions used by eigensolvers and solver managers to get the necessary information from the eigenvalue problem. In addition, there are two methods for storing and retrieving the results of the eigenvalue computation:

```
const EigenSolverSolution & getSolution();
void setSolution(const EigenSolverSolution & sol);
```

In order to verify if all the parameters are set, EigenProblem provide a method isProblemSet()

### The EigenSolverSolution structure

The EigenSolution structure was developed in order to facilitate setting and retrieving of solution data.

```
//!  Struct for storing an eigenproblem solution.
template <class ScalarType, class MV>
struct EigenSolverSolution {
  //! The computed eigenvectors
  SmartPtr<MV> evecs;
  //! An orthonormal basis for the computed eigenspace
  SmartPtr<MV> espace;
  //! The computed eigenvalues
  std::vector<ValueEigenSolver<ScalarType> >  evals;
  /*! \brief An index into evecs to allow compressed storage of eigenvectors for real,
      non-Hermitian problems.
   *
   *  index has length numVecs, where each entry is 0, +1, or -1. These have the following
      interpretation:
   *    - index[i] == 0: signifies that the corresponding eigenvector is stored as the i
      column of evecs. This will usually be the
   *        case when ScalarType is complex, an eigenproblem is Hermitian, or a real,
      non-Hermitian eigen problem has a real eigenvector.
   *    - index[i] == +1: signifies that the corresponding eigenvector is stored in two
      vectors: the real part in the i column of evecs and the <i><b>positive</b></i>
      imaginary part in the i+1 column of evecs.
   *    - index[i] == -1: signifies that the corresponding eigenvector is stored in two
      vectors: the real part in the i-1 column of evecs and the <i><b>negative</b></i>
      imaginary part in the i column of evecs
   */
  std::vector<int>          index;
  //! The number of computed eigenpairs
  int numVecs;

  EigenSolverSolution() : evecs(),espace(),evals(0),index(0),numVecs(0) {}
};
```

All *eigenSparse* solver managers place the results of the computation in the EigenProblem class using an EigenSolverSolution structure. The number of eigen solutions computed is given by field numVecs. The eigenvalues are always stored as two real values, even when templated on a complex data type or when the eigenvalues are real. Similarly, the eigen space can always be represented by a multivector of width numVecs, even for non-symmetric eigen problems over the real field. The storage scheme for eigenvectors requires more finesse.

When solving real symmetric eigen problems, the eigenvectors can always be chosen to be real, and therefore can be stored in a single column of a real multivector. When solving eigenproblems over a complex field, whether Hermitian or non-Hermitian, the eigenvectors may be complex, but the multivector is defined over the complex field, so that this poses no problem. However, real non-symmetric problems can have complex eigenvectors, which prohibits a one-for-one storage scheme using a real multivector. Fortunately, the eigenvectors in this scenario occur as complex conjugate pairs, so the pair can be stored in two real vectors. This permits a compressed storage scheme, which uses an index vector stored in the EigenSolverSolution, allowing conjugate pair eigenvectors to be easily retrieved from evecs. The integers in EigenSolverSolution::index take one of three values: $\{0,+1,-1\}$. These values allow the eigenvectors to be retrieved as follows:

- $index[i] = 0$: the i-th eigenvector is stored uncompressed in column $i$ of evecs

- $index[i] = +1$: the i-th eigenvector is stored compressed, with the real component in column $i$ of evecs and the positive complex component stored in column $i+1$ of evecs
- $index[i] = -1$: the i-th eigenvector is stored compressed, with the real component in column $i$ -1 of evecs and the negative complex component stored in column $i$ of evecs

Because this storage scheme is only required for non-symmetric problems over the real field, all other eigenproblems will result in an index vector composed entirely of zeroes. For the real non-symmetric case, the +1 index will always immediately precede the corresponding -1 index.

### The `EigenSolver` class

The `EigenSolver` class defines the basic interface that must be met by any eigen solver class in *eigenSparse*. The specific eigensolvers are implemented as derived classes of `EigenSolver`. There are two eigen solvers currently implemented in *eigenSparse*

- `BlockDavidson` : A block Davidson solver for Hermitian eigenvalue problems
- `BlockKrylovSchur` : A block Krylov Schur solver for Hermitian or non-Hermitian eigenvalue problems.

The class `EigenSolver`, like `EigenProblem`, is templated on the scalar type, multivector type and operator type. The options for the eigen solver are passed through the constructor, defined by `EigenSolver` to have the following form:

```
template<class ScalarType, class MV, class OP>
class EigenSolver {
  public:

  //! name Constructors/Destructor//{


  //! Default Constructor.
  EigenSolver() {};

  //! Basic Constructor.
  /*! This constructor, implemented by all xlifepp eigensolvers, takes an xlifepp::Eigenproblem,
    xlifepp::SortManager, xlifepp::OutputManager, and Parameters as input.  These
    four arguments are sufficient enough for constructing any xlifepp::EigenSolver object.
  */
  EigenSolver( const SmartPtr<EigenProblem<ScalarType,MV,OP> >& problem,
               const SmartPtr<SortManager<ScalarType> >&        sorter,
               const SmartPtr<OutputManager<ScalarType> >&      printer,
               const SmartPtr<StatusTest<ScalarType,MV,OP> >&   tester,
               const SmartPtr<OrthoManager<ScalarType,MV> >&    ortho,
               Parameters& params );
...
```

These classes are used as follows:

- **problem** - the eigenproblem to be solved; the solver will get the problem operators from here.
- **sorter** - the sort manager selects the significant eigenvalues
- **printer** - the output manager dictates verbosity level in addition to processing output streams
- **tester** - the status tester dictates when the solver should quit iterate() and return to the caller
- **ortho** - the orthogonalization manager defines the inner product and other concepts related to orthogonality, in addition to performing these computations for the solver

- **params** - the parameter list specifies eigensolver-specific options; see the documentation for a list of options support by individual solvers

In addition to specifying an iteration, an eigensolver also specifies a concept of state, i.e. the current data associated with the iteration. After declaring an Eigensolver object, the state of the solver is in an uninitialized state. For most solver, to be initialized mean to be in a valid state, containing all of the information necessary for performing eigen solver iterations.
Eigensolver provides two methods concerning initialization: *isInitialized()* indicates whether the solver is initialized or not, and *initialize()* (with no arguments) instructs the solver to initialize itself using random data or the initial vectors stored in the eigenvalue problem.
To ensure that solvers can be used as efficiently as possible, the user needs access to the state of the solver. To this end, each eigensolver provides low-level methods for getting and setting the state of the solver:

- `getState()` - returns a solver-specific structure with read-only pointers to the current state of the solver.
- `initialize(...)` - accepts a solver-specific structure enabling the user to initialize the solver with a particular state.

The combination of these two methods, along with the flexibility provided by status tests, allows the user almost total control over eigen solver iterations.
Moreover, each eigen solver provides two significant types of methods: status methods and solver- specific state methods. The status methods are defined by the Eigensolver abstract base class and represent the information that a generic status test can request from any eigensolver. A list of these methods is given in following table

| *Method name* | *Description* |
|---|---|
| `getNumIters` | Get the current number of iterations. |
| `getRitzValues` | Get the most recent Ritz values. |
| `getRitzVectors` | Get the most recent Ritz vectors. |
| `getRitzIndex` | Get the Ritz index needed for indexing compressed Ritz vectors. |
| `getResNorms` | Get the most recent residual norms, with respect to the OrthoManager. |
| `getRes2Norms` | Get the most recent residual 2-norms. |
| `getRitzRes2Norms` | Get the most recent Ritz residual 2-norms. |
| `getCurSubspaceDim` | Get the current subspace dimension. |
| `getMaxSubspaceDim` | Get the maximum subspace dimension. |
| `getBlockSize` | Get the block size. |

### The `SolverManager` class

Using *eigenSparse* by interfacing directly with eigensolvers is extremely powerful, but can be tedious. Solver managers provide a way for users to encapsulate specific solving strategies inside of an easy-to-use class. Novice users may prefer to use existing solver managers, while advanced user may prefer to write custom solver managers. `SolverManager` defines only two methods: a constructor accepting an `EigenProblem` and a parameter list of solver manager-specific options; and a `solve()` method, taking no arguments and returning either `_converged` or `_unconverged`. Consider the following example code:

```
// Create an eigen problem
SmartPtr<EigenProblem<ST,MV,OP> > problem =
// Create parameter list to pass into the solver manager
  Parameters pl;
  pl.set("Verbosity", (int)verbosity);
  pl.set("Which", which);
  pl.set("Orthogonalization", ortho);
  pl.set("Block Size", blockSize);
  pl.set("Num Blocks", numBlocks);
  pl.set("Maximum Restarts", maxRestarts);
// Create a solver manager
  BlockDavidsonSolMgr<ST,MV,OP> bdSolverMan(problem, pl);
```

```
// Solve the eigenvalue problem
  ComputationInfo returnCode = bdSolverMan.solve();
// Get the solution from the problem
  EigenSolverSolution<ST,MV> sol = problem->getSolution();
```

As has been stated before, the goal of the solver manager is to create an eigensolver object, along with the support objects needed by the eigensolver. Another purpose of many solver managers is to manage and initiate the repeated calls to the underlying solver's `iterate()` method. For solvers that build a Krylov subspace to some maximum dimension (e.g., `BlockKrylovSchur` and `BlockDavidson`), the solver manager will also assume the task of restarting the solver when the subspace is full. This is something for which multiple approaches are possible. Also, there may be substantial flexibility in creating the support classes (e.g., sort manager, status tests) for the solver. An aggressive solver manager could even go so far as to construct a preconditioner for the eigenvalue problem.
These examples are meant to illustrate the flexibility that specific solver managers may have in implementing the `solve()` routine. Some of these options might best be incorporated into a single solver manager, which takes orders from the user via the parameter list given in the constructor. Some of these options may better be contained in multiple solver managers, for the sake of code simplicity. It is even possible to write solver managers that contain other solvers managers; motivation for something like this would be to select the optimal solver manager at runtime based on some expert knowledge, or to create a hybrid method which uses the output from one solver manager to initialize another one.

### The `StatusTest` class

the purpose of the `StatusTest` should be clear: to give the user or solver manager flexibility in stopping the eigen solver iterations in order to interact directly with the solver.
Many reasons exist for why a user would want to stop the solver from iterating:

- some convergence criterion has been satisfied and it is time to quit;
- some part of the current solution has reached a sufficient accuracy to removed from the iteration ("locking");
- the solver has performed a sufficient or excessive number of iterations.

These are just some commonly seen reasons for ceasing the iteration, and each of these can be so varied in implementation/parametrization as to require some abstract mechanism controlling the iteration.
Below is a list of status tests:

- `StatusTestCombo` - this status test allows for the boolean combination of other status tests, creating near unlimited potential for complex status tests.
- `StatusTestOutput` - this status test acts as a wrapper around another status test, allowing for printing of status information on a call to checkStatus()
- `StatusTestMaxIters` - this status test monitors the number of iterations performed by the solver; it can be used to halt the solver at some maximum number of iterations or even to require some minimum number of iterations.
- `StatusTestResNorm` - this status test monitors the residual norms of the current iterate.
- `StatusTestWithOrdering` - this status test also monitors the residual norms of the current iterate, but only considers the residuals along with a set of auxiliary eigenvalues.

### The SortManager class

The purpose of a sort manager is to separate the eigensolver classes from the sorting functionality required by those classes. This satisfies the flexibility principle sought by *eigenSparse*, by giving users the opportunity to perform the sorting in whatever manner is deemed to be most appropriate. *eigenSparse* defines an abstract class SortManager with two methods, one for sorting real values and one for sorting complex values:

```
// Sorting with real value
virtual void sort(std::vector<MagnitudeType>& evals, SmartPtr<std::vector<int> > perm =
    _smPtrNull, int n = -1) const = 0;
// Sorting with complex value
virtual void sort(std::vector<MagnitudeType>& rEvals,
                          std::vector<MagnitudeType>& iEvals,
                          SmartPtr<std::vector<int> > perm = _smPtrNull,
                           int n = -1) const = 0;
```

### The BasicSort class

The concrete derived class implements sorting scheme for sorting real values and one for sorting complex values.

```
template<class MagnitudeType>
class BasicSort : public SortManager<MagnitudeType>
{
public:
    /*! \brief Parameter list driven constructor

        This constructor accepts a paramter list with the following options:
      - \c "Sort Strategy" - a \c string specifying the desired sorting strategy. See
           setSortType() for valid options.
    */
    BasicSort(Parameters& pl);

    /*! \brief String driven constructor

        Directly pass the string specifying sort strategy. See setSortType() for valid options.
    */
    BasicSort(const String& which = "LM");

    //! Destructor
    virtual ~BasicSort();
    ...
```

By default, sort strategy Largest Magnitude (LM) is used. So as to change the strategy, user can easily specify it with setSortType method.

### The OrthoManager class

Orthogonalization and orthonormalization are commonly performed computations in iterative eigensolvers; in fact, for some eigensolvers, they represent the dominant cost. Different scenarios may require different approaches (e.g, Euclidean inner product versus $M$ inner product, orthogonal projections versus oblique projections). Combined with the plethora of available methods for performing these computations, Anasazi has left as much leeway to the users as possible.
Orthogonalization of multivectors is performed by derived classes of the abstract class OrthoManager that provides five methods:

- innerProd(X,Y,Z) - performs the inner product defined by the manager.
- norm(X) - computes the norm induced by innerProd().

- `project(X,C,Q)` - given an orthonormal basis Q, projects X onto to the space perpindicular to colspan(Q), optionally returning the coefficients of X in Q.

- `normalize(X,B)` - returns an orthonormal basis for colspan(X), optionally returning the coefficients of X in the computed basis.

- `projectAndNormalize(X,C,B,Q)` - computes an orthonormal basis for subspace colspan(X) - colspan(Q), optionally returning the coefficients of X in Q and the new basis.

It should be noted that a call to `projectAndNormalize()` is not necessarily equivalent to a call to `project()` followed by `normalize()`. This follows from the fact that, for some orthogonalization managers, a call to `normalize()` may augment the column span of a rank- deficient multivector in order to create an orthonormal basis with the same number of columns as the input multivector. In this case, the code

```
orthoman.project(X,C,Q);
orthoman.normalize(X,B);
```

could result in an orthonormal basis $X$ that is not orthogonal to the basis in $Q$.
XLIFE++ provides two orthogonalization managers:

- `BasicOrthoManager` - performs orthogonalization using multiple steps of classical Gram-Schmidt.

- `SVQBOrthoManager` - performs orthogonalization using the SVQB orthogonalization technique described by Stathapoulos and Wu

The core function of these orthogonalization managers is `findBasis`, which find an operator-orthonormal basis for a span, with the option of extending the subspace.

### The `OutputManager` class

The output manager exists to provide flexibility with regard to the verbosity of the eigen solver. Each output manager has two primary concerns: what output is printed and where the output is printed to. When working with the output manager, output is classified into one of the following message types:

```
enum MsgEigenType
{
  _errorsEigen = 0,                 /*!< Errors [ always printed ] */
  _warningsEigen = 0x1,               /*!< Internal warnings */
  _iterationDetailsEigen = 0x2,       /*!< Approximate eigenvalues, errors */
  _orthoDetailsEigen = 0x4,           /*!< Orthogonalization/orthonormalization details */
  _finalSummaryEigen = 0x8,          /*!< Final computational summary */
  _timingDetailsEigen = 0x10,         /*!< Timing details */
  _statusTestDetailsEigen = 0x20,     /*!< Status test details */
  _debugEigen = 0x40                 /*!< Debugging information */
};
```

Output manager are subclasses of the abstract base class `OutputManager`. This class provides the following output-related methods:

```
template <class ScalarType>
class OutputManager {
  public:
   ...
  //! Find out whether we need to print out information for this message type.
  /*! This method is used by the solver to determine whether computations are
      necessary for this message type.
  */
  virtual bool isVerbosity(MsgEigenType type) const = 0;

  //! Send output to the output manager.
  virtual void print(MsgEigenType type, const String output) = 0;

  //! Create a stream for outputting to.
  virtual std::ostream& stream(MsgEigenType type) = 0;
...
```

XLIFE++ provides a single output manager, `BasicOutputManager`. This class accepts an output stream from the user. The output corresponding to the verbosity level of the manager is sent to this stream.

### The `SolverUtils` class

Most of the large-scale eigenvalue algorithms exploit projection processes so as to extract approximate eigenvectors from a given subspace. Inside this subspace, a small matrix eigenvalue problem is obtained. XLIFE++ provides `SolverUtils` class, a collection of utilities necessary for the solvers. These utilities include sorting, orthogonalization, projecting/solving local eigen systems,

```
  template<class ScalarType, class MV, class OP>
  class SolverUtils
  {
  public:
    typedef typename NumTraits<ScalarType>::RealScalar MagnitudeType;
    typedef typename NumTraits<ScalarType>::Scalar  SCT;
    typedef MatrixEigenDense<SCT> MatrixDense;

    //! name Constructor/Destructor//{


    //! Constructor.
    SolverUtils();

    //! Destructor.
    virtual ~SolverUtils() {};
    ...
```

In fact, all utilities along with this class make use of functions of *eigenCore*. The most important function of this class is `directSolver`, a routine for computing eigen pairs of Hermitian pencil. This method is heavily used during the projection of vectors into a subspace and normalization of these vector with a specified norm.

## 15.2.4 Examples

The following gives sample code for solving a symmetric eigenvalue problem using the Block Davidson solver manager.
The first step in solving an eigenvalue problem is to define the eigenvalue problem. However, before that, we need to make sure define the operator and the multivector.

```
// Load LargeMatrix from file
LargeMatrix<Real> rMatSym(dataPathTo(rMatrixSym), _dense, 782, _cs, _symmetric);
// Define the operator (in this case, it's LargeMatrix)
SmartPtr< const LargeMatrixAdapter<ST> > K(new LargeMatrixAdapter<ST>(&rMatSym));
// Sometimes, we need a preconditioner to be able to solve the eigenvalue problem
SmartPtr< const LargeMatrixAdapter<ST> > Prec(new LargeMatrixAdapter<ST>(&matPrec));
// Define multivector
SmartPtr<MV> ivec = SmartPtr<MultiVecAdapter<ST> >(new MultiVecAdapter<ST>(rMatSym.nbCols,
    blockSize));
// Initialize the multivector  with random values
ivec->mvRandom();
```

Everything is fine then eigenvalue problem is defined as follow:

```
SmartPtr<EigenProblem<ST,MV,OP> > problem = SmartPtr<EigenProblem<ST,MV,OP> >(new
    EigenProblem<ST,MV,OP>(K,ivec));
// Inform the eigenProblem that the operator cK is symmetric
problem->setHermitian(true);
// Set the number of eigenvalues requested
problem->setNEV(nev);
```

The second step is to specify parameters for the solver manager, depending on algorithm (Block Davidson or Block Krylov Schur), we can have a different parameters. Nevertheless, there are some essential ones to be specified

```
const int nev = 4; //6
int blockSize = 5;//6;
int numBlocks = 5;//14;
int maxRestarts = 25;//8;
Real tol = 1.0e-6;
String which("SM"), ortho("SVQB");
bool locking = true;
bool insitu = false;
MsgEigenType verbosity = _errorsEigen;

Parameters pl;
pl.set("Verbosity", (int)verbosity);
pl.set("Which", which);
pl.set("Orthogonalization", ortho);
pl.set("Block Size", blockSize);
pl.set("Num Blocks", numBlocks);
pl.set("Maximum Restarts", maxRestarts);
pl.set("Convergence Tolerance", tol);
pl.set("Use Locking", locking);
pl.set("Locking Tolerance", tol/10);
pl.set("In Situ Restarting", insitu);
```

Till now, we have all the information needed to declare the solver manager and solve the problem:

```
BlockDavidsonSolMgr<ST,MV,OP> bdSolverMan(problem, pl);
ComputationInfo returnCode = bdSolverMan.solve();
```

The return value of the solver indicate whether the algorithm succeeds or not.(i.e: whether the requested number of eigenpairs were found to a sufficient accuracy (as defined by the solver manager). Output from `solve()` routine in this example might look as follows:

```
BlockDavidson Eigen Solver Test : Standard symmetric matrix test with Smallest Magnitude
------------------------------------------------------------------------------

  Direct residual norms computed
          Eigenvalue          Residual(M)
----------------------------------------
        -1.29891e-06          8.63079e-08
        -1.29973e-06          6.27415e-08
        -1.30048e-06          7.99246e-08
        -1.33992e-06          7.09023e-07
```

# 16 The *arpackppSupport* library

The *arpackppSupport* library contains the interface of XLiFE++ with ARPACK library through ARPACK++. Because of commonality and stability, ARPACK library is chosen as the external eigen solver.

ARPACK is a well known collection of FORTRAN subroutines designed to compute a few eigenvalues and eigenvectors of large scale sparse matrices and pencils. It implements a variant of the Arnoldi process for finding eigenvalues called Implicit restarted Arnoldi method (IRAM) and is capable of solving a great variety of problems from single precision positive definite symmetric problems to double precision complex non-Hermitian generalized problems. ARPACK++ is the C++ an interface of ARPACK.

XLiFE++ offers an interface to ARPACK++ through a well-organized collection of classes which hide all the complexity of ARPACK++. User can easily call an eigen solver like a call to an iterative solver. Moreover, this interface offers advanced users a flexible way to make use of all features of ARPACK++ with a minimum effort by modifying some classes. This package is organized into 2 layers:

- `Users Interface` wraps all ARPACK++ interface and provides simple call prototype to user
- `Arpack++ Interface` is collection of classes interacting directly with ARPACK++

In order to use ARPACK++, ARPACK must be already installed. ARPACK++ package can be found at `http://www.ime.unicamp.br/~chico/arpack++/`. However, because of the deprecation of this version, a patch at `http://reuter.mit.edu/index.php/software/arpackpatch/` needs applied to make sure a correct compilation. The following is organized in "bottom-up", the ARPACK++ interface is described then Users Interface.

## 16.1 ARPACK++ interface layer

ARPACK++ interface is a group of class which is an interface between XLiFE++ and ARPACK++. Each class of this group corresponds to a specific eigen problem with a computational mode.

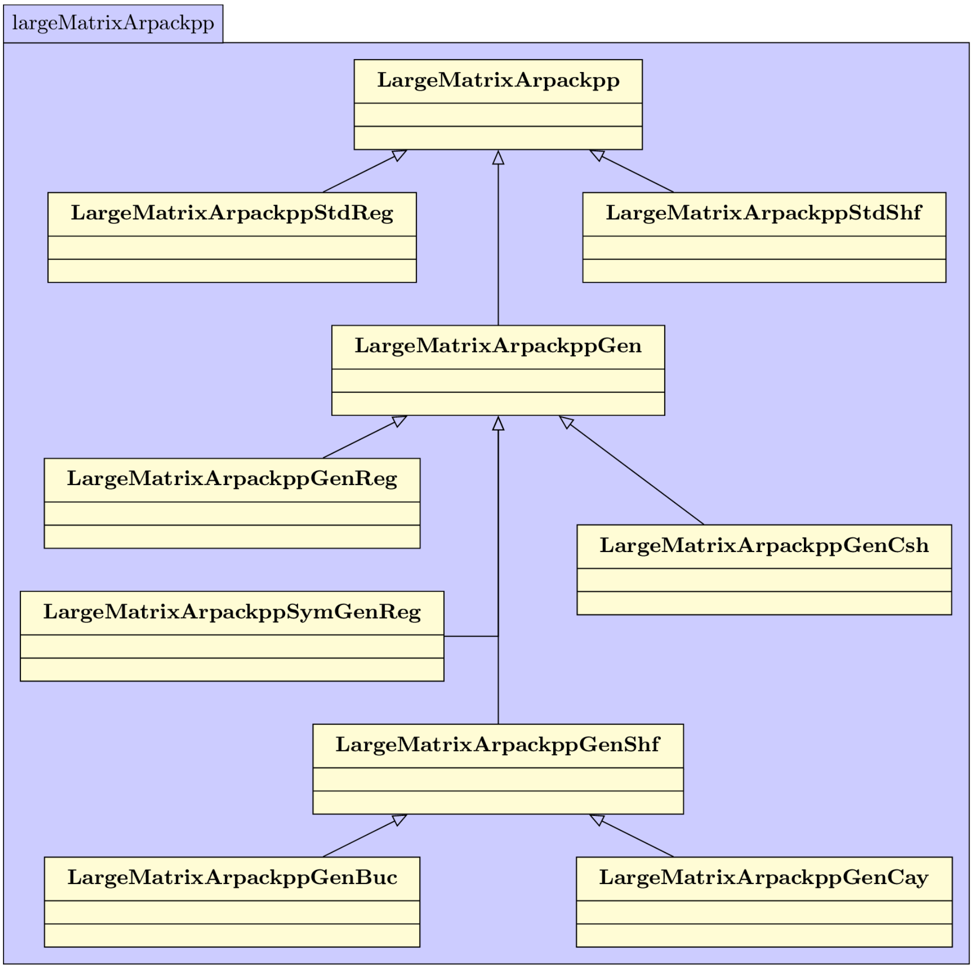

largeMatrixArpackpp
LargeMatrixArpackpp
LargeMatrixArpackppStdReg
LargeMatrixArpackppStdShf
LargeMatrixArpackppGen
LargeMatrixArpackppGenReg
LargeMatrixArpackppGenCsh
LargeMatrixArpackppSymGenReg
LargeMatrixArpackppGenShf
LargeMatrixArpackppGenBuc
LargeMatrixArpackppGenCay

Figure 16.1: Hierarchy of LargeMatrixArpackpp

LargeMatrixArpackpp is an interface class between XLiFE++ and ARPACK++. This class is an abstract base class so that all classes to be used in the program are derived from this one. This class defines some basic properties and methods which are used in all derived classes.

```
template<typename K, class Mat>
class LargeMatrixArpackpp
{
  public:
    LargeMatrixArpackpp(const Mat& matA, const Number sizeProblem);
    LargeMatrixArpackpp(const Mat& matA, const Number sizeProblem, const String name);
    virtual ~LargeMatrixArpackpp();
    virtual void multOPx (K* x, K* y) = 0;
    String kindOfFactorization() const {return factName_;}

  protected:
    const Mat* matA_p;      //< Left hand-side matrix A, generally stiffness matrix (given data)
    Number size_;     //< Size of problem
    String name_;      //< Name of problem
    String factName_;      //< Name of the algorithm used to compute the factorization pointed to by fact_p
    Mat* fact_p;   //<Factorization of matB, matAsI or matAsB in order to speed up linear  systems solving.

  protected:
    void (Mat::*solver_)(std::vector<K>& b, std::vector<K>& x);
    void checkDims(const Mat* mat);
    void factorize(const Mat* mat);
    void bzMultAx(K* x, K* y);      //< Matrix-vector product y <- A * x
    void array2Vector(const K*, std::vector<K>&);      //< Convert array to Vector
    void vector2Array(std::vector<K>&, K*);      //< Convert Vector to Array
}; // end of Class LargeMatrixArpackpp
```

| | |
|---|---|
| library : | **eigenSolvers** |
| header : | |
| implementation : | |
| unitary tests : | **test_EigenSolverArpackpp.hpp** |
| header dependences : | |

### 16.1.1 The `LargeMatrixArpackppStdReg` class

`LargeMatrixArpackppStdReg` class is an interface between XLIFE++ and ARPACK++ designed to enable the use of Arpack++'s own classes for standard problems in regular mode. This class allows XLIFE++ users to solve real symmetric, non-symmetric and complex standard eigen problem in regular mode. This class holds informations of matrices and some methods related to product matrix-vector. In general, only matrix-vector product $y \leftarrow Ax$ is needed.

```
template<typename K, class Mat>
class LargeMatrixArpackppStdReg: public LargeMatrixArpackpp<K, Mat>
{
  public:
    LargeMatrixArpackppStdReg(const Mat& matA, const Number sizeProblem);
    virtual ~LargeMatrixArpackppStdReg() {}
    virtual void multOPx(K* x, K* y);      //< Matrix-vector product y <- A * x

  private:
    //! Duplicating such object is disabled
    LargeMatrixArpackppStdReg(const LargeMatrixArpackppStdReg&);
    LargeMatrixArpackppStdReg& operator=(const LargeMatrixArpackppStdReg&);
}; // end of Class LargeMatrixArpackppStdReg
```

| | |
|---|---|
| library : | **eigenSolvers** |
| header : | |
| implementation : | |
| unitary tests : | **test_EigenSolverArpackpp.hpp** |
| header dependences : | **LargeMatrixArpackpp.hpp** |

### 16.1.2 The `LargeMatrixArpackppStdShf` class

`LargeMatrixArpackppStdShf` class is an interface between XLIFE++ and ARPACK++ designed to enable the use of ARPACK++'s own classes for standard problems in shift and inverse mode. This class allows XLIFE++ users to solve real symmetric, non-symmetric and complex standard eigen problem in shift and inverse mode. This class holds informations of matrices and some methods related to product matrix-vector. In general, we need to provide matrix-vector product $y \leftarrow (A-\sigma I)^{-1}x$. However, thanks to some built-in special solvers of XLIFE++, only $(A-\sigma I)$ is enough.

```
template<typename K, class Mat>
class LargeMatrixArpackppStdShf: public LargeMatrixArpackpp<K, Mat>
{
  public:
    LargeMatrixArpackppStdShf(const Mat& matA, const Number sizeProblem, const K sigma);
    virtual ~LargeMatrixArpackppStdShf();
    virtual void multOPx (K* x, K* y);      //< Matrix-vector product y <- inv(A-sigma*Id) * x
  private:
    const Mat* matAsI_p; //<          A - sigma Id matrix for shift and invert mode in standard
        problems
    bool localAlloc_;      //< flag to indicate if dynamic memory is allocated to store the matrix
        (A - sigma*Id)

    //! Duplicating such object is disabled
    LargeMatrixArpackppStdShf(const LargeMatrixArpackppStdShf&);
    LargeMatrixArpackppStdShf& operator=(const LargeMatrixArpackppStdShf&);
}; // end of Class LargeMatrixArpackppStdShf
```

| | |
|---:|---|
| library : | **eigenSolvers** |
| header : | |
| implementation : | |
| unitary tests : | **test_EigenSolverArpackpp.hpp** |
| header dependences : | **LargeMatrixArpackpp.hpp** |

### 16.1.3 The LargeMatrixArpackppGen class

LargeMatrixArpackppGen is an abstract class which plays a role of an interface between XLIFE++ and ARPACK++ designed to enable the use of ARPACK++'s own classes for generalized eigen problem $Ax = \lambda Bx$. All classes for generalized problem are derived from this one.

```
template<typename K, class Mat>
class LargeMatrixArpackppGen: public LargeMatrixArpackpp<K, Mat>
{
  public:
    LargeMatrixArpackppGen(const Mat& matA, const Mat& matB, const Number sizeProblem);
    LargeMatrixArpackppGen(const Mat& matA, const Mat& matB, const Number sizeProblem, const
        String name);
    virtual ~LargeMatrixArpackppGen() {}
    virtual void multBx (K* x, K* y); //<   Matrix-vector product y <- B * x required for all
        derived classes

  protected:
    const Mat* matB_p; //< Right hand-side matrix B, e.g. mass matrix (given data)
    Mat* matAsB_p; //!< Matrix (A - sigma*B)
    bool localAlloc_; //<     flag to indicate if dynamic memory is allocated to store A - sigma
        B,

  private:
    //! Duplicating such object is disabled
    LargeMatrixArpackppGen(const LargeMatrixArpackppGen&);
    LargeMatrixArpackppGen& operator=(const LargeMatrixArpackppGen&);
}; // end of Class LargeMatrixArpackppGen
```

| | |
|---:|---|
| library : | **eigenSolvers** |
| header : | |
| implementation : | |
| unitary tests : | **test_EigenSolverArpackpp.hpp** |
| header dependences : | **LargeMatrixArpackpp.hpp** |

### 16.1.4 The LargeMatrixArpackppGenReg class

LargeMatrixArpackppGenReg class is interface classes between XLIFE++ and ARPACK++ designed to enable the use of ARPACK++'s own classes for generalized problems in regular mode except for real symmtric generalize problem. This class holds informations of matrices and some methods related to product matrix-vector. In general, we need to provide matrix-vector product $w \leftarrow (B)^{-1}Ax$ and $z \leftarrow Bx$

```
template<typename K, class Mat>
class LargeMatrixArpackppGenReg: public LargeMatrixArpackppGen<K, Mat>
{
  public:
    LargeMatrixArpackppGenReg(const Mat& matA, const Mat& matB, const Number sizeProblem);
    virtual ~LargeMatrixArpackppGenReg() {};
    virtual void multOPx (K* x, K* y);  //< Matrix-vector product y <- inv(B)*A * x

  private:
    //! Duplicating such object is disabled
    LargeMatrixArpackppGenReg(const LargeMatrixArpackppGenReg&);
    LargeMatrixArpackppGenReg& operator=(const LargeMatrixArpackppGenReg&);
}; // end of Class LargeMatrixArpackppGenReg
```

| | |
|---|---|
| library : | **eigenSolvers** |
| header : | |
| implementation : | |
| unitary tests : | **test_EigenSolverArpackpp.hpp** |
| header dependences : | **LargeMatrixArpackppGen.hpp** |

### 16.1.5 The LargeMatrixArpackppSymGenReg class

LargeMatrixArpackppGenReg is basically not different from classLargeMatrixArpackppGenReg except on how the calculation results are returned. Maybe in the future, we don't need this class anymore.

```
template<typename K, class Mat>
class LargeMatrixArpackppSymGenReg: public LargeMatrixArpackppGen<K, Mat>
{
  public:
    LargeMatrixArpackppSymGenReg(const Mat& matA, const Mat& matB, const Number sizeProblem);
    virtual ~LargeMatrixArpackppSymGenReg() {}
    virtual void multOPx (K* x, K* y);  //< Matrix-vector product y <- inv(B)*A * x

  private:
    //! Duplicating such object is disabled
    LargeMatrixArpackppSymGenReg(const LargeMatrixArpackppSymGenReg&);
    LargeMatrixArpackppSymGenReg& operator=(const LargeMatrixArpackppSymGenReg&);
}; // end of Class LargeMatrixArpackppSymGenReg
```

| | |
|---|---|
| library : | **eigenSolvers** |
| header : | |
| implementation : | |
| unitary tests : | **test_EigenSolverArpackpp.hpp** |
| header dependences : | **LargeMatrixArpackppGen.hpp** |

### 16.1.6 The `LargeMatrixArpackppGenShf` class

Class `LargeMatrixArpackppGenShf` is interface between XLiFE++ and ARPACK++ designed to enable the use of ARPACK++'s own classes for generalized problems in shift and invert mode. All classes for generalized problem in relevant shift and invert mode (including Buckling and Cayley) are derived from this one.

```
template<typename K, class Mat>
class LargeMatrixArpackppGenShf: public LargeMatrixArpackppGen<K, Mat>
{
  public:
    LargeMatrixArpackppGenShf(const Mat& matA, Mat& matB, const Number sizeProblem, const K
        sigma, const String name = "Generalized Shift and Invert");
    virtual ~LargeMatrixArpackppGenShf() {}
    virtual void multOPx (K* x, K* y); //< Matrix-vector product y <- inv(A-sigma B)*x

  private:
    //! Duplicating such object is disabled
    LargeMatrixArpackppGenShf(const LargeMatrixArpackppGenShf&);
    LargeMatrixArpackppGenShf& operator=(const LargeMatrixArpackppGenShf&);
}; // end of Class LargeMatrixArpackppGenShf
```

| | |
|---:|:---|
| library : | **eigenSolvers** |
| header : | |
| implementation : | |
| unitary tests : | **test_EigenSolverArpackpp.hpp** |
| header dependences : | **LargeMatrixArpackppGen.hpp** |

### 16.1.7 The `LargeMatrixArpackppGenBuc` class

Class `LargeMatrixArpackppGenBuc` is derived from class `LargeMatrixArpackppGenShf` to solve generalized problems Buckling mode. Two products matrix-vector need provided: $w \leftarrow (A-\sigma B)^{-1}x$ and $z \leftarrow Ax$

```
template<typename K, class Mat>
class LargeMatrixArpackppGenBuc: public LargeMatrixArpackppGenShf<K, Mat>
{
  public:
    LargeMatrixArpackppGenBuc(const Mat& matA, Mat& matB, const Number sizeProblem, const K
        sigma);
    virtual ~LargeMatrixArpackppGenBuc() {}
    virtual void multBx (K* x, K* y);//<  Matrix-vector product y <- A * x

  private:
    //! Duplicating such object is disabled
    LargeMatrixArpackppGenBuc(const LargeMatrixArpackppGenBuc&);
    LargeMatrixArpackppGenBuc& operator=(const LargeMatrixArpackppGenBuc&);
}; // end of Class LargeMatrixArpackppGenBuc
```

| | |
|---:|:---|
| library : | **eigenSolvers** |
| header : | |
| implementation : | |
| unitary tests : | **test_EigenSolverArpackpp.hpp** |
| header dependences : | **LargeMatrixArpackppGen.hpp** |

### 16.1.8 The LargeMatrixArpackppGenCay class

Class LargeMatrixArpackppGenCay is derived from class LargeMatrixArpackppGenShf to solve generalized problems in Cayley mode. Three products matrix-vector need provided: $y \leftarrow (A-\sigma B)^{-1}z$, $w \leftarrow Az$ and $u \leftarrow Bz$

```
template<typename K, class Mat>
class LargeMatrixArpackppGenBuc: public LargeMatrixArpackppGenShf<K, Mat>
{
  public:
    LargeMatrixArpackppGenBuc(const Mat& matA, Mat& matB, const Number sizeProblem, const K
        sigma);
    virtual ~LargeMatrixArpackppGenBuc() {}
    virtual void multBx (K* x, K* y);//<  Matrix-vector product y <- A * x

  private:
    //! Duplicating such object is disabled
    LargeMatrixArpackppGenBuc(const LargeMatrixArpackppGenBuc&);
    LargeMatrixArpackppGenBuc& operator=(const LargeMatrixArpackppGenBuc&);
}; // end of Class LargeMatrixArpackppGenBuc
```

| | |
|---|---|
| library : | **eigenSolvers** |
| header : | |
| implementation : | |
| unitary tests : | **test_EigenSolverArpackpp.hpp** |
| header dependences : | **LargeMatrixArpackppGen.hpp** |

### 16.1.9 The LargeMatrixArpackppGenCsh class

Class LargeMatrixArpackppGenCsh is derived from class LargeMatrixArpackppGen to solve real non-symmetric generalized problem in complex shift and invert mode. Three products matrix-vector need provided: $y \leftarrow (A-\sigma B)^{-1}z$, $w \leftarrow Az$ and $u \leftarrow Bz$

```
template<typename K, class Mat>
class LargeMatrixArpackppGenCsh : public LargeMatrixArpackppGen<K, Mat>
{
  public:
    LargeMatrixArpackppGenCsh(const Mat& matA, Mat& matB, const Number sizeProblem, Complex
        sigma, const char part);
    virtual ~LargeMatrixArpackppGenCsh() {};
    /*!
        Matrix-vector product y <- real(inv(A - sigma*B)) if part = 'R'
                              y <- imag(inv(A - sigma*B)) if part = 'I'
    */
    void virtual multOPx (K* x, K* y);
    void multAx (K* x, K* y); //< Matrix-vector product y <- A * x
  private:
    //! Duplicating such object is disabled
    LargeMatrixArpackppGenCsh(const LargeMatrixArpackppGenCsh&);
    LargeMatrixArpackppGenCsh& operator=(const LargeMatrixArpackppGenCsh&);
}; // end of Class LargeMatrixArpackppGenCsh
```

| | |
|---|---|
| library : | **eigenSolvers** |
| header : | |
| implementation : | |
| unitary tests : | **test_EigenSolverArpackpp.hpp** |
| header dependences : | **LargeMatrixArpackppGen.hpp** |

## 16.2 Users interface layer

User interface contains classes which wrap all ARPACK++ interface layer and provide user a simple prototype. All eigen solvers are invoked by operator(), which is similar to other iterative solvers of *solvers* library. There are two principal classes, each of which solves a specific eigen problem

- `EigenSolverStdArpackpp` for standard eigen problem $Ax = \lambda x$
- `EigenSolverGenArpackpp` for generalized eigen problem $Ax = \lambda Bx$

For each type of eigen problem, input matrix `A` decides the value type (Real or Complex) of eigenvalue and/or eigenvector found. There are three cases corresponding to input matrix `A`: real symmetric, complex and real non-symmetric. For the first two cases, the eigenvalue and/or eigenvector found have the same value type of matrix `A` (i.e: Real if matrix `A` is real symmetric and Complex if matrix `A` is complex). For the real non-symmetric case, eigenvalue and/or eigenvector can be complex. Based on value type of input matrix and output eigenvalue (and/or eigenvector), an operator () can be invoked to solve an eigen problem correctly. There are three prototypes of operator() corresponding to three cases:

- `real symmetric case`: input matrix `A` is real symmetric and output eigenvalues/eigenvectors are real
- `real non-symmetric case`: input matrix `A` is real non-symmetric and output eigenvalues/eigenvectors are complex
- `complex case` : input matrix `A` is complex and output eigenvalues/eigenvectors are complex

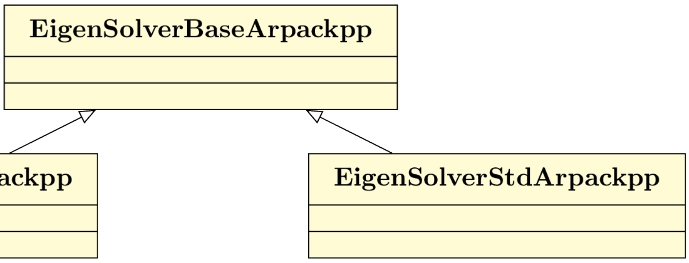


Figure 16.2: `EigenSolverBaseArpackpp` class

### 16.2.1 The `EigenSolverBaseArpackpp` class

The `EigenSolverBaseArpackpp` is the base class which provides some methods to construct object and retrieve eigenvalue/eigenvector returned by ARPACK++. All other wrapper classes are derived from this one.

```
class EigenSolverBaseArpackpp
{
  public:
    EigenSolverBaseArpackpp(const String& nam);
    EigenSolverBaseArpackpp(const String& nam, const Number maxOfIt, const Real epsilon);
    virtual ~EigenSolverBaseArpackpp();
    // Iterative solver name for documentation purposes
    String name() { return name_; }
    // Some functions to extract Eigenvalue and EigenVector returned from Arpack
    // Extract EigenValue and EigenVector
    template<class ArProblem, class EigValue, class EigVector>
    Number extractEigenValueVector(ArProblem& arProb,
                                   EigValue& eigValue, EigVector& eigVector,
                                   Number nev, Number size, bool isReturnVector);

    // Extract EigenValue and EigenVector for non-symmetric problem
    template<class ArProblem, class EigValue, class EigVector>
    Number extractEigenValueVectorNonSym(ArProblem& arProb,
                                          EigValue& eigValue, EigVector& eigVector,
                                          Number nev, Number size, bool isReturnVector);

    // Set some parameters with user-defined value
    template<class ArProblem>
    void setParameters(ArProblem& arProb);
  protected:
    // Extract result EigenVector
    template<typename K, class ArProblem>
    void extractEigenVector(ArProblem& arProb, std::vector<K>& result, Number size, Number idx);

    // Extract result EigenVector of non-symmetric problem
    template<class ArProblem>
    void extractEigenVectorNonSym(ArProblem& arProb, std::vector<Complex>& result, Number size,
        Number idx, bool isNegative, bool isNegativeLeft);
 ...
};
```

### 16.2.2 The EigenSolverStdArpackpp class

The EigenSolverStdArpackpp class enables the use of ARPACK++ to solve the standard eigen problem $Ax = \lambda x$ in all computational modes. Moreover, this class simplifies the post-processing stage, the found eigenvalues/eigenvectors are returned directly to user. However, advanced user can easily customize the some lines of code to get more features of ARPACK++ (e.g Schur vector, etc, ...). There are three prototypes of operator () corresponding to three cases: real symmetric, complex and real non-symmetric.

- Real symmetric:

```
template<class Mat>
Number operator()(Mat& matA, Vector<Real>& eigValue, std::vector<Vector<Real> >& eigVector,
    Number nev, EigenComputationalMode compMode, Real sigma, const char* calMode = "LM")
```

- Real non-symmetric:

```
template<class Mat>
Number operator()(Mat& matA, Vector<Complex>& eigValue, std::vector<Vector<Complex> >& eigVector,
    Number nev, EigenComputationalMode compMode, Complex sigma, const char* calMode = "LM")
```

- Complex:

```
template<class Mat>
Number operator()(Mat& matA, Vector<Complex>& eigValue, std::vector<Vector<Complex> >& eigVector,
    Number nev, EigenComputationalMode compMode, Real sigma, const char* calMode = "LM")
```

If compMode isn't _regular, only largeMatrix with storage of skylineStorage can be used as matrix input.

The operator() returns a value specifying the number of eigenvalues/eigenvectors being have found by ARPACK++. This value is equal or less than the input nev, which determines the number of eigenvalues/eigenvectors which user needs. sigma determines shift value in Shift mode (also in Buckling and Cayley mode). By default, nev eigenvalues with largest magnitude are turned; however, the function can return eigenvalues with smalles magnitude by changing calMode to "SM".
The EigenComputationalMode is enumeration:

```
enum EigenComputationalMode {_regular, _buckling, _cayley, _shiftInv, _cplxShiftInv};
```

In order to solve eigen problem with ARPACK++, it is necessary to define a ARPACK++ problem then link this problem to XLIFE++ through ARPACK++ interface layer (i.e LargeMatrixArpackpp, etc, ...). There are three ARPACK++ classes which are used to define a standard eigen problem: ARSymStdEig, ARNonSymStdEig, ARCompStdEig.

The following functions define ARPACK++ problem and make link to XLIFE++ via ARPACK++ interface layer.

```
template<typename K, class MatArpackpp, class Arpackpp, class Mat, class EigValue, class
    EigVector>
Number regMode(Mat& matA, Number size, Number nev, EigValue& eigValue, EigVector& eigVector,
    const char* calMode);
Number shfInvMode(Mat& matA, Number size, Number nev, K sigma, EigValue& eigValue, EigVector&
    eigVector, const char* calMode);
Number regModeNonSym(Mat& matA, Number size, Number nev, EigValue& eigValue, EigVector&
    eigVector, const char* calMode);
Number shfInvModeNonSym(Mat& matA, Number size, Number nev, K sigma, EigValue& eigValue,
    EigVector& eigVector, const char* calMode);
```

Users can easily customize the parameters of ARPACK++ problem corresponding to their need.

| | |
|---|---|
| library : | **eigenSolvers** |
| header : | |
| implementation : | |
| unitary tests : | **test_EigenSolverArpackpp.hpp** |
| header dependences : | **EigenSolverBaseArpackpp.hpp, LargeMatrixArpackppStdReg.hpp, LargeMatrixArpackppStdShf.hpp** |

### 16.2.3 The EigenSolverGenArpackpp class

The EigenSolverStdArpackpp class enables the use of ARPACK++ to solve the generalized eigen problem $Ax = \lambda Bx$ in all computational modes. Moreover, this class simplifies the post-processing stage, the found eigenvalues/eigenvectors are returned directly to user. However, advanced user can easily customize several lines of code to get more features of ARPACK++ (e.g Schur vector, etc, ...). There are three prototypes of operator () corresponding to three cases: real symmetric, complex and real non-symmetric.

- Real symmetric:

```
template<class Mat>
Number operator()(const Mat& matA, Mat& matB, Vector<Real>& eigValue, std::vector<Vector<Real> >&
    eigVector, Number nev, EigenComputationalMode compMode, Real sigmaR, const char* calMode =
    "LM");
```

- Real non-symmetric:

```
template<class Mat>
Number operator()(const Mat& matA, Mat& matB, Vector<Complex>& eigValue,
    std::vector<Vector<Complex> >& eigVector, Number nev, EigenComputationalMode compMode,
    Complex sigma, const char* calMode = "LM");
```

- Complex:

```
template<class Mat>
Number operator()(const Mat& matA, Mat& matB, Vector<Complex>& eigValue,
    std::vector<Vector<Complex> >& eigVector, Number nev, EigenComputationalMode compMode, Real
    sigmaR, const char* calMode = "LM");
```

- Real non-symmetric with complex shift:

```
template<class Mat>
Number operator()(const Mat& matA, Mat& matB, Vector<Complex>& eigValue,
    std::vector<Vector<Complex> >& eigVector, Number nev, EigenComputationalMode compMode, const
    char mode, Complex sigma, const char* calMode = "LM");
```

If compMode isn't _regular, only largeMatrix with storage of skylineStorage can be used as matrix input.

Having matrix B as an additional input, the operator() of EigenSolverGenArpackpp class is called with the same parameters as the case of EigenSolverStdArpackpp. Moreover, it has one more prototype which is served for real non-symmetric case with complex shift value. Besides the same parameters like other prototypes, it is necessary for user to specify which part of complex shift value:real or imaginary, to use in the shift mode by parameter mode. This input can be 'R' for real part or 'I' for imaginary part of complex shift value sigma. Same as EigenSolverStdArpackpp, it needs to define ARPACK++ problems and link them to XLIFE++. ARSymGenEig, ARNonSymGenEig and ARCompGenEig class are used to define ARPACK++ generalized problem.
The following functions define ARPACK++ problem and make link to XLIFE++ via ARPACK++ interface layer.

```
template<typename K, class MatArpackpp, class Arpackpp, class Mat, class EigValue, class
    EigVector>
Number regMode(const Mat& matA, const Mat& matB, Number size, Number nev, EigValue& eigValue,
    EigVector& eigVector, const char* calMode);
Number regModeNonSym(const Mat& matA, const Mat& matB, Number size, Number nev, EigValue&
    eigValue, EigVector& eigVector, const char* calMode);
Number symShfBucMode(const Mat& matA, Mat& matB, Number size, Number nev, K sigma, const char
    mode, EigValue& eigValue, EigVector& eigVector, const char* calMode);
Number symCaleyMode(const Mat& matA, Mat& matB, Number size, Number nev, K sigma, EigValue&
    eigValue, EigVector& eigVector, const char* calMode);
Number shfMode(const Mat& matA, Mat& matB, Number size, Number nev, K sigma, EigValue& eigValue,
    EigVector& eigVector, const char* calMode);
Number shfModeNonSym(const Mat& matA, Mat& matB, Number size, Number nev, K sigma, EigValue&
    eigValue, EigVector& eigVector, const char* calMode);
Number complexShfInvMode(const Mat& matA, Mat& matB, Number size, Number nev, Real sigmaR, Real
    sigmaI, const char mode, EigValue& eigValue, EigVector& eigVector, const char* calMode);
```

Users can easily customize the parameters of ARPACK++ problem corresponding to their need.

| | |
|---:|:---|
| library : | **eigenSolvers** |
| header : | |
| implementation : | |
| unitary tests : | **test_EigenSolverArpackpp.hpp** |
| header dependences : | **EigenSolverBaseArpackpp.hpp, LargeMatrixArpackppGenReg.hpp, LargeMatrixArpackpp-GenShf.hpp** |

### 16.2.4 Examples

The following matrices and vectors are used for all examples below.

```
const Number rowNum = 20;
const Number colNum = 20;
const Number nev = 15;
const String rMatrixDataSym("rSym20.data");
const String rMatrixDataSymPosDef("rSymPos20.data");
const String rMatrixDataNoSym("rnonSym20.data");
const String cMatrixDataSym("c20.data");
const String cMatrixData("c20b.data");
Vector<Real> rEigValue(colNum);
Vector<Complex> cEigValue(colNum);
std::vector<Vector<Real> > rEigVector(nev, rEigValue);
std::vector<Vector<Complex> > cEigVector(nev, cEigValue);

LargeMatrix<Real> rMatSkylineSym(dataPathTo(rMatrixDataNoSym), _dense, rowNum, colNum, _skyline,
    _sym);
LargeMatrix<Real> rMatSkylineSymSym(dataPathTo(rMatrixDataSym), _dense, rowNum, _skyline,
    _symmetric);

// A trick to make matrix A and matrix B have the same storage (just for testing purpose)
LargeMatrix<Real> rMatPosDefTemp(dataPathTo(rMatrixDataSymPosDef), _dense, rowNum, _skyline,
    _symmetric);
LargeMatrix<Real> rMatPosDefSym(rMatSkylineSymSym);
  for (Number i = 1; i < rowNum + 1; i++)
    for (Number j = 1; j < colNum + 1; j++)
    { rMatPosDefSym(i, j) = rMatPosDefTemp(i, j); }

// Positive definite in real non-symmetric case
LargeMatrix<Real> rMatPosDefNoSymTemp(dataPathTo(rMatrixDataSymPosDef), _dense, rowNum, colNum,
    _skyline, _sym);
LargeMatrix<Real> rMatPosDefNoSym(rMatSkylineSym);
  for (Number i = 1; i < rowNum + 1; i++)
    for (Number j = 1; j < colNum + 1; j++)
    { rMatPosDefNoSym(i, j) = rMatPosDefNoSymTemp(i, j); }

//  Complex Large Matrix
LargeMatrix<Complex> cMatSkylineSymSym(dataPathTo(cMatrixDataSym), _dense, rowNum, _skyline,
    _symmetric);

Real sigma = 10.0;
Complex csigma(-700, 20.0);
EigenSolverStdArpackpp eigenSolverStd;
EigenSolverGenArpackpp eigenSolverGen;
```

#### Standard eigenvalue problem

Real symmetric case

```
// Regular mode
if ( 0 != eigenSolverStd(rMatSkylineSymSym, rEigValue, rEigVector, nev, _regular, sigma) ) {
    out << "Eigenvalue regular mode (Skyline Sym) : " << rEigValue << std::endl;
    out << "Eigenvector regular mode (Skyline Sym) : " << rEigVector << std::endl;
}
// Shift and invert mode
if ( 0 != eigenSolverStd(rMatSkylineSymSym, rEigValue, rEigVector, nev, _shiftInv, sigma) ) {
    out << "Eigenvalue shift and inverse mode :" << rEigValue << std::endl;
    out << "Eigenvalue shift and inverse mode: " << rEigVector << std::endl;
}
```

Real non -symmetric case

```
// Regular mode
if ( 0 != eigenSolverStd(rMatSkylineSym, cEigValue, cEigVector, nev, _regular, sigma)) {
    out << "Eigenvalue regular mode (Skyline Sym) : " << cEigValue << std::endl;
    out << "Eigenvector regular mode (Skyline Sym) : " << cEigVector << std::endl;
 }
//Shift and invert mode
if ( 0 != eigenSolverStd(rMatSkylineSym, cEigValue, cEigVector, nev, _shiftInv, sigma)) {
    out << "Eigenvalue shift and inverse mode (Skyline Sym) :" << cEigValue << std::endl;
    out << "Eigenvalue shift and inverse mode (Skyline Sym): " << cEigVector << std::endl;
}
```

Complex case

```
// Regular mode
if ( 0 != eigenSolverStd(cMatSkylineSymSym, cEigValue, cEigVector, nev, _regular, csigma)) {
    out << "Eigenvalue regular mode (Skyline Sym) : " << cEigValue << std::endl;
    out << "Eigenvector regular mode (Skyline Sym) : " << cEigVector << std::endl;
}
// Shift and invert mode
if ( 0 != eigenSolverStd(cMatSkylineSymSym, cEigValue, cEigVector, nev, _shiftInv, csigma)) {
    out << "Eigenvalue shift and inverse mode (Skyline Sym) : " << cEigValue << std::endl;
    out << "Eigenvector shift and inverse mode (Skyline Sym) : " << cEigVector << std::endl;
}
```

### Generalized eigenvalue problem

Real symmetric case

```
// Regular mode
if ( 0 != eigenSolverGen(rMatSkylineSymSym, rMatPosDefSym, rEigValue, rEigVector, nev, _regular,
     sigma) ) {
    out << "Eigenvalue regular mode (Skyline Sym):" << rEigValue << std::endl;
    out << "Eigenvalue regular mode (Skyline Sym): " << rEigVector << std::endl;
}
// Shift and invert mode
if ( 0 != eigenSolverGen(rMatSkylineSymSym, rMatPosDefSym, rEigValue, rEigVector, nev, _shiftInv,
     sigma) ) {
    out << "Eigenvalue shift and inverse mode (Skyline Sym) :" << rEigValue << std::endl;
    out << "Eigenvalue shift and inverse mode (Skyline Sym) : " << rEigVector << std::endl;
}
// Buckling mode
if ( 0 != eigenSolverGen(rMatPosDefSym, rMatSkylineSymSym, rEigValue, rEigVector, nev, _buckling,
     sigma) ) {
    out << "Eigenvalue buckling mode (Skyline Sym) (positive definite):" << rEigValue <<
         std::endl;
    out << "Eigenvalue buckling mode (Skyline Sym) (positive definite): " << rEigVector <<
         std::endl;
}
// Cayley mode
if ( 0 != eigenSolverGen(rMatSkylineSymSym, rMatPosDefSym, rEigValue, rEigVector, nev, _cayley,
     sigma) ) {
    out << "Eigenvalue cayley mode (Skyline Sym):" << rEigValue << std::endl;
    out << "Eigenvalue cayley mode (Skyline Sym): " << rEigVector << std::endl;
}
```

Real non -symmetric case

```
// Regular mode
if ( 0 != eigenSolverGen(rMatSkylineSym, rMatPosDefSym, cEigValue, cEigVector, nev, _regular,
     sigma) ) {
```

```
    out << "Eigenvalue regular mode  (Skyline Dual) : " << cEigValue << std::endl;
    out << "Eigenvector regular mode (Skyline Dual) : " << cEigVector << std::endl;
}
// Shift and invert mode
if ( 0 != eigenSolverGen(rMatSkylineSym, rMatPosDefNoSym, cEigValue, cEigVector, nev, _shiftInv,
    sigma) ) {
    out << "Eigenvalue shift and inverse mode :" << cEigValue << std::endl;
    out << "Eigenvalue shift and inverse mode: " << cEigVector << std::endl;
}
// Complex shift with real part
if ( 0 != eigenSolverGen(rMatSkylineSym, rMatPosDefNoSym, cEigValue, cEigVector, nev,
    _cplxShiftInv, 'R', csigma) ) {
    out << "Eigenvalue complex shift and inverse mode (Real part) :" << cEigValue << std::endl;
    out << "Eigenvalue complex shift and inverse mode (Real part): " << cEigVector << std::endl;
}
// Complex shift with imaginary part
if ( 0 != eigenSolverGen(rMatSkylineSym, rMatPosDefNoSym, cEigValue, cEigVector, nev,
    _cplxShiftInv, 'I', csigma) ) {
    out << "Eigenvalue complex shift and inverse mode (Imaginary part):" << cEigValue <<
        std::endl;
    out << "Eigenvalue complex shift and inverse mode (Imaginary part): " << cEigVector <<
        std::endl;
}
```

Complex case

```
// Regular mode
if ( 0 != eigenSolverGen(cMatSkylineSymSym, cMatPosDef, cEigValue, cEigVector, nev, _regular,
    csigma)) {
    out << "Eigenvalue regular mode (Skyline Sym) : " << cEigValue << std::endl;
    out << "Eigenvector regular mode (Skyline Sym) : " << cEigVector << std::endl;
}
// Shift and invert mode
if ( 0 != eigenSolverGen(cMatSkylineSymSym, cMatPosDef, cEigValue, cEigVector, nev, _shiftInv,
    csigma, "LM")) {
    out << "Eigenvalue shift and inverse mode (Skyline Sym) : " << cEigValue << std::endl;
    out << "Eigenvector shift and inverse mode (Skyline Sym) : " << cEigVector << std::endl;
}
```

Besides making use of class `EigenSolverStdArpackpp` and class `EigenSolverGenArpackpp`, we can call ARPACK++ problem object directly. However, it's only recommended for advanced users!! The following examples describe how to use ARPACK++ object directly.

```
//1. Create interface object
LargeMatrixArpackppStdReg<Real, LargeMatrix<Real> > intMat(rMatSkylineSymSym, size);

//2. Create Arpack++ problem object
ARSymStdEig<Real, LargeMatrixArpackppStdReg<Real, LargeMatrix<Real> > >  arProb(size, nev,
    &intMat, &LargeMatrixArpackppStdReg<Real, LargeMatrix<Real> >::multOPx, (char *)"LM");

//3. Compute eigenvalues
Int nconv = arProb.FindEigenvalues();

for (Int i = 0; i < nconv; ++i) {
    out << arProb.Eigenvalue(i) << "  ";
}
out << "\n";
//4. Change some parameters
arProb.ChangeNev(nev-2);
arProb.ChangeTol(1.e-6);

nconv = arProb.FindEigenvectors();
```

```
for (Int i = 0; i < nconv; ++i) {
  out << arProb.Eigenvalue(i) << "  ";
}
out << "\n";

//4. Retrieve eigenVector
Real* eigenVec_p = 0;
for (Int i = 0; i < nconv; ++i) {
    eigenVec_p = arProb.RawEigenvector(i);
    out << "Eigenvector [" << i << "] :" ;
    for (Int j = 0; j < size; j++) {
        out <<   *eigenVec_p << "  ";
        eigenVec_p++;
    }
    out << "\n";
}

out << "\n";
```

# 17 The *mathResources* library

The *mathResources* library collects all stuff related to special functions, standard Green's functions, exact solutions and useful numerical tools such as basic quadratures, fast Fourier transform, spline approximations, root finding, ODE solvers.

## 17.1 Some basic numerical tools

Are collected here various basic numerical tools : binomial coefficients, roots of low degree polynomials, simple quadratures, fft, ode solver, random generators.

### 17.1.1 Binomial coefficients and polynomial roots

XLIFE++ provides 3 functions related to binomial coefficients:

```
Number_t binomialCoefficient(int n, int k); // compute C_n^k = = n!/(k!*(n-k)!)
void binomialCoefficients(vector<number_t>& row); // compute n-th row of Pascal binomial
     coefficients
void binomialCoefficientsScaled(vector<real_t>& row); // compute n-th row of Pascal binomial
     coefficients scaled by (n-1)!
```

and functions given roots of polynomials of degree 2, 3 (Cardan formula), 4 (Ferrari formula):

```
vector<complex_t> quadratic(real_t a, real_t b, real_t c);           //roots of degree 2
     polynomial (real)
vector<complex_t> quadratic(complex_t a, complex_t b, complex_t c); //roots of degree 2
     polynomial (complex)
vector<complex_t> cardan(real_t a, real_t b, real_t c, real_t d);    //roots of degree 3
     polynomial (real)
vector<complex_t> cardan(complex_t a, complex_t b, complex_t c, complex_t d);// roots of degree 3
     polynomial (complex)
vector<complex_t> ferrari(real_t a, real_t b, real_t c, real_t d, real_t e); // roots of degree 4
     polynomial
```

### 17.1.2 Basic quadrature methods and FFT

XLIFE++ proposes some useful basic quadrature methods (rectangle, trapeze, Simpson, Laguerre, adaptive trapeze) to compute 1D integrals. They compute integrals of real/complex function either given by a C++ function of the form (T being a real value (float, double, ...) type or a complex type (complex<float>, complex<double>, ...)

```
T f(real_t){...}
T f(real_t,Parameters&){...}
```

or by a vector of values given by an explicit vector or an iterator. So, all the methods are templated by the type T of function values and possibly by a generic iterator (say Iterator).

```
T rectangle(number_t n, real_t h, Iterator itb, T& intg);
T rectangle(const vector<T>& f, real_t h);
T rectangle(T(*f)(real_t), real_t a, real_t b, number_t n);
T rectangle(T(*f)(real_t, Parameters&), Parameters& pars, real_t a, real_t b, number_t n);

T trapz(number_t n, real_t h, Iterator itb, T& intg);
```

```
T trapz(const vector<T>& f, real_t h);
T trapz(T(*f)(real_t), real_t a, real_t b, number_t n);
T trapz(T(*f)(real_t, Parameters&), Parameters& pars, real_t a, real_t b, number_t n);

T simpson(number_t n, real_t h, Iterator itb, T& intg);
T simpson(const vector<T>& f, real_t h);
T simpson(T(*f)(real_t), real_t a, real_t b, number_t n);
T simpson(T(*f)(real_t, Parameters&), Parameters& pars, real_t a, real_t b, number_t n);

T laguerre(T(*f)(real_t), real_t t0, real_t a, number_t nq, vector<real_t>& points,
    vector<real_t>& weights);
T laguerre(T(*f)(real_t,Parameters&), Parameters& pars, real_t t0, real_t a, number_t nq,
    vector<real_t>& points, vector<real_t>& weights);

T adaptiveTrapz(T(*f)(real_t), real_t a, real_t b, real_t eps=1E-6)
T adaptiveTrapz(T(*f)(real_t,Parameters&), Parameters& pars, real_t a, real_t b, real_t eps=1E-6)
```

Note that Laguerre's quadrature uses a table of points and weights created by the function

```
void LaguerreTable(number_t n, std::vector<real_t>& points, std::vector<real_t>& weights);
```

and adaptativeTrapz uses the class

```
template<typename T> class TrapzInterval
{public :
  real_t x1,x2;
  T f1, f2;
  TrapzInterval(real_t a, real_t b, const T& fa, const T& fb)   : x1(a), x2(b), f1(fa), f2(fb) {}
};
```

Besides, some elementary FFT (Fast Fourier Transformation-1d) tools are provided doing the fft or inverse fft of a vector of real/complex values (template T), the number $N$ of values being of the form $2^n$. If not, the number used in fft and ifft is the closest $\tilde{N} = 2^n$ not greater than $N$. This vector of values can be passed either as an explicit vector or an implicit one through an iterator:

```
template<typename IterA, typename IterB>
 void ffta(IterA ita, IterB itb, number_t log2n, real_t q)
 void fft(IterA ita, IterB itb, number_t log2n)
 void ifft(IterA ita, IterB itb, number_t log2n)

template<typename T>
 vector<complex_t> fft(const vector<T>& f);
 vector<complex_t>& fft(const vector<T>& f, vector<complex_t>& g);
 vector<complex_t> ifft(const std::vector<T>& f);
 vector<complex_t>& ifft(const std::vector<T>& f, std::vector<complex_t>& g);

number_t bitReverse(number_t x, int log2n);
```

Implementation of the FFT comes from C++ Cookbook by Jeff Cogswell, Jonathan Turkanis, Christopher Diggins, D. Ryan Stephen.

### 17.1.3 ODE solvers

XLiFE++ provides some ODE solvers : Euler, Runge-Kutta 4 and Runge-Kutta 45 that is an adaptive step time solver based on the Dortmand-Prince method (see http://en.wikipedia.org/wiki/Dormand-Prince_method). All solvers are templated by the type of the state $y \in V$ involved in the first order differential equation:

$$\begin{cases} y'(t) = f(t, y(t)) & t \in ]t_0, t_f[ \\ y(t_0) = y_0 \end{cases}$$

with $f : ]t_0, t_f[ \times V \rightarrow V$ a non stiff function.

ODE solvers are based on template abstract class `OdeSolver` that collects common stuff:

```
template <class T> class OdeSolver
{protected :
  T& (*f_)(real_t, const T&, T&);     // f(t,x) : R x K -> K (K=R, C, Rn, Cn, ...)
  real_t t0_,tf_;          // initial and final time
  real_t dt_;              // time step
  T y0_;                   // initial state
  std::list<std::pair<real_t,T> > tys_;     // list of (time step, state)
  string_t name_;          // name of solver
  public :
  OdeSolver(T& (*f)(real_t, const T&, T&),real_t t0, real_t tf, real_t dt, const T& y0, const
      string_t& na="");
  virtual compute()=0;  //abstract class
  const std::list<std::pair<real_t,T> >& tys() const; // access to (time, state) sequence
  vector<T> states() const; // access to states y
  vector<T> times() const   // access to time step t
  void saveToFile(const string_t& fn) const;
};
```

The user function $f$ may be any C++ function of the form (T any scalar/vector/matrix type):

```
T& f(real_t t, const T& y, T& fty);  //fty the returned value
// for instance, with XLiFE++ common types
Real f(Real t, const Real& y, Real& fty){...; return fty;}                  // real scalar ODE
Complex& f(Real t, const Complex& y, Complex& fty){...; return fty;}        // complex scalar ODE
Reals& f(Real t, const Reals& y, Reals& fty){...; return fty;}              // real vector ODE
Complexes& f(Real t, const Complexes& y, Complexes& fty){...; return fty;} // complex vector ODE
```

Particular solvers are classes inheriting from `OdeSolver` that handle some additional data and provide a constructor and the `compute` function:

```
template <class T> class EulerT : public OdeSolver<T>
{ public :
  EulerT(T& (*f)(real_t, const T&, T&), real_t t0, real_t tf, real_t dt,const T& y0);
  void compute();
};

template <class T> class RK4T : public OdeSolver<T>
{ public :
    RK4T(T& (*f)(real_t, const T&, T&), real_t t0, real_t tf, real_t dt,const T& y0);
    void compute();
};

template <class T> class Ode45T : public OdeSolver<T>
{public :
 real_t a,b,c,d,s;             //coefficients of RK45
 number_t nbTry_;              // number of try when adapting time step
 real_t minScale_, maxScale_;  // min and max scale of time step
 real_t prec_;                 // precision required
 Ode45T(T& (*f)(real_t, const T&, T&), real_t t0, real_t tf, real_t dt,const T& y0, real_t
     prec=1E-6);
 Ode45T(T& (*f)(real_t, const T&, T&), real_t t0, real_t tf, real_t dt,const T& y0,
        number_t nbtry, real_t minscale, real_t maxscale,real_t prec=1E-6)
 void compute();
 real_t rk45(real_t t, T& y, T& yy, real_t dt);  //one step of Runge-Kutta 4-5
};
```

When solving real scalar ODE, the following aliases are available:

```
typedef EulerT<real_t> Euler;
typedef RK4T<real_t> RK4;
typedef Ode45T<real_t> Ode45;
```

In adaptive RK45 method, the time step may grow to becomes very large. To still get a meaningful number of times step, the time step is limited by the initial guess `dt`. Even if the initial guess `dt` is very large, the method should be convergent if the problem is not stiff.

The following example deals with the linear pendulum (ODE of order 2):

```
Real omg=1., th0=pi_/4, thp0=0.;
Reals& f(Real t, const Reals& y, Reals& fyt)
{fyt.resize(2);
 fyt[0]=y[1]; fyt[1]=-omg*omg*y[0];
 return fyt;}
Reals yex(Real t) //exact solution
{Reals yy(2,0.);
 yex[0] = thp0*sin(omg*t)/omg+ th0*cos(omg*t);
 yex[1] = thp0*cos(omg*t)- th0*omg*sin(omg*t);
 return yex;}
...
Real a=0,b=1,dt=0.01, errsup=0;
Reals y0(2,0.);y0[0]=th0; y0[1]=thp0;
list<pair<Real,Reals>> ty = EulerT<Reals>(f,a,b,dt,y0).tys();
for(auto it=ty.begin();it!=ty.end();++it)
    errsup=max(errsup,norm(it->second-yex(it->first)));
theCout<<"Euler : nb dt="<<ty.size()<<" error sup = "<<errsup<<eol;

ty = RK4T<Reals>(f,a,b,dt,y0).tys(); errsup=0.;
for(auto it=ty.begin();it!=ty.end();++it)
    errsup=max(errsup,norm(it->second-yex(it->first)));
theCout<<"RK4   : nb dt="<<ty.size()<<" error sup = "<<errsup<<eol;

ty = Ode45T<Reals>(f,a,b,0.1,y0).tys(); errsup=0.;
for(auto it=ty.begin();it!=ty.end();++it)
   errsup=max(errsup,norm(it->second-yex(it->first)));
theCout<<"Ode45 : nb dt="<<ty.size()<<" error sup = "<<errsup<<eol;
```

As the `compute()` function is called by the constructors, so once the object is created, the field is computed! The previous code gives

```
Euler : nb dt=101 error sup = 0.00393671
RK4   : nb dt=101 error sup = 6.54499e-11
Ode45 : nb dt=12  error sup = 5.25629e-08
```

showing the advantage to use Ode45!

The following end user functions (wrapping ode objects) are also provided:

```
template <typename T>
  Vector<T> euler(T& (*f)(real_t,const T&,T&), real_t a, real_t b, real_t dt, const T& y0);
  Vector<T> rk4(T& (*f)(real_t,const T&,T&), real_t a, real_t b, real_t dt, const T& y0);
  pair<Vector<real_t>,Vector<T> > ode45(T& (*f)(real_t,const T&,T&), real_t a, real_t b,
                                        real_t dt, const T& y0, real_t prec=1.E-6);
```

### 17.1.4 Random generators

XLiFE++ provides two random generators : uniform distribution and normal distribution. When C+11 is available (most of the time), it wraps STL random generators. If not, uniform distribution is based on the standard C random generator (rand) and normal distribution is built from the Box-Muller or Marsaglia methods. The proposed methods address either scalar or vector distribution :

```
template <typename T>
void uniformDistribution(vector<T>& v, real_t a=0., real_t b=1.);
void uniformDistribution(vector<T>& mat, number_t n, number_t m, real_t a=0., real_t b=1.);
vector<T> uniformDistribution(number_t n, real_t a=0., real_t b=1.);
vector<T> uniformDistribution(number_t n, number_t m, real_t a=0., real_t b=1.);
```

```
void normalDistribution(vector<T>& v, real_t mu=0., real_t sigma=1.);
void normalDistribution(vector<T>& mat, number_t n, number_t m, real_t mu=0., real_t sigma=1.);
vector<T> normalDistribution(number_t n, real_t mu=0., real_t sigma=1.);
vector<T> normalDistribution(number_t n, number_t m, real_t mu=0., real_t sigma=1.);
```

These end user functions call effective random generators:

```
//uniform distribution using <random> if C++11 available else using rand();
real_t uniformDistribution(real_t a=0., real_t b=1.);
void uniformDistribution(real_t* mat, real_t a, real_t b,number_t n=1, number_t m=1);
void uniformDistribution(real_t* mat,number_t n=1, number_t m=1);
void uniformDistribution(complex_t* mat, real_t a, real_t b, number_t n=1, number_t m=1);
void uniformDistribution(complex_t* mat, number_t n=1, number_t m=1);

//uniform distribution using C style rand() function
real_t uniformDistributionC(real_t a=0., real_t b=1.);
void uniformDistributionC(real_t* mat, real_t a, real_t b,number_t n=1, number_t m=1);
void uniformDistributionC(real_t* mat,number_t n=1, number_t m=1);
void uniformDistributionC(complex_t* mat, real_t a, real_t b, number_t n=1, number_t m=1);
void uniformDistributionC(complex_t* mat, number_t n=1, number_t m=1);

//normal distribution using <random> if C++11 available else using rand();
real_t normalDistribution(real_t mu=0., real_t sigma=1.,GaussianGenerator gg=_MarsagliaGenerator);
void normalDistribution(real_t* mat, number_t n=1, number_t m=1);
void normalDistribution(real_t* mat, real_t mu, real_t sigma, number_t n=1, number_t m=1);
void normalDistribution(complex_t* mat, real_t mu, real_t sigma, number_t n=1, number_t m=1);
void normalDistribution(complex_t* mat, number_t n=1, number_t m=1);

//normal distribution based on C style rand() function
real_t normalBoxMuller(real_t mu=0., real_t sigma=1.);
real_t normalMarsaglia(real_t mu=0., real_t sigma=1.);
real_t normalDistributionC(real_t mu=0., real_t sigma=1.,GaussianGenerator
    gg=_MarsagliaGenerator);
void normalDistributionC(real_t* mat, real_t mu, real_t sigma, number_t n=1, number_t m=1);
void normalDistributionC(real_t* mat, number_t n=1, number_t m=1);
void normalDistributionC(complex_t* mat, real_t mu, real_t sigma, number_t n=1, number_t m=1);
void normalDistributionC(complex_t* mat, number_t n=1, number_t m=1);
void normalDistributionC(real_t* mat, real_t mu, real_t sigma, GaussianGenerator gg, number_t
    n=1, number_t m=1);
void normalDistributionC(real_t* mat, GaussianGenerator gg, number_t n=1, number_t m=1);
void normalDistributionC(complex_t* mat, real_t mu, real_t sigma, GaussianGenerator gg,number_t
    n=1, number_t m=1);
void normalDistributionC(complex_t* mat, GaussianGenerator gg, number_t n=1, number_t m=1);
```

The random engine has to be initialized before. It is done by the `init()` function of XLiFE++ using `srand()` or the Mersenne Twister 19937 random engine if C++11 is available.

## 17.2 Special functions, Green kernels and exact solutions

XLiFE++ provides some special functions. Some are parts of XLiFE++, others are provided by the AMOS library through a wrapper. Besides, classical Green functions (Helmhotz, Laplace, Maxwell) and exact solutions of scattering problem are proposed.

### 17.2.1 Special functions

Notations of special functions follow the HANDBOOK Of MATHEMATICAL FUNCTIONS, Ed. M.ABRAMOWITZ & I.A. STEGUN. They are computed using either local implementation or the AMOS library that it is provided by default when installing XLiFE++.

### Bessel functions

```
vector<real_t> besselJ0N(real_t x, number_t n);   // internal
real_t     besselJ0(real_t x);                    // internal
real_t     besselJ1(real_t x);                    // internal
real_t     besselJ(real_t x, int_t n);            // internal
complex_t besselJ0(const complex_t& z);           // AMOS
complex_t besselJ1(const complex_t& z);           // AMOS
complex_t besselJ(const complex_t& z, real_t n); // AMOS
real_t     besselJ(real_t x, real_t nu);          // AMOS
complex_t besselJ(const complex_t& z, real_t nu);// AMOS

vector<real_t> besselY0N(real_t x, number_t n);   // internal
... same as J
vector<real_t> besselI0N(real_t x, number_t n);   // internal
... same as J
vector<real_t> besselK0N(real_t x, number_t n);   // internal
... same as J
vector<real_t> besseH10N(real_t x, number_t n);   // internal
... same as J
vector<real_t> besseH20N(real_t x, number_t n);   // internal
... same as J

real_t struveNotH0(real_t x);   // Struve function of order 0, internal
real_t struveNotH1(real_t x);   // Struve function of order 1, internal
pair<real_t, real_t> struveNotH01(real_t x); // returns both H_0(x) and H_1(x), internal

// spherical Bessel function, of first and second kind for 0..N
vector<real_t> sphericalbesselJ0N(real_t x, number_t N);
vector<real_t> sphericalbesselY0N(real_t x, number_t N);
```

### Airy functions

```
complex_t airy(real_t x, DiffOpType d=_id);           // Ai(x) or Ai'(x), AMOS
complex_t airy(const complex_t& z, DiffOpType d=_id);// Ai(z) or Ai'(z), AMOS
complex_t biry(real_t x, DiffOpType d=_id);           // Bi(x) or Bi'(x), AMOS
complex_t biry(const complex_t& z, DiffOpType d=_id);// Bi(z) or Bi'(z), AMOS
```

### Exponential integral

$$E1(z) = \int_z^\infty t^{-1} e^{-t} dt = -\gamma - log(z) + \sum_{n>0} \frac{(-z)^n}{nn!}.$$

```
complex_t e1z(const complex_t& z);    // return E1(z)
complex_t eInz(const complex_t& z);   // return E1(z) + gamma + log(z)
complex_t expzE1z(const complex_t&); // return exp(z)*E1(z)
complex_t zexpzE1z(const complex_t&);// return z*exp(z)*E1(z)
complex_t ascendingSeriesOfE1(const complex_t& z);    // ascending series in E1  (small z)
complex_t continuedFractionOfE1(const complex_t& z); // continued fraction in E1 (large z)
```

### Erf function

The erf function

$$\operatorname{erf} z = \frac{2}{\sqrt{\pi}} \int_0^z e^{-t^2} dt$$

is available from

```
complex_t erf(complex_t z);
```

that wraps erf stuff coming from libcerf (https://jugit.fz-juelich.de/mlz/libcerf) developped by Steven G. Johnson and Joachim Wuttke.

### Gamma function

$$\Gamma(z) = \int_0^\infty t^{z-1} e^{-t} dt \text{ for } Re(z) > 0$$

with $\Gamma(1-z) = \dfrac{\pi}{\sin(\pi z)\Gamma(z)}$, $\Gamma(z+1) = z\Gamma(z)$ and $\Gamma(n+1) = n!$ for integer $n > 0$.

```
real_t gammaFunction(int_t n);              // return Gamma(n) = (n-1)!
real_t gammaFunction(real_t);               // return Gamma(x) for x > 0
complex_t gammaFunction(const complex_t&);  // return Gamma(z) for re(z) > 0
real_t logGamma(real_t);                    // return Log(Gamma(x))
complex_t logGamma1(const complex_t&);      // return Log(Gamma(z))
complex_t logGamma(const complex_t&);       // Paul Godfrey's Lanczos implementation
real_t diGamma(int_t n);                    // return -gamma + sum_1^{n-1} 1/n
real_t diGamma(real_t);                     // return dx Log(Gamma(x)) for x > 0
complex_t diGamma(const complex_t&);        // return dz Log(Gamma(z)) for re(z) > 0
```

### Polynomials

See http://en.wikipedia.org/wiki for definition of following polynomials :

```
void chebyshevPolynomials(real_t, vector<real_t>&);
void gegenbauerPolynomials(real_t lambda, real_t, vector<real_t>&);
void jacobiPolynomials(real_t a, real_t b, real_t, vector<real_t>&);
void jacobiPolynomials01(real_t a, real_t b, real_t, vector<real_t>&);
void legendrePolynomials(real_t, vector<real_t>&);
void legendrePolynomialsDerivative(real_t, vector<real_t>&);
void legendreFunctions(real_t, vector<vector<real_t> >& Pml);
void legendreFunctionsDerivative(real_t,const vector<vector<real_t>>&,vector<vector<real_t>>&);
```

## 17.2.2 Green kernels

XLIFE++ provides kernel (Green function) for Laplace and Helmholtz problems in 2D or 3D and Maxwell problem in 3D. For each problem, the functions computing the kernel and its derivatives are available and a build function constructing the related Kernel object is also provided. We detail the case of Helmholtz Green function, other kernels being similar.

### Helmholtz kernels

The 2D Helmholtz kernel in free space is :

$$K(x,y) = \frac{i}{4} H_0^{(1)}(k|x-y|)$$

where $H_0^{(1)}$ is the Hankel function of the first kind of order 0. Its implementation is the following

```
Kernel Helmholtz2dKernel(Parameters& = defaultParameters);      // construct a Helmholtz2d kernel
Kernel Helmholtz2dKernelReg(Parameters& = defaultParameters);   // construct a Helmholtz2d kernel
     regular part
Kernel Helmholtz2dKernelSing(Parameters& = defaultParameters);  // construct a Helmholtz2d kernel
     singular part
Kernel Helmholtz2dKernel(const real_t& k);          // construct a Helmholtz2d kernel from real k
void initHelmholtz2dKernel(Kernel&, Parameters&);  // initialize kernel data
// computation functions
complex_t Helmholtz2d(const Point& x, const Point& y, Parameters& pa = defaultParameters);
                         // value
```

```
Vector<complex_t> Helmholtz2dGradx(const Point& x, const Point& y, Parameters& pa =
    defaultParameters);      // gradx
Vector<complex_t> Helmholtz2dGrady(const Point& x, const Point& y, Parameters& pa =
    defaultParameters);      // grady
Matrix<complex_t> Helmholtz2dGradxy(const Point& x, const Point& y, Parameters& pa =
    defaultParameters);     // gradxy
complex_t Helmholtz2dNxdotGradx(const Point& x, const Point&y, Parameters& pa =
    defaultParameters);          // nx.gradx
complex_t Helmholtz2dNydotGrady(const Point& x, const Point&y, Parameters& pa =
    defaultParameters);          // ny.grady
complex_t Helmholtz2dReg(const Point& x, const Point& y, Parameters& pa = defaultParameters);
                  // reg value
Vector<complex_t> Helmholtz2dGradxReg(const Point& x, const Point& y, Parameters& pa =
    defaultParameters);  // reg gradx
Vector<complex_t> Helmholtz2dGradyReg(const Point& x, const Point& y, Parameters& pa =
    defaultParameters);  // reg grady
Matrix<complex_t> Helmholtz2dGradxyReg(const Point& x, const Point& y, Parameters& pa =
    defaultParameters); // reg gradxy
complex_t Helmholtz2dSing(const Point& x, const Point& y, Parameters& pa = defaultParameters);
                 // sing value
Vector<complex_t> Helmholtz2dGradxSing(const Point& x, const Point& y, Parameters& pa =
    defaultParameters); // sing gradx
Vector<complex_t> Helmholtz2dGradySing(const Point& x, const Point& y, Parameters& pa =
    defaultParameters); // sing grady
Matrix<complex_t> Helmholtz2dGradxySing(const Point& x, const Point& y, Parameters& pa =
    defaultParameters);// sing gradxy
```

`reg` and `sing` versions are required when computing integral involving $x = y$ case and using particular integration method (see Quadrature). The pseudo Kernel constructors call the `initHelmholtz2dKernel` function that associates computing functions to the Kernel object:

```
void initHelmholtz2dKernel(Kernel& K, Parameters& pars)
{
 K.dimPoint=2;
 K.name="Helmholtz 2D kernel";
 K.shortname="Helmz2D";
 K.singularType = _logr;
 K.singularOrder = 1;
 K.singularCoefficient= -over2pi_;
 K.symmetry=_symmetric;
 K.userData.push(pars);
 K.kernel = Function(Helmholtz2d, 2,K.userData);
 K.gradx = Function(Helmholtz2dGradx, 2, K.userData);
 K.grady = Function(Helmholtz2dGrady, 2, K.userData);
 K.gradxy = Function(Helmholtz2dGradxy, 2, K.userData);
 K.ndotgradx = Function(Helmholtz2dNxdotGradx, 2, K.userData);
 K.ndotgrady = Function(Helmholtz2dNydotGrady, 2, K.userData);
 K.singPart = new Kernel(Helmholtz2dKernelSing(pars));
 K.regPart = new Kernel(Helmholtz2dKernelReg(pars));
}
```

This function shows how to proceed to create a new kernel type. But, to use the Helmholtz kernel it is sufficient to build the Kernel object:

```
Kernel H2d = Helmholtz2dKernel(k);
```

Besides the free space kernel, XLiFE++ provides the 2D Helmholtz kernel in half-space and the 2D Helmholtz kernel in the strip $]-\infty,+\infty[\times]0,h[$:

```
Kernel Helmholtz2dHalfPlaneKernel(real_t k, real_t t1=1., real_t t2=0., real_t a=0., real_t b=0.,
                                  BoundaryCondionType bct=_Dirichlet);
Kernel Helmholtz2dStripKernel(BoundaryCondionType bct, real_t k, real_t h=1.,
                              number_t n=1000, real_t l=-1., real_t e=1.E-6);
```

Only Dirichlet or Neumann boundary condition are handled. In case of the strip, $n$ is the maximum of terms in the modal expansion used to compute the kernel.

The Helmholtz kernel in 3d free space

$$K(x,y)=\frac{e^{ik|x-y|}}{4\pi|x-y|}$$

is also available:

```
Kernel Helmholtz3dKernel(const real_t& k);     // construct a Helmholtz3d kernel from real k
Kernel Helmholtz3dKernel(const complex_t& k);  // construct a Helmholtz3d kernel from complex k
```

### Laplace kernels

The Laplace kernels in 2d and 3d free space are given by

$$K(x,y)=\frac{\log(|x-y|}{2\pi} \text{ and } K(x,y)=\frac{1}{4\pi|x-y|}$$

and can be constructed using:

```
Kernel Laplace2dKernel(Parameters& pars = defaultParameters);
Kernel Laplace3dKernel(Parameters& pars = defaultParameters);
```

For the moment, they do not provide singular and regular parts!

### Maxwell kernel

Only the 3D free space kernel is available :

$$K(x,y)=H_k(x,y)\mathbb{I}_3+\frac{1}{k^2}\text{Hess}\big(H_k(x,y)-H_{k\sqrt{s}}(x,y)\big)$$

where $H_k$ is the 3d Helmholtz kernel. $s$ is a regularization parameter (0 by default and means no regularization):

```
Kernel Maxwell3dKernel(const real_t& k, const real_t& s=0);
Kernel Maxwell3dKernel(const complex_t& k, const real_t& s=0);
```

### 17.2.3 Exact solutions

## 17.3 Spline

Generally speaking, a spline is a piecewise polynomial curve that approaches, in a sense to be specified, an ordered list of points. The simplest spline is the spline of degree 1 (linear spline) which connects the points by segments. There are various way to construct splines. We focus here on quadratic spline (C1-spline), Hermite cubic spline (C2-spline) , Catmull-Row spline, B-spline and nurbs. The first ones are interpolation splines while the last ones are approximation splines but also be designed to interpolate some points .

The stuff presented here is quite standard and can be found in several documents available on the web, for instance : *Courbes B-Spline* (Pansu 2004), *Spline Methods* (Lych,Morken 2008), *Controlling the interpolation of nurbs curves and surfaces* (Lockyer 2006).

In the following we consider the vectors $(t_i)_{0\le i\le n}$ and $(y_i)_{0\le i\le n}$. We set

$$h_i=t_i-t_{i-1},\ 1\le i\le n.$$

We are looking for a piecewise polynomial function, say $q$, such that $q(t_i)=y_i$ for $0\le i\le n$.

### 17.3.1 Quadratic and cubic interpolation spline

For each interval $[t_{i-1}, t_i]$ $(1 \le i \le n)$, we define the quadratic polynomial

$$\begin{array}{ll} q_i(t) & = a_i + b_i(t - t_{i-1}) + c_i(t - t_{i-1})^2 \\ q_i'(t) & = b_i + 2\,c_i(t - t_{i-1}) \\ q_i''(t) & = 2\,c_i \end{array}$$

Imposing the matching of values $y_i$ at $t_i$ $(i = 0, n)$ and the C1 matching at $t_i$ $(i = 1, n-1)$:

$$\begin{array}{ll} q_i(t_{i-1}) = y_{i-1} \text{ and } q_i(t_i) = y_i & \text{for } i = 1, n \\ q_i'(t_i) = q_{i+1}'(t_i) & \text{for } i = 1, n-1 \end{array}$$

gives

$$\left|\begin{array}{ll} b_i + b_{i+1} = \dfrac{2}{h_i}(y_i - y_{i-1}) & \text{for } i = 1, n-1 \\ a_i = y_{i-1} & \text{for } i = 1, n \\ c_i = \dfrac{1}{h_i^2}(y_i - y_{i-1} - h_i b_i) & \text{for } i = 1, n \end{array}\right. \tag{17.1}$$

say a linear system of $3n-1$ equations. As there is $n$ quadratic polynomials to be found ($3n$ unknown coefficients), it remains one free coefficient that can be fixed in various ways:

- given derivative $y_0'$ at first end point : $q_1'(t_0) = b_1 = y_0'$, leading to the linear system

$$\begin{bmatrix} 1 & & & \\ 1 & 1 & & \\ & \ddots & \ddots & \\ & & 1 & 1 \end{bmatrix} \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{bmatrix} = \begin{bmatrix} y_0' \\ \frac{2}{h_1}(y_1 - y_0) \\ \vdots \\ \frac{2}{h_{n-1}}(y_{n-1} - y_{n-2}) \end{bmatrix}$$

- given derivative $y_n'$ at last end point : $q_n'(t_n) = b_n + 2\,c_n h_n = y_n' \Rightarrow b_n = \dfrac{2}{h_n}(y_n - y_{n-1}) - y_n'$, leading to the linear system

$$\begin{bmatrix} 1 & 1 & & \\ & \ddots & \ddots & \\ & & 1 & 1 \\ & & & 1 \end{bmatrix} \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{bmatrix} = \begin{bmatrix} \frac{2}{h_1}(y_1 - y_0) \\ \vdots \\ \frac{2}{h_{n-1}}(y_{n-1} - y_{n-2}) \\ \frac{2}{h_n}(y_n - y_{n-1}) - y_n' \end{bmatrix}$$

- $b_n = 0 \Rightarrow q_n'(t_n) = \dfrac{2}{h_n}(y_n - y_{n-1})$ meaning the derivative is twice the slope of the last segment

$$\begin{bmatrix} 1 & 1 & & \\ & \ddots & \ddots & \\ & & 1 & 1 \\ & & & 1 \end{bmatrix} \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{bmatrix} = \begin{bmatrix} \frac{2}{h_1}(y_1 - y_0) \\ \vdots \\ \frac{2}{h_{n-1}}(y_{n-1} - y_{n-2}) \\ 0 \end{bmatrix}$$

- periodic derivative : $q_1'(t_0) = q_n'(t_n) \Rightarrow b_1 + b_n = \dfrac{2}{h_n}(y_n - y_{n-1})$

$$\begin{bmatrix} 1 & 1 & & \\ & \ddots & \ddots & \\ & & 1 & 1 \\ 1 & & & 1 \end{bmatrix} \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{bmatrix} = \begin{bmatrix} \frac{2}{h_1}(y_1 - y_0) \\ \vdots \\ \frac{2}{h_{n-1}}(y_{n-1} - y_{n-2}) \\ \frac{2}{h_n}(y_n - y_{n-1}) \end{bmatrix}$$

Note that it is not possible to impose both derivatives at end points! The first linear system can be solved by a straight forward loop and the second and third one by a straight backward loop. But the last linear system requires more loops (LU factorization or Gauss reduction).
Following the same approach, for each interval $[t_{i-1}, t_i]$ $(1 \leq i \leq n)$, we define the cubic polynomial

$$\begin{aligned}
q_i(t) &= a_i + b_i(t - t_{i-1}) + c_i(t - t_{i-1})^2 + d_i(t - t_{i-1})^3 \\
q_i'(t) &= b_i + 2\,c_i(t - t_{i-1}) + 3\,d_i(t - t_{i-1})^2 \\
q_i''(t) &= 2\,c_i + 6\,d_i(t - t_{i-1}) \\
q_i'''(t) &= 6\,d_i
\end{aligned}$$

Now impose the matching of values $y_i$ at $t_i$ $(i = 0, n)$ and the C2 matching at $t_i$ $(i = 1, n-1)$:

$$\begin{aligned}
q_i(t_i) = q_{i+1}(t_i) &\longrightarrow \quad y_{i-1} + b_i h_i + c_i h_i^2 + d_i + h_i^3 = y_i \\
q_i'(t_i) = q_{i+1}'(t_i) &\longrightarrow \quad b_i + 2\,c_i h_i + 3 d_i h_i^3 = b_{i+1} \\
q_i''(t_i) = q_{i+1}''(t_i) &\longrightarrow \quad 2\,c_i + 6\,d_i h_i = 2\,c_{i+1}
\end{aligned}$$

The two first relations give

$$\left|\begin{aligned}
c_i &= 3\frac{y_i - y_{i-1}}{h_i^2} - \frac{2\,b_i + b_{i+1}}{h_i} \\
d_i &= 2\frac{y_{i-1} - y_i}{h_i^3} + \frac{b_i + b_{i+1}}{h_i^2}
\end{aligned}\right. \tag{17.2}$$

and writing the second derivative matching $(i = 1, n-1)$:

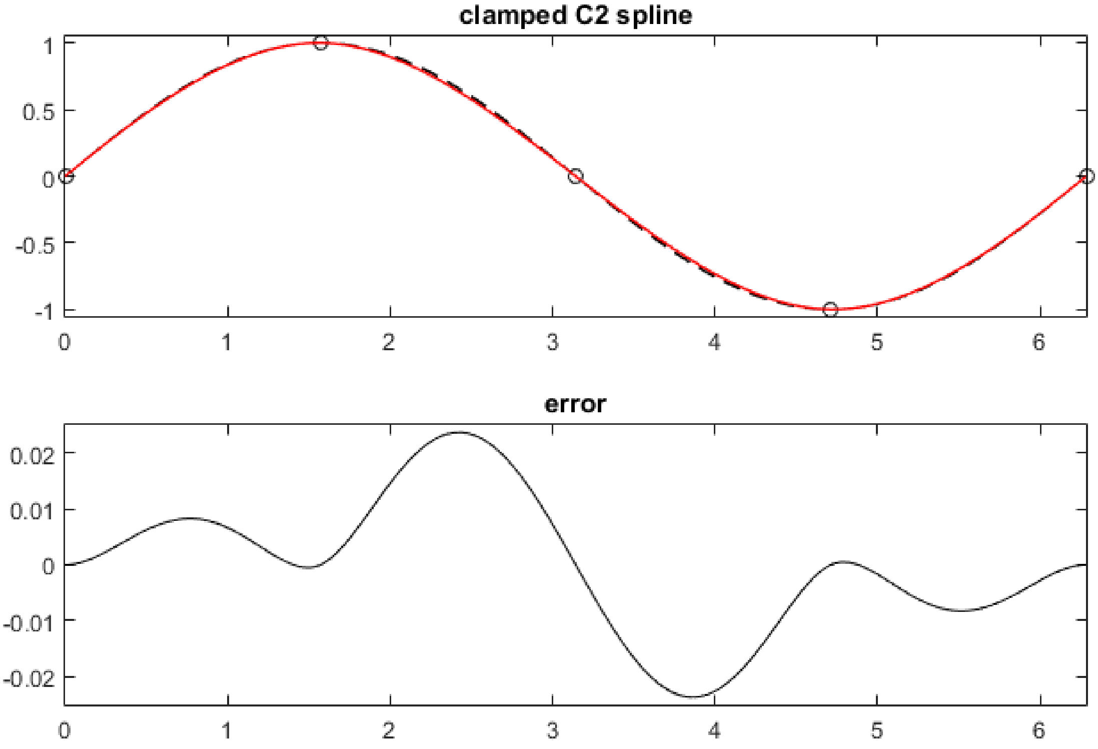
$$h_{i+1} b_i + 2(h_i + h_{i+1}) b_{i+1} + h_i b_{i+2} = \frac{3}{h_i h_{i+1}}\left(h_i^2(y_{i+1} - y_i) + h_{i+1}^2(y_i - y_{i-1})\right)$$

where $b'_{n+1} = q'_n(t_n)$. It is a linear system of $n-1$ equations with $n+1$ unknowns. Two more equations are required to close it. Usual choices are

- clamped spline : $b_1 = y'_0$, $b_{n+1} = y'_n$ leading to the linear system

$$\begin{bmatrix}
1 & 0 & & & & & \\
h_2 & h_{1,2} & h_1 & & & & \\
 & \ddots & \ddots & \ddots & & & \\
 & & h_{i+1} & h_{i,i+1} & h_i & & \\
 & & & \ddots & \ddots & \ddots & \\
 & & & & h_n & h_{n-1,n} & h_{n-1} \\
 & & & & & 0 & 1
\end{bmatrix}
\begin{bmatrix}
b_1 \\ b_2 \\ \vdots \\ b_i \\ \vdots \\ b_n \\ b_{n+1}
\end{bmatrix}
=
\begin{bmatrix}
y'_0 \\
\frac{3}{h_1 h_2}\left(h_1^2(y_2 - y_1) + h_2^2(y_1 - y_0)\right) \\
\vdots \\
\frac{3}{h_i h_{i+1}}\left(h_i^2(y_{i+1} - y_i) + h_{i+1}^2(y_i - y_{i-1})\right) \\
\vdots \\
\frac{3}{h_{n-1} h_n}\left(h_{n-1}^2(y_n - y_{n-1}) + h_n^2(y_{n-1} - y_{n-2})\right) \\
y'_n
\end{bmatrix}$$

  where $h_{i,j} = 2(h_i + h_j)$.

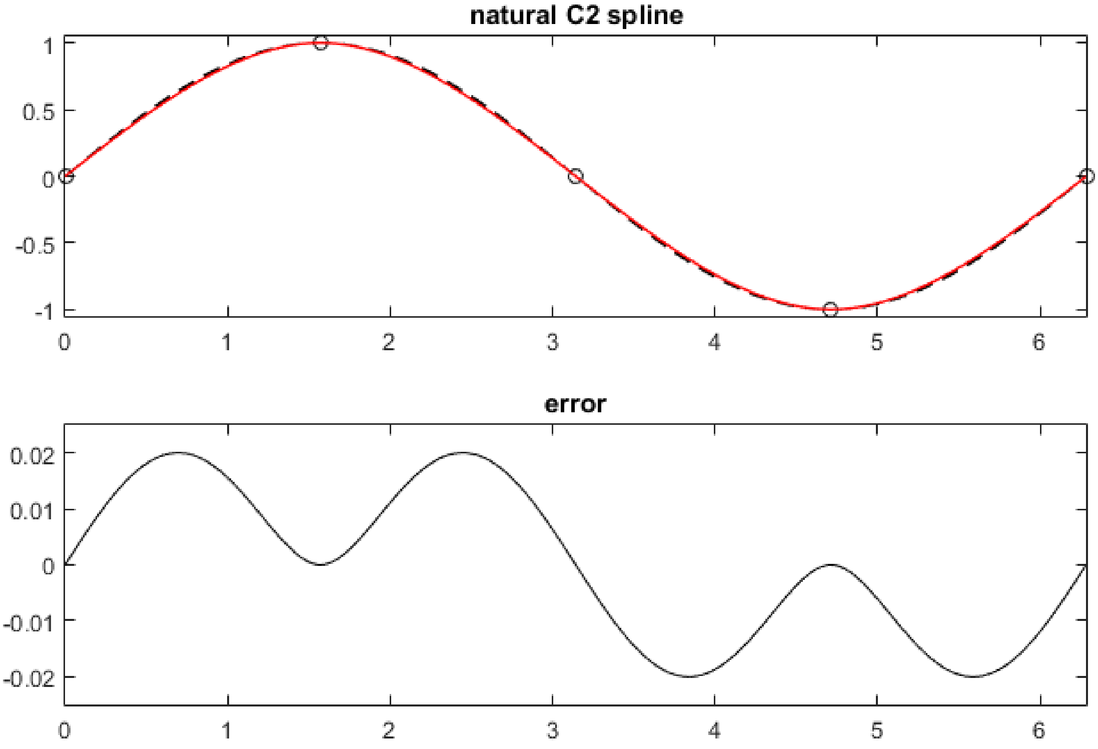


- natural spline : $q_1''(t_0) = q_n''(t_n) = 0$ that reads

$$h_1(2b_1 + b_2) = 3(y_1 - y_0) \text{ and } h_n(b_n + 2b_{n+1}) = 3(y_n - y_{n-1})$$

leading to the linear system

$$\begin{bmatrix} 2h_1 & h_1 & & & & & \\ h_2 & h_{1,2} & h_1 & & & & \\ & \ddots & \ddots & \ddots & & & \\ & & h_{i+1} & h_{i,i+1} & h_i & & \\ & & & \ddots & \ddots & \ddots & \\ & & & & h_n & h_{n-1,n} & h_{n-1} \\ & & & & & h_n & 2h_n \end{bmatrix} \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_i \\ \vdots \\ b_n \\ b_{n+1} \end{bmatrix} = \begin{bmatrix} 3(y_1 - y_0) \\ \frac{3}{h_1 h_2}\left(h_1^2(y_2 - y_1) + h_2^2(y_1 - y_0)\right) \\ \vdots \\ \frac{3}{h_i h_{i+1}}\left(h_i^2(y_{i+1} - y_i) + h_{i+1}^2(y_i - y_{i-1})\right) \\ \vdots \\ \frac{3}{h_{n-1} h_n}\left(h_{n-1}^2(y_n - y_{n-1}) + h_n^2(y_{n-1} - y_{n-2})\right) \\ 3(y_n - y_{n-1}) \end{bmatrix}$$

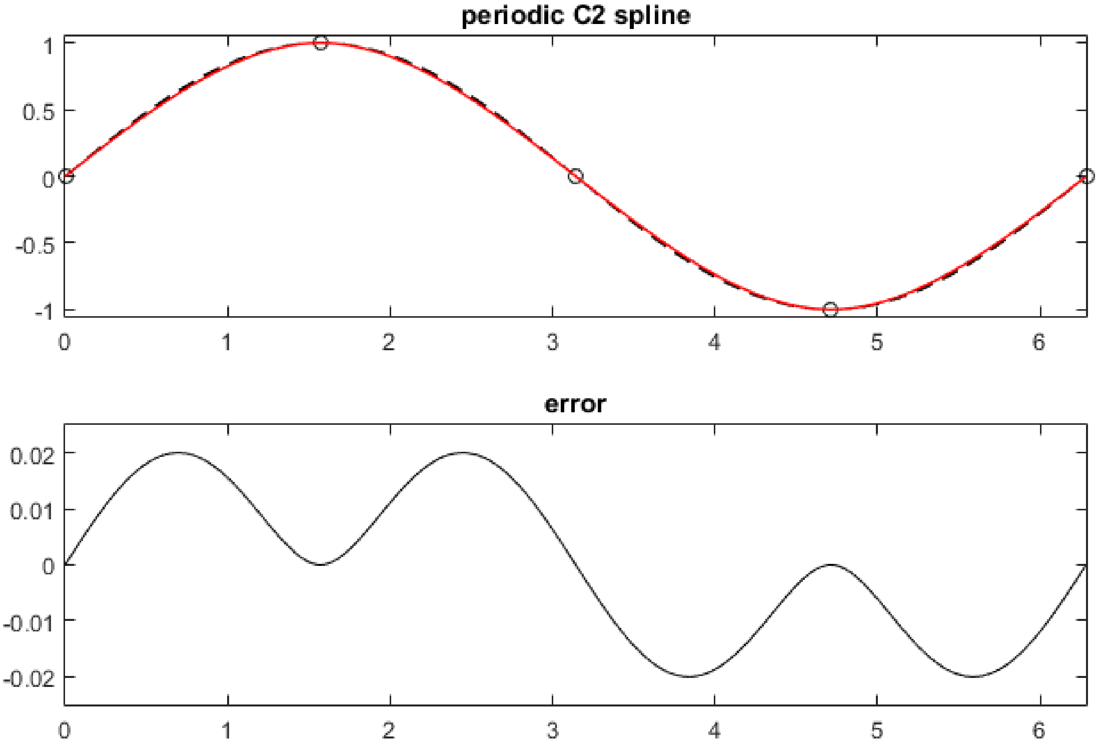


- periodic spline : $q_1'(t_0) = q_n'(t_n)$ and $q_1''(t_0) = q_n''(t_n)$ that reads

$$b_1 = b_{n+1}, \text{ and } h_n(2b_1 + b_2) + h_1(b_n + 2b_{n+1}) = 3\frac{h_n}{h_1}(y_1 - y_0) + 3\frac{h_1}{h_n}(y_n - y_{n-1})$$

leading to the modified linear system

$$\begin{bmatrix} 2h_n & h_n & & & & h_1 & 2h_1 \\ h_2 & h_{1,2} & h_1 & & & & \\ & \ddots & \ddots & \ddots & & & \\ & & h_{i+1} & h_{i,i+1} & h_i & & \\ & & & \ddots & \ddots & \ddots & \\ & & & & h_n & h_{n-1,n} & h_{n-1} \\ 1 & & & & & & -1 \end{bmatrix} \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_i \\ \vdots \\ b_n \\ b_{n+1} \end{bmatrix} = \begin{bmatrix} 3\frac{h_n}{h_1}(y_1 - y_0) + 3\frac{h_1}{h_n}(y_n - y_{n-1}) \\ \frac{3}{h_1 h_2}\left(h_1^2(y_2 - y_1) + h_2^2(y_1 - y_0)\right) \\ \vdots \\ \frac{3}{h_i h_{i+1}}\left(h_i^2(y_{i+1} - y_i) + h_{i+1}^2(y_i - y_{i-1})\right) \\ \vdots \\ \frac{3}{h_{n-1} h_n}\left(h_{n-1}^2(y_n - y_{n-1}) + h_n^2(y_{n-1} - y_{n-2})\right) \\ 0 \end{bmatrix}$$



### Interpolating points in $\mathbb{R}^2$ or $\mathbb{R}^3$

Let us consider now an ordered list of $n+1$ points, say $(P_i)_{0\le i\le n}$ and the following parametrization:

$$t_0 = 0 \text{ and } t_i = t_{i-1} + \|P_i - P_{i-1}\|,\ i = 1, n.$$

If $\mathscr{S}(\mathscr{X},\mathscr{T})$ denotes a 1D spline related to the set $\mathscr{X} = (x_i)_{i=0,n}$, $\mathscr{T} = (t_i)_{i=0,n}$, the spline in $\mathbb{R}^2$ or $\mathbb{R}^3$ will be defined as:

$$Q(t) = (\mathscr{S}(\mathscr{P}_1, T)(t), \mathscr{S}(\mathscr{P}_2, T)(t), \mathscr{S}(\mathscr{P}_3, T)(t))$$

where $\mathscr{P}_k = (P_i^k)_{i=0,n}$ with $P_i^k$ the $k^{th}$ coordinate of the point $P_i$.

### 17.3.2 Catmull-Rom spline

Let us associate a set of tangent vectors $(T_i)_{0\le i\le n}$ to the set of points $(P_i)_{0\le i\le n}$. All the methods presented here are local (moving a point or a tangent vector will modify only the curve in the neighborhood of the point) but there are no longer $C^2$ but only $C^1$!

To construct a curve interpolating $P_i$ at $x_i$ with tangent $T_i$, let us introduce the Hermite polynomials

$$h_{00}(t) = 2t^3 - 3t^2 + 1,\ h_{10}(t) = t^3 - 2t^2 + t,\ h_{01}(t) = -2t^3 + 3t^2,\ h_{11}(t) = t^3 - t^2$$

and the polynomials, $i = 0, n-1$

$$Q_i(x) = h_{00}(t)P_i + h_{10}(t)(x_{i+1} - x_i)T_i + h_{01}(t)P_{i+1} + h_{11}(t)(x_{i+1} - x_i)T_{i+1},\ \ t = \frac{x - x_i}{x_{i+1} - x_i}\ \ x \in [x_i, x_{i+1}].$$

By construction, $Q_i$ is the unique cubic polynomial such that $Q_i(x_i) = P_i$, $Q_i(x_{i+1}) = P_{i+1}$, $Q_i'(x_i) = T_i$, $Q_i'(x_{i+1}) = T_{i+1}$. Obviously, the curve is $C^1$

Different choices to approximate the tangent vectors are available:

- Finite differences : $\begin{cases} T_i = & \frac{1}{2}\left(\frac{P_{i+1}-P_i}{x_{i+1}-x_i}+\frac{P_i-P_{i-1}}{x_i-x_{i-1}}\right),\ i=1,n-1 \\ T_0 = & \frac{1}{2}\frac{P_1-P_0}{x_1-x_0} \\ T_n = & \frac{1}{2}\frac{P_n-P_{n-1}}{x_n-x_{n-1}} \end{cases}$

- Cardinal spline : $T_i = (1-\tau)\dfrac{P_{i+1}-P_{i-1}}{x_{i+1}-x_{i-1}}, i = 1, n-1,$
  where $\tau$ is a tension factor. $\tau = 0$ corresponds to the standard Catmull-Rom spline.

The Catmull-Rom spline may be generalized using the following process. Let us define for each $(P_{i-1}, P_i, P_{i+1}, P_{i+2}),\ i = 1, n-1$

$$t_0 = 0 \text{ and } t_{j+1} = t_j + \left\|P_{i-1+j} - P_{i+j}\right\|^{\alpha},\ j = 0,2 \text{ with } \alpha \in [0,1],$$

$$A_i^1 = \frac{t_1-t}{t_1-t_0}P_{i-1} + \frac{t-t_0}{t_1-t_0}P_i,\ \ A_i^2 = \frac{t_2-t}{t_2-t_1}P_i + \frac{t-t_1}{t_2-t_1}P_{i+1},\ \ A_i^3 = \frac{t_3-t}{t_3-t_2}P_{i+1} + \frac{t-t_2}{t_3-t_2}P_{i+2}$$

$$B_i^1 = \frac{t_2-t}{t_2-t_0}A_i^1 + \frac{t-t_0}{t_2-t_0}A_i^2,\ \ B_i^2 = \frac{t_3-t}{t_3-t_1}A_i^2 + \frac{t-t_1}{t_3-t_1}A_i^3$$

$$Q_i(t) = \frac{t_2-t}{t_2-t_1}B_i^1 + \frac{t-t_1}{t_2-t_1}B_i^2,\ t \in [t_1, t_2].$$

The standard choices of $\alpha$ are:

- $\alpha = 0$ : the standard Catmull-Rom spline,

- $\alpha = 1$ : the chordal Catmull-Rom spline,

- $\alpha = \frac{1}{2}$ : the centripetal Catmull-Rom spline.

The centripetal Catmull-Rom spline has some good properties : there is no self-intersection, cusp will never occur and it follows the control points in a better way.

Catmull-Rom spline may be constructed in a compact way using the following formula:

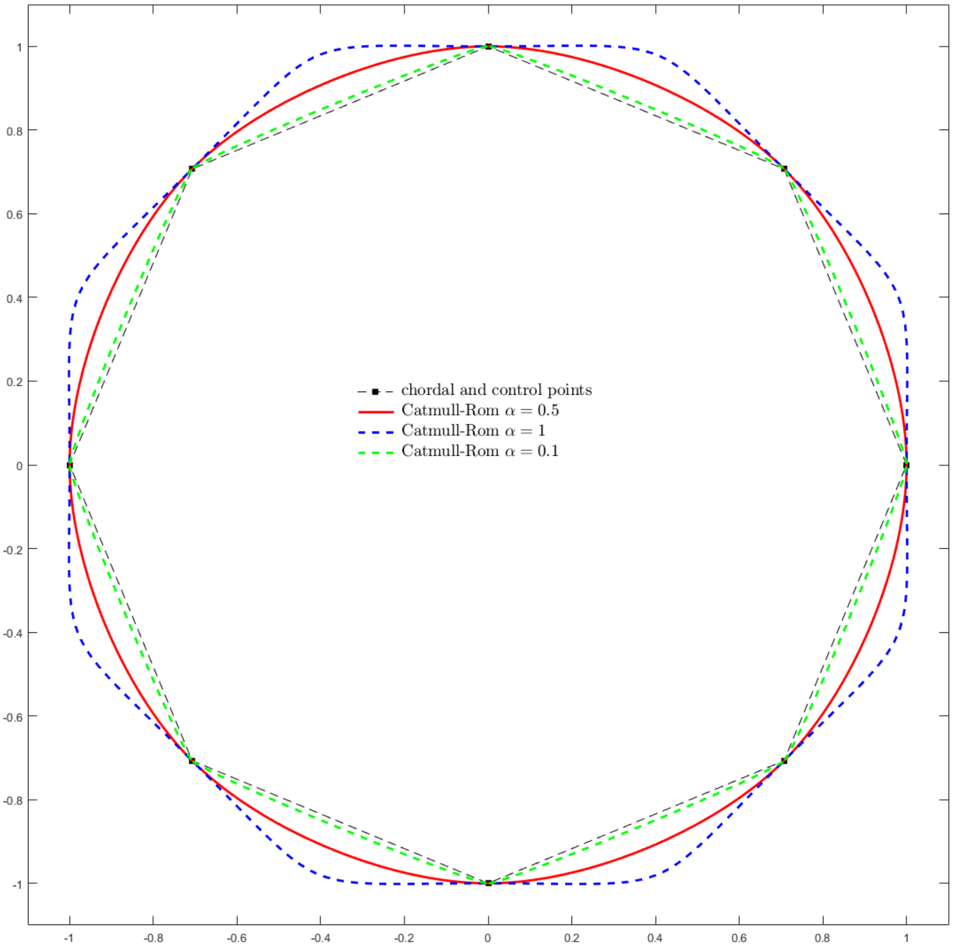
$$Q(t) = \begin{bmatrix} 1 & t & t^2 & t^3 \end{bmatrix} \begin{bmatrix} 0 & 1 & 0 & 0 \\ -\alpha & 0 & \alpha & 0 \\ 2\alpha & \alpha-3 & 3-2\alpha & -\alpha \\ -\alpha & 2-\alpha & \alpha-2 & \alpha \end{bmatrix} \begin{bmatrix} P_{i-1} \\ P_i \\ P_{i+1} \\ P_{i+2} \end{bmatrix}$$

$$Q'(t) = \begin{bmatrix} 0 & 1 & 2t & 3t^2 \end{bmatrix} \begin{bmatrix} 0 & 1 & 0 & 0 \\ -\alpha & 0 & \alpha & 0 \\ 2\alpha & \alpha-3 & 3-2\alpha & -\alpha \\ -\alpha & 2-\alpha & \alpha-2 & \alpha \end{bmatrix} \begin{bmatrix} P_{i-1} \\ P_i \\ P_{i+1} \\ P_{i+2} \end{bmatrix}$$

To close a curve add the two last points at the beginning and the two first points at the end:

$$(P_1\ P_2\ P_3\ \ldots P_{n-2}\ P_{n-1}\ P_n) \longrightarrow (P_{n-1}\ P_n\ \ P_1\ P_2\ P_3\ \ldots P_{n-2}\ P_{n-1}\ P_n\ \ P_1\ P_2)$$

and build Catmull-Rom spline on segments $[P_n, P_1],\ [P_1, P_2],\ \ldots,\ [P_{n-2}, P_{n-1}],\ [P_{n-1}, P_n]$.



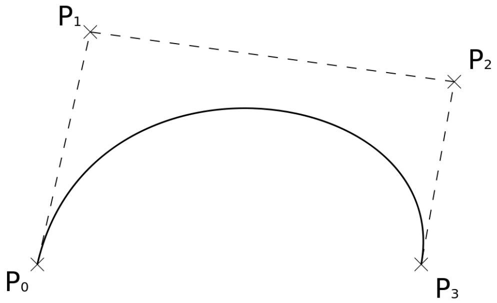
### 17.3.3 B-Spline

For the set of control points $(P_i)_{0\leq i\leq n}$, the **Bezier curve** is defined by

$$Q(t) = \sum_{i=0}^{n} B_i^n(t)P_i \ \text{ for } t \in [0,1]$$

where $B_i^n = C_n^i\, t^i(1-t)^{n-i}$ are the Bernstein polynomials ($\sum_{i=0}^{n} B_i^n = 1$). There are the following properties

- $Q(0) = P_0$ and $Q(1) = P_n$ but the curve does not interpolate the interior points $(P_1,\ldots,P_{n-1})$,
- $\overrightarrow{P_0P_1}$ (resp. $\overrightarrow{P_{n-1}P_n}$) is a tangent vector to the curve at $P_0$ (resp. $P_n$),
- the curve is inside the convex hull of the control points,
- the curve is $C^\infty$.



The **B-spline** curve is a generalization of the Bezier curve. Let $t_0 \le t_1 \cdots \le t_m$ a set of $m+1$ knots and the B-spline functions of degree $k$ defined by recurrence:

$$\begin{array}{ll} \text{for } 0 \le i \le m-1 & B_{i,0}(t) = \begin{cases} 1 & t_i \le t < t_{i+1} \\ 0 & \text{else} \end{cases} \\ \text{for } k \ge 1,\ 0 \le i \le m-k-1 & B_{i,k}(t) = \dfrac{t-t_i}{t_{i+k}-t_i} B_{i,k-1}(t) + \dfrac{t_{i+k+1}-t}{t_{i+k+1}-t_{i+1}} B_{i+1,k-1}(t) \end{array}$$

with the convention $\frac{\bullet}{0} = 0$.
The B-spline functions have a lot of properties, in particular

- $B_{i,k}$ is a polynomial of order $k$ on intervals $[t_j, t_{j+1}]$ with support $[t_i, t_{i+k+1}]$,
- $0 < B_{i,k}(t) < 1$ for $t \in ]t_i, t_{i+k+1}]$,
- $B_{i,k}$ is $C^\infty$ at right and is $C^{k-r}$ at knots of multiplicity $r$

For the set of $n+1$ control points $P_0, P_1, \ldots, P_n$ and the set of knots $t_0 \le t_1 \cdots \le t_m$ with $m \ge n+k+1$, the B-spline curve is defined by

$$Q(t) = \sum_{i=0}^{n} B_{i,k}(t) P_i \ \text{ for } t_k \le t \le t_{n+1}.$$

The B-spline curve is inside the convex hull of the control points, it is $C^{k-1}$ if all the knots are of multiplicity 1, moving a point $P_i$ induces a modification of the points related to the interval $[t_i, t_{i+k}]$. A Bezier curve is a B-Spline with a knots vector of the form [0,0,...0,1,1,...1].

To clamp the curve at $P_0$ choose $t_0 = t_1 \cdots = t_k < t_{k+1}$ and to close the curve duplicate the $k+1$ first points at the end of the set of points.

To compute a point on the B-spline, previous formula or the DeBoor's algorithm may be used:

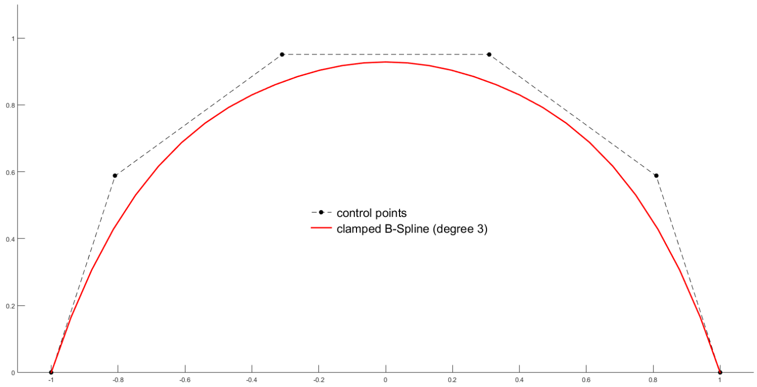
```
• $P_0, P_1, \ldots, P_n$ , $t_0 \le t_1 \cdots \le t_m$, $k$, $t$ given
• find $i$ such that $t_i \le t < t_{i+1}$
• for $j = i-k, k$ set $P_j^0 = P_j$
• for $\ell = 1, k$ do
    for $j = i, i-k+\ell$ (step $-1$) do
        $\alpha_j^\ell = \dfrac{t-t_j}{t_{j+k+1-\ell}-t_j}$ and $P_j^\ell = (1-\alpha_j^\ell)P_{j-1}^{\ell-1} + \alpha_j^\ell P_j^{\ell-1}$
• return $P_i^k$
```

Hereafter, a C++ recursive implementation of the De Boor algorithm using a `Point` class:

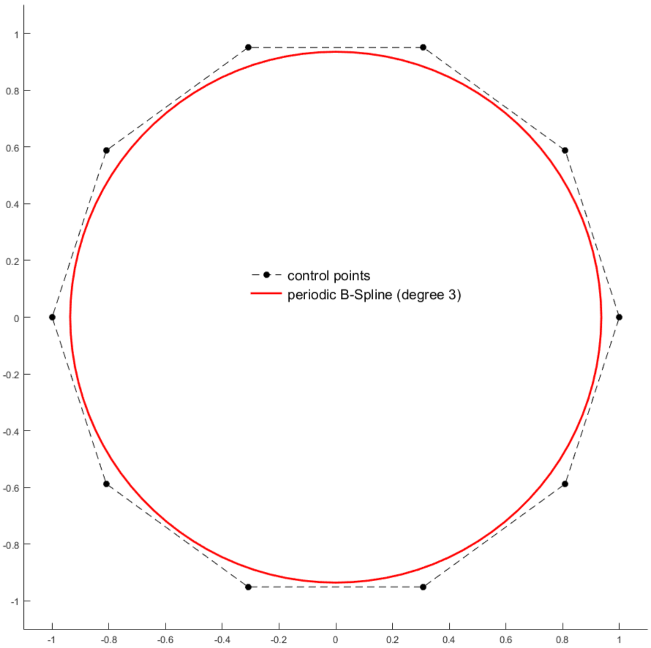
```
Point deBoor(int k,int degree, int i, double x, vector<double>& knots,
             vector<Point>& ctrlPoints)
{if( k == 0) return ctrlPoints[i];
 double alpha = (x-knots[i])/(knots[i+degree+1-k]-knots[i]);
 return  deBoor(k-1,degree,i-1,x,knots,ctrlPoints)*(1-alpha)
       + deBoor(k-1,degree,i,x,knots,ctrlPoints)*alpha ;
}
```

Note that the computation of B-shape functions $(B_{i,k})$ may be done in an efficient way by restricting the computation to four indexes around $i$. That gives an algorithm as fast as DeBoor algorithm! Besides, using the elegant recursive de Boor algorithm may not be so efficient in C++, because the construction of temporary points in the stack!

• Clamped B-spline of degree 3 with 5 control points and knots [0,0,0,0,1,2,3,3,3,3] plotted on [0,3]:



- Periodic B-spline of degree 3 with 10 control points and knots [0,1,2,3,4,5,6,7,8,9,10,11,12,13,14,15,16] plotted on $[3, 13]$:

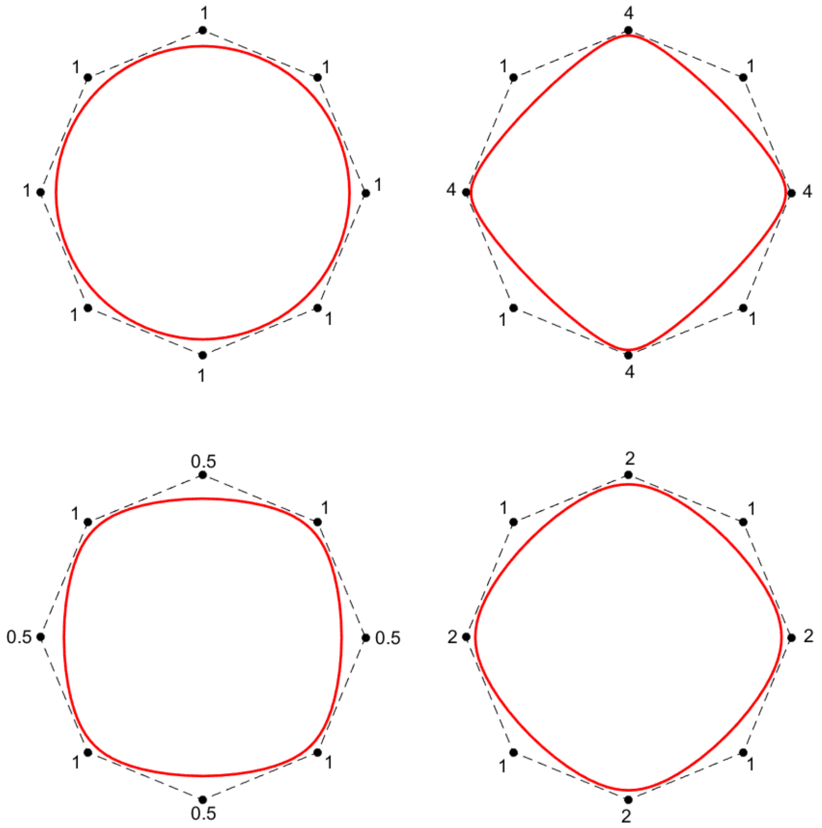


Note that the B-spline curves are inside the convex hull of the control points and there are approximations, not interpolations.

A rational B-spline is defined as following:

$$Q(t) = \frac{\sum_{i=0}^{n} \omega_i B_{i,k}(t) P_i}{\sum_{i=0}^{n} \omega_i B_{i,k}(t)} \quad \text{for } t_k \leq t \leq t_{n+1}$$

where $(\omega_i)_{i=0,n}$ are some weights. When the weight $\omega_i$ is large, the curve goes to the control point $P_i$. When all the weights are equal to 1, the rational B-spline coincides with the B-spline.



If $t_0 = t_1 = \cdots = t_k < t_{k+1}$ and $P_0 \neq P_1$ then

$$\begin{aligned}
&Q(t_k) = P_0,\\
&Q'(t_k) = \frac{k}{t_{k+1} - t_k}\,\frac{w_1}{w_0}(P_1 - P_0),\\
&Q'(t_k) \times Q''(t_k) = \frac{k^2(k-1)}{(t_{k+1} - t_k)^2(t_{k+2} - t_k)}\,\frac{w_1 w_2}{w_0^2}(P_1 - P_0) \times (P_2 - P_0),\\
&\kappa = \frac{k-1}{k}\,\frac{t_{k+1} - t_k}{t_{k+2} - t_k}\,\frac{w_1 w_2}{w_0^2}\,\frac{2A}{c^3} \quad \text{(curvature)}
\end{aligned}$$

with $A$ the surface of the triangle $(P_0, P_1, P_2)$ and $c = ||P_1 - P_0||$. That gives a way to match the rational B-spline to an other curve up to $C^2$.

### B-spline interpolation

To build a (rational) B-spline interpolating a set of points, say $(Q_i)_{0\le i\le n}$ at parameters $(s_i)_{0\le i\le n}$, the following inverse problem is addressed :

$$\left|\begin{array}{l}
\text{find } (P_j)_{0\le j\le n} \text{ such that } \forall i,\ 0 \le i \le n\\
\displaystyle\sum_{j=0}^{n} \omega_j B_{j,k}(s_i) P_j = \sum_{j=0}^{n} \omega_j B_{j,k}(s_i) Q_i.
\end{array}\right.$$

Introducing the matrices ($0 \le i, j \le n,\ 1 \le \ell \le d$ =dimension of points)

$$\mathbb{B}_{ij} = \omega_j B_{j,k}(s_i),\ \ \mathbb{D}_{ii} = \sum_{j=0}^{n} \omega_j B_{j,k}(s_i),\ \ \mathbb{P}_{i\ell} = (P_i)_\ell,\ \ \mathbb{Q}_{i\ell} = (Q_i)_\ell$$

the previous system is rewritten as

$$\mathbb{B}\mathbb{P} = \mathbb{D}\mathbb{Q} \ \text{ and } \mathbb{P} = \mathbb{B}^{-1}\mathbb{D}\mathbb{Q} \ \text{ if } \mathbb{B} \text{ is invertible.}$$

Note that $\mathbb{D} = \mathbb{I}$ for a standard B-spline (non rational). Because the $B_{jk}$ functions are locally supported, the $\mathbb{B}$ matrix is sparse.

When the starting control point is free, the interval of definition of the spline starts at $t_k > t_0$ and the previous linear system may be used. But when the starting point is clamped ($t_0 = t_1 \cdots = t_k$), the previous linear system may be adapted to impose the tangent vector (say $dQ_0$) at the first point. Indeed

$$\frac{k}{t_{k+1} - t_k} \frac{w_1}{w_0}(P_1 - P_0) = dQ_0$$

As a consequence, the two first rows of the linear system are substituted by the rows:

$$\begin{aligned} P_0 &= Q_0 \\ \frac{k}{t_{k+1} - t_k} \frac{w_1}{w_0}(P_1 - P_0) &= dQ_0 \end{aligned}$$

The parameters $s_i$ are not equal to the abstract parameters $t_i$ used to build the B-spline. They only have to belong to the interval of definition of the spline $[t_k, t_{n+1}]$. Let the function $t(s) = t_k + s(t_{n+1} - t_k)$ which maps $[0,1]$ onto $[t_k, t_{n+1}]$. The parameters are constructed as $s_i = t(\tilde{s}_i)$ $(0 \le i \le n)$ where $\tilde{s}_i$ are usually chosen using one of the following rules :

- uniform: $\tilde{s}_i = \frac{i}{n}$
- chordal: $\tilde{s}_i = \tilde{s}_{i-1} + \dfrac{\|Q_i - Q_{i-1}\|}{\sum_{j=1,n} \|Q_j - Q_{j-1}\|}$ with $\tilde{s}_0 = 0$
- centripetal: $\tilde{s}_i = \tilde{s}_{i-1} + \dfrac{\sqrt{\|Q_i - Q_{i-1}\|}}{\sum_{j=1,n} \sqrt{\|Q_j - Q_{j-1}\|}}$ with $\tilde{s}_0 = 0$

Other rules have been proposed (see Lockyer). By the way, it is also possible to play with the weights $(w_j)$ of rational B-splines to build an interpolating B-spline or to improve the interpolation (see for instance the choice of weights to get a circle).

### 17.3.4 Approximate surfaces

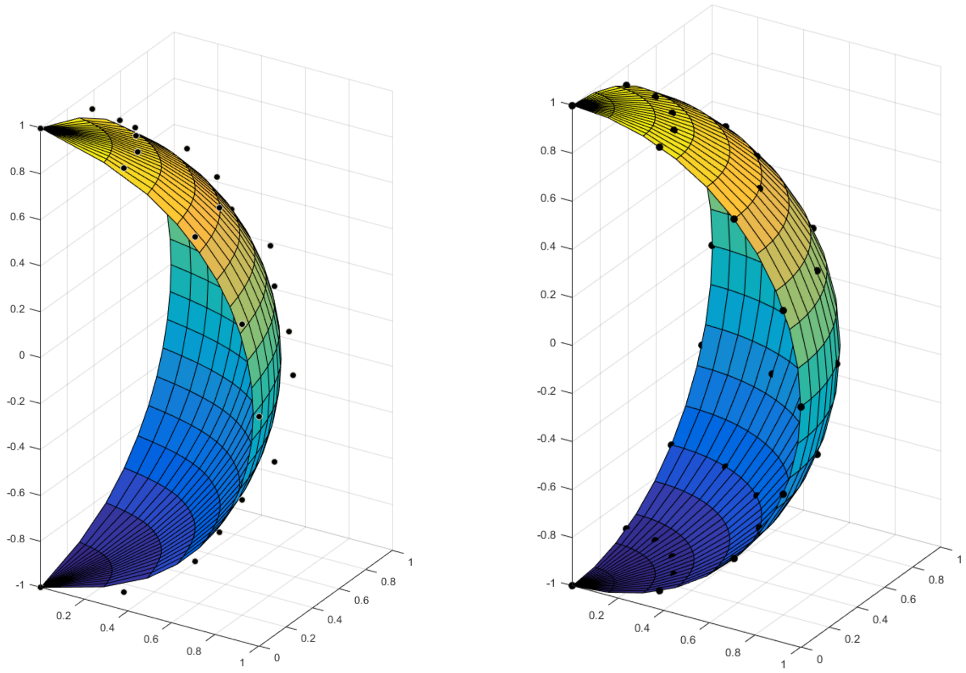
The most common method to approximate surface are NURBS (non uniform rational B-spline) that are no more than the cross-product of two rational B-splines. Let

- a set of $(m+1) \times (n+1)$ control points $P_{ij}$, $0 \le i \le m$ and $0 \le j \le n$
- a knot vector in $u$-direction and $v$-direction : $U = [u_0, u_1, \dots u_k]$ and $V = [v_0, v_1, \dots v_\ell]$,
- the degree $p$ in $u$-direction and the degree $q$ in $v$-direction
- $k = m + p + 1$ and $\ell = n + q + 1$

The NURBS surface is defined by

$$(u, v) \longrightarrow Q(u, v) = \frac{\sum_{i=0}^{m} \sum_{j=0}^{n} \omega_{ij} B_{i,p}(u) B_{j,q}(v) P_{ij}}{\sum_{i=0}^{m} \sum_{j=0}^{n} \omega_{ij} B_{i,p}(u) B_{j,q}(v)}.$$

The following example shows the NURBS surface get from 45 control points on a quarter of sphere and clamped cubic B-Splines (no weights).



NURBS approximation and NURBS interpolation

**Nurbs interpolation**

In a same way as B-Spline, Nurbs can be used to interpolate a set of $(m+1)\times(n+1)$ points $Q_{k\ell}$ arranged in a grid related to a 2D parametrization $(u,v)$. A simple way to build an interpolating nurbs consists in solving the linear system

$$\sum_{i=0}^{m}\sum_{j=0}^{n}\omega_{ij}B_{i,p}(s_k)\,B_{j,q}(t_\ell)P_{ij}=\left(\sum_{i=0}^{m}\sum_{j=0}^{n}\omega_{ij}B_{i,p}(t_k)\,B_{j,q}(t_\ell)\right)Q_{k\ell}\ \ \forall 0\le k\le m\ ,0\le\ell\le n$$

where $(s_k)_{0\le k\le m}$ and $(t_\ell)_{0\le\ell\le n})$ are some parameter values picked following the uniform, chordal or centripetal rule presented above. Note that both the B-Spline in $u$, $v$ direction has to be clamped at the ends or periodic if the last point coincides with the first one.

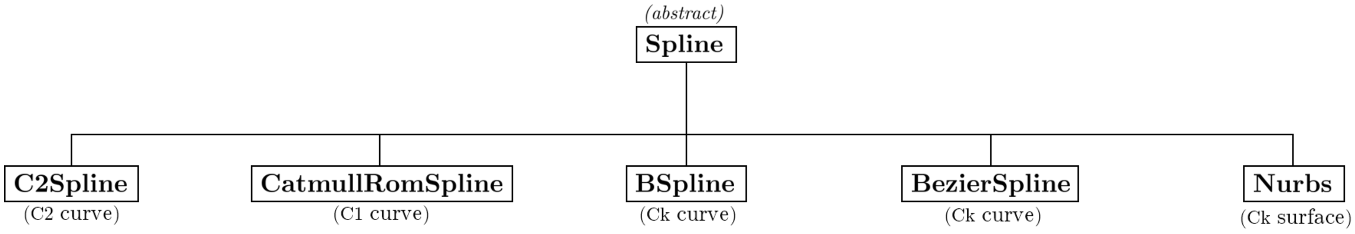
When B-splines are not rational (weights equal to 1), the system is simplified :

$$\sum_{i=0}^{m}\sum_{j=0}^{n}B_{i,p}(s_k)\,B_{j,q}(t_\ell)P_{ij}=Q_{k\ell}\ \ \forall 0\le k\le m\ ,0\le\ell\le n.$$

Note that more sophisticated nurbs interpolations can be considered by finding both control points and weights minimizing some quality criteria under the constraint defined by the previous linear system.

### 17.3.5 XLiFE++ spline classes

Spline stuff in XLiFE++ is handled using the following class hierarchy (either curve and surface):



### • Spline abstract class

The Spline abstract class collects the following general data:

```
vector<Point> controlPoints_;       //list of control points
multimap<real_t,number_t> knots_;   //ordered list of knots
number_t degree_;                   //spline degree (default 3)
bool isClosed_;                     //true if first and last points are the same
SplineType type_;                   //type of the spline
SplineSubtype subtype_;             //subtype (interpolation or approximation)
SplineBC bcs_,bce_;                 //type of boundary condition at end points
SplineParametrization splinePar_;   //type of knots parametrization
vector<real_t> yp0_, yp1_;          //optional tangent vector at end points
Parametrization* parametrization_;  //pointer to parametrization if not 0
```

Parametrization is a class dealing with 1d, 2d and 3d parametrization. Once a function giving values and derivatives is linked to a Parametrization object, this object provides a lot of quantities such as curvatures, curvilinear abscissas, normal and tangent vectors, ... (see Parametrization class)

For commodity, it has been chosen that the parameters of spline, say $t$ or $(u,v)$, always belongs to the interval $[0,1]$ whereas splines are not really designed with this choice. The evaluate function does the parameters mapping.

The types of spline are defined with the following enumeration:

```
enum SplineType {_noSpline, _C2Spline, _CatmullRomSpline, _BSpline, _BezierSpline, _Nurbs};
```

and a subtype for some of them (BSpline and Nurbs):

```
enum SplineSubtype{_noSplineSubtype,_SplineInterpolation,_SplineApproximation};
```

The type of parametrization describing how the spline parameter varies between knots is given by:

```
enum SplineParametrization{
  _xParametrization,              //using x-coordinates of points
  _uniformParametrization,        //using uniform distribution
  _chordalParametrization,        //using point distances
  _centripetalParametrization     //using square root of point distances
}
```

The _xParametrization is managed only by C2Spline.

To deal with several boundary conditions, the following enumeration is available:

```
enum SplineBC {
  _undefBC,         //not defined
  _naturalBC,       //free condition
  _clampedBC,       //to clamp the ends
  _periodicBC       //to enforce periodicity
}
```

There is a useful tool to check and set the default boundary conditions

```
  void checkBC(SplineBC defBC);
```

This class provides several basic accessors:

```
[const] vector<Point>& controlPoints() [const];
SplineType type() const;
SplineSubtype subtype() const;
number_t degree() const;
number_t nbcp() const;
number_t dim()const;
bool isClosed() const;
bool isPeriodic() const;
const Parametrization& parametrization() const;
const std::multimap<real_t,number_t>& knots()const;
RealPair knotsBounds() const;
```

The Spline class declares the following virtual member functions, some of them providing default behavior:

```
Spline* clone() const =0;     //copy like constructor
RealPair parameterBounds() const;
vector<const Point> boundNodes();

multimap<real_t,number_t>::const_iterator locate(real_t t) const;
Point evaluate(real_t t, DiffOpType d=_id) const;
Vector<Point> evaluate(const std::vector<real_t>& ts, DiffOpType d=_id) const;
Point operator()(real_t t, DiffOpType d=_id) const
Vector<Point> operator()(const std::vector<real_t>& ts, DiffOpType d=_id) const;

void print(std::ostream&) const;
void print(PrintStream&) const;
```

While knotsBounds returns the bounds of knots list, parameterBounds returns the bounds of the interval where the parameter can be really selected (always (0,1)). The member function evaluate() is one of the most important. It computes the spline or its derivatives at any admissible parameter. Obviously, this function will be overridden by the Spline child classes.

It proposes also safe downcast functions either const or non-const:

```
virtual [const] C2Spline* c2Spline() [const];
virtual [const] CatmullRomSpline* catmullRomSpline() [const];
virtual [const] BSpline* bSpline() [const];
virtual [const] BezierSpline* bezierSpline() [const];
virtual [const] Nurbs* nurbs() [const];
```

### • C2Spline class

The C2Spline class handles cubic interpolation splines. Inheriting from Spline class, it manages only one additional data handling the coefficients of polynomials:

```
class C2Spline : public Spline
{
  vector<Vector<real_t> > P_; //polynomial coefficients
  ...
```

It provides two end-user constructors calling the init() member function that constructs the polynomial coefficients related to the spline:

```
C2Spline(const vector<Point>& cpts, SplineParametrization sp=_xParametrization,
   SplineBC bcs=_naturalBC, SplineBC bce=_naturalBC,
    const vector<real_t>& yp0=vector<real_t>(3,0.), const vector<real_t>&
        yp1=vector<real_t>(3,0.));
C2Spline(real_t a, real_t b, const vector<real_t>& ys, SplineParametrization sp=_xParametrization,
   SplineBC bcs=_naturalBC, SplineBC bce=_naturalBC,
    const vector<real_t>& yp0=vector<real_t>(3,0.), const vector<real_t>&
        yp1=vector<real_t>(3,0.));
void init();
```

Because a deep copy of Parametrization has to done for safety, the copy constructor, the assign operator and the destructor are also defined:

```
C2Spline(const C2Spline&);
C2Spline& operator=(const C2Spline&);
void copy(const C2Spline&);
virtual ~C2Spline();
```

To link the parametrization of the spline to a Parametrization object (done by init), the class handles two following member functions:

```
Vector<real_t> funParametrization(const Point& pt, Parameters& pars, DiffOpType d=_id) const;
Vector<real_t> invParametrization(const Point& pt, Parameters& pars, DiffOpType d=_id) const;
```

that are called by the two extern functions (wrapper):

```
Vector<real_t> parametrization_C2Spline(const Point& pt, Parameters& pars, DiffOpType d=_id);
Vector<real_t> invParametrization_C2Spline(const Point& pt, Parameters& pars, DiffOpType d=_id);
```

Because the function pointers used in the definition of the Parametrization class can not be initialized with a member function pointer, even if their signature are the same, so the real parametrization functions are wrapped.The mechanism is the following :

- When initializing a C2Spline object, its parametrization_ pointer is allocated using the external function parametrization_C2Spline and a Parameters object that handles the pointer to the C2Spline object.

- When it is called, the parametrization_C2Spline external function uses this Parameters object to get the address of the C2Spline object and calls the funParametrization member function attached to this object.

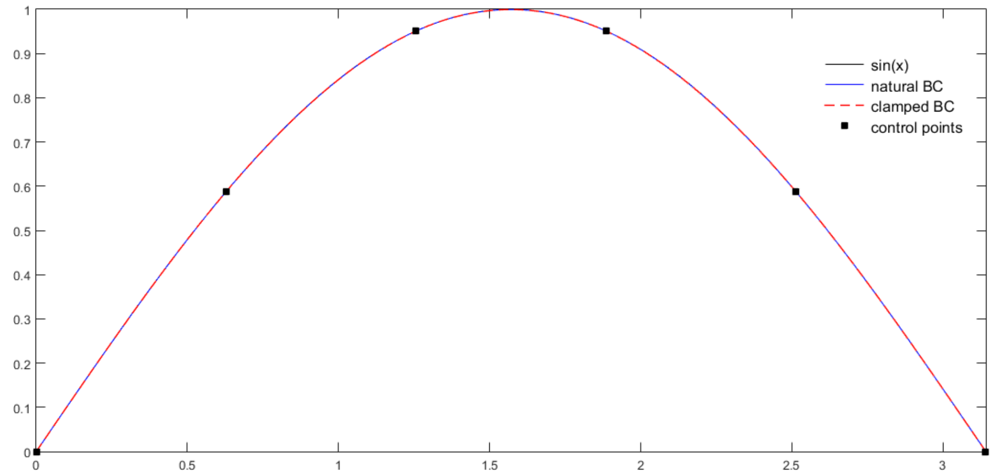
In addition, this class implements the following virtual functions (in particular the fundamental evaluate function that computes the C2Spline at a parameter $x \in [0,1]$):

```
virtual C2Spline* clone() const;
virtual [const] C2Spline* c2Spline() [const];
virtual std::vector<Point> boundNodes() const;
Point evaluate(real_t t, DiffOpType d=_id) const;
void print(std::ostream&) const;
void print(PrintStream& os) const;
```

The following example illustrates how to use the C2Spline class

```
number_t n=5; Real x=0, dx=pi_/n;
vector<Point> points(n+1);
for(number_t i=0;i<=n;i++, x+=dx) points[i]=Point(x,sin(x));

//natural spline
C2Spline cs(points);
theCout<<cs;
const Parametrization& pa=cs.parametrization();
theCout<<"pa(0.5) = "<<pa(0.5)<<eol;
theCout<<"pa.curvature(0.5) = "<<pa.curvature(0.5)<<eol;
theCout<<"pa.curabc(0.5) = "<<pa.curabc(0.5)<<eol;
theCout<<"pa.normal(0.5) = "<<pa.normal(0.5)<<eol;
```

```
theCout<<"pa.tangent(0.5) = "<<pa.tangent(0.5)<<eol;

//clamped spline (imposed derivatives at end points)
C2Spline csc(points,_xParametrization,_clampedBC,_clampedBC,Reals(1.,1.),Reals(1.,-1.));
dx=0.01;
ofstream of("c2spline_nat.dat");
for(real_t x=0; x<=1; x+=dx)
  of<<x*pi<<" "<<sin(x*pi)<<" "<<cs(x)[0]<<" "<<csc(x)[0]<<eol;
of.close();
```



- `CatmullRomSpline` **class**

The `CatmullRomSpline` class inherits from the `Spline` class and manage one additional parameter, the tension factor:

```
class CatmullRomSpline : public Spline
{
real_t tau_;  //tension factor (0<=tau<=1, default 0.5)
...
```

It offers only one end-user constructor, calling the `init()` function that initializes the knots list according to the boundary conditions and the spline parametrization type:

```
CatmullRomSpline(const vector<Point>& cpts,
                 SplineParametrization =_chordalParametrization, real_t tau=0.5,
                 SplineBC bcs=_naturalBC, SplineBC bce=_naturalBC,
                 const vector<real_t>& yp0=vector<real_t>(3,0.),
                 const vector<real_t>& yp1=vector<real_t>(3,0.));
void init();
```

Besides, copy constructor and assign operator are also provided:

```
CatmullRomSpline(const CatmullRomSpline&);
CatmullRomSpline& operator=(const CatmullRomSpline&);
void copy(const CatmullRomSpline&);
virtual ~CatmullRomSpline();
```

It proposes the virtual member functions:

```
CatmullRomSpline* clone() const;
CatmullRomSpline* catmullRomSpline();
[const] CatmullRomSpline* catmullRomSpline() [const];
```

```
Point evaluate(real_t t, DiffOpType d=_id) const;
void print(std::ostream&) const;
void print(PrintStream& os) const;
```

and the two member functions related to the parametrization

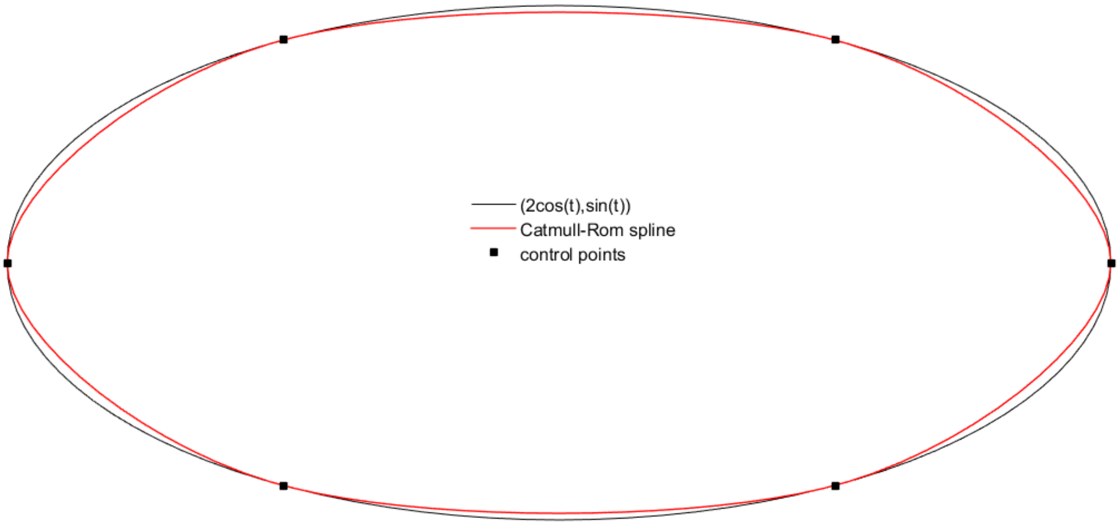
```
Vector<real_t> funParametrization(const Point& pt, Parameters&, DiffOpType d=_id) const;
Vector<real_t> invParametrization(const Point& pt, Parameters&, DiffOpType d=_id) const;
```

wrapped to the extern functions:

```
Vector<real_t> parametrization_CatmullRomSpline(const Point& pt, Parameters&,
                                                DiffOpType d=_id);
Vector<real_t> invParametrization_CatmullRomSpline(const Point& pt, Parameters&,
                                                   DiffOpType d=_id);
```

The following code is a simple example of using the CatmullRomSpline class to interpolate an ellipse with 7 control points:

```
Number n=6;
Real s=0, ds=2*pi_/n;
vector<Point> pts(n+1);
for(Number i=0;i<=n;i++,s+=ds) pts[i]=Point(2*cos(s),sin(s));
CatmullRomSpline cmr(pts);
of.open("catmullspline.dat");
dt=0.01;
for(Real t=0.;t<1.+theTolerance;t+=dt)
{
  Point p=cmr(t);
  of<<p[0]<<" "<<p[1]<<eol;
}
of.close();
```



- BSpline **class**

Because B-spline are rational B-spline with a constant weights, the BSpline class encapsulates in a same framework the classic B-spline and the rational B-spline. As a consequence, the BSpline class inheriting from Spline class manages some additional parameters related to the weights. Using interpolation B-spline requires to store also the original list of interpolation points that differs from the list of control points.

```
class BSpline : public Spline
{
 vector<Point> interpolationPoints_;   //interpolation points
 vector<real_t> weights_;              //weights related to control points (default 1)
 bool noWeight_;                       //true if weight=(1,1, ...,1) or empty
 real_t t0_=0, tf_=0;                  //internal parameter bounds
 map<real_t,number_t> paramMap_;       //for non uniform parametrization
  ...
```

Do not confuse the bounds of internal parameter (knot parameter) with the bounds of the parametrization (set to (0,1)). The `toKnotsParameter` member function do the linear mapping $[0,1] \to [t_0, t_f]$.

The `paramMap_` indexing intermediate values of non uniform parametrizations, is used to locate knot intervals faster.

A general constructor and a shortcut constructor (approximation B-spline) are provided:

```
BSpline(SplineSubtype, const vector<Point>& cpts, number_t degree=3,
        SplineParametrization = _uniformParametrization,
        SplineBC bcs=_undefBC, SplineBC bce=_undefBC,
        const vector<real_t>& yp0=vector<real_t>(),
        const vector<real_t>& yp1=vector<real_t>(),
        const vector<real_t>& weights=std::vector<real_t>());
BSpline(const vector<Point>& cpts, number_t degree=3,
        SplineBC bcs=_undefBC, SplineBC bce=_undefBC,
        const vector<real_t>& weights=vector<real_t>());
void init();
void initInterp();
```

These constructors call the `init()` function that initializes the knot list regarding the boundary conditions and `initInterp()` function that solves the inverse problem to construct control points from interpolation points.

Default spline subtype is `_splineApproximation`.

Besides, copy constructor and assign operator (managing parametrization pointer allocation) are also available

```
BSpline(const BSpline&);
BSpline& operator=(const BSpline&);
void copy(const BSpline&);
virtual ~BSpline();
```

The following virtual member functions are implemented:

```
BSpline* clone() const;
[const] BSpline* bSpline() [const];
Point evaluate(real_t t, DiffOpType d=_id) const;
void print(std::ostream&) const;
void print(PrintStream& os) const;
```

The `evaluate` function uses the member function

```
void computeB(real_t,DiffOpType,number_t&, Vector<real_t>& B,
              Vector<real_t>& dB, Vector<real_t>& d2B) const;
```

that computes the quantities $B_{ik}(t)$ and its derivative, involved in the B-spline definition.

The stuff related to the parametrization are available:

```
real_t toKnotsParameter(real_t t);
Vector<real_t> funParametrization(const Point&, Parameters&, DiffOpType d=_id) const;
Vector<real_t> invParametrization(const Point&, Parameters&, DiffOpType d=_id) const;
```

wrapped to the extern functions:

```
Vector<real_t> parametrization_BSpline(const Point&, Parameters&, DiffOpType d=_id);
Vector<real_t> invParametrization_BSpline(const Point&, Parameters&, DiffOpType d=_id);
```

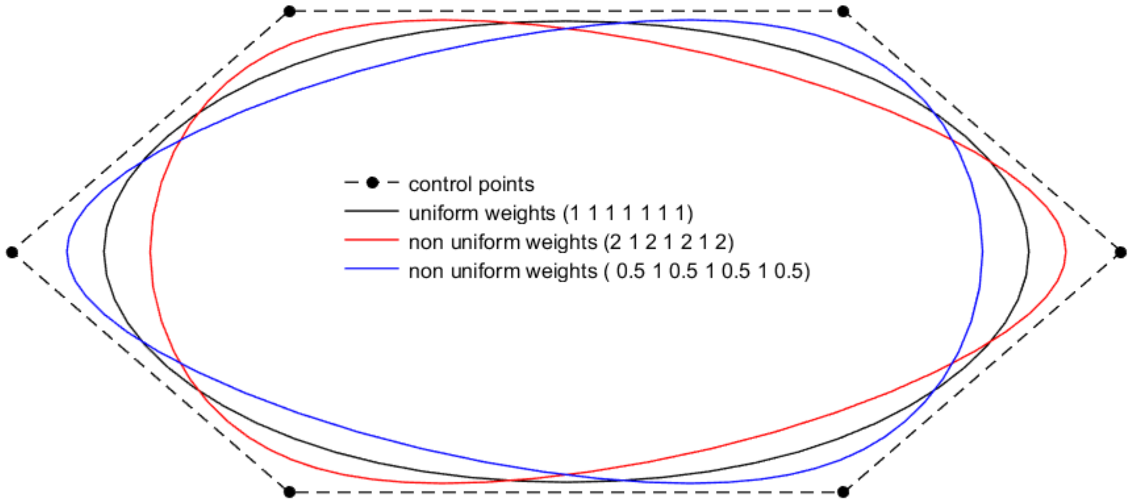
The next code show how to create a B-spline from control points located on an ellipse:

```
Number n=6; Real s=0, ds=2*pi_/n;
vector<Point> pts(n+1);
for(Number i=0;i<=n;i++,s+=ds) pts[i]=Point(2*cos(s),sin(s));
BSpline bsp(pts,3,_periodicBC);
dt=0.01;
of.open("BSpline.dat");
for(Real t=0;t<=1;t+=dt)
{
  Point p=bsp(t);
  of<<p[0]<<" "<<p[1]<<eol;
}
of.close();
```

To handle a rational B-spline with weights 0.5,1,0.5,1,0.5,1,0.5 with the same control points, the code looks like

```
vector<real_t> we(pts.size(),1.);
for(number_t k=0;k<we.size();k+=2) we[k]=0.5;
BSpline bspw(pts,3,_periodicBC,_periodicBC,we);
for(Real t=1;t<=1+theTolerance;t+=dt)
{
  Point p=bspw(t);
  of<<p[0]<<" "<<p[1]<<eol;
}
of.close();
```

The next figure illustrates the influence of weights.



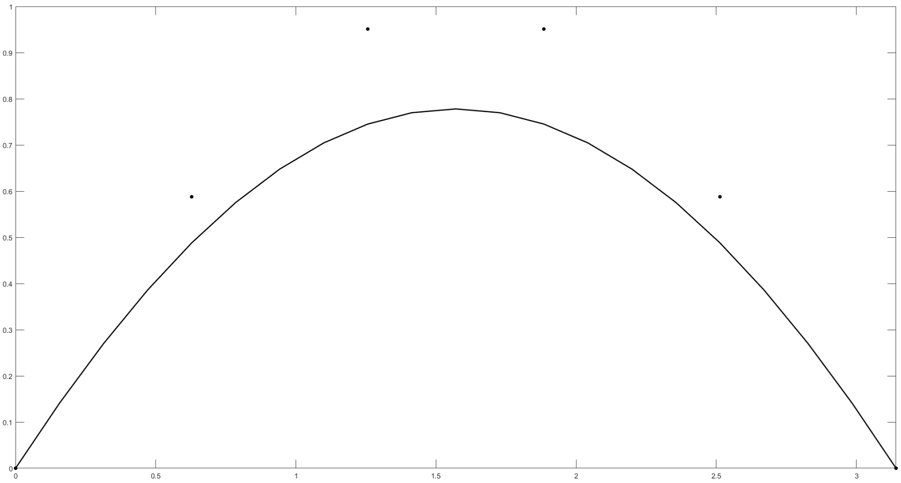
- BezierSpline **class**

Although the Bezier curves are a special case of B-spline, for a sake of efficiency they are implemented as a separate class in XLiFE++. In particular, the BezierSpline class does not manage the knot list, nor the parametrization type (uniform parametrization by construction) and the boundary conditions (clamped by definition). As a consequence, the only parameter to set is the list of control points that fix the polynomial degree (number of points - 1) and the class is very simple:

```
class BezierSpline : public Spline
{
public:
  BezierSpline(const std::vector<Point>&);
  BezierSpline(const BezierSpline&);
  virtual BezierSpline* clone() const;
  void copy(const BezierSpline&);
  BezierSpline& operator=(const BezierSpline&);
  virtual ~BezierSpline(){}
  [const] BezierSpline* bezierSpline() [const];

  RealPair parameterBounds() const;
  virtual Point evaluate(real_t t, DiffOpType d=_id) const;
  Vector<real_t> funParametrization(const Point&, Parameters&, DiffOpType =_id) const;
  Vector<real_t> invParametrization(const Point&, Parameters&, DiffOpType =_id) const;

  virtual void print(std::ostream&) const;
  virtual void print(PrintStream& os) const;
};

Vector<real_t> parametrization_BezierSpline(const Point&, Parameters&, DiffOpType =_id);
Vector<real_t> invParametrization_BezierSpline(const Point&, Parameters&,DiffOpType =_id) ;
```

Hereafter is a simple example of using Bezier spline with 6 control points:

```
number_t n=5; std::vector<Point> points(n+1);
Real x=0, dx=pi_/n;
for(number_t i=0;i<=n;i++, x+=dx) points[i]=Point(x,sin(x));
BezierSpline bz(points);
Real dt=0.05,t0=0,tf=1.;
of.open("bezierspline.dat");
for(real_t t=t0;t<tf;t+=dt)
{ Point p=bz(t);  of<<p[0]<<" "<<p[1]<<eol;}
of.close();
```



Note that the Bezier curve does not well approximate the control points!

- Nurbs **class**

This class implements the non uniform rational B-Spline (nurbs) that approximates surface. It inherits from Spline class and manages the list of control points $P_{ij}$ as a vector of vectors of points, an optional list of weights $w_{ij}$ as a vector of vectors of scalars (same sizes), two B-Spline pointers to handles data of B-splines along $u, v$ (knot vector, boundary conditions, degree) and a parametrization pointer:

```
class Nurbs
{
 protected:
 vector<vector<Point> > controlPointsM_; //list of control points as matrix
 vector<vector<real_t> > weightsM_;      //list of weights as matrix
 BSpline* bs_u, *bs_v;                   //u/v-Bspline
 bool noWeight_;                         //true if weightsM_ is empty
```

⚠ The vectors contropl Points_ and weights_ handled by the Spline class parent are no longer used!

The BSpline objects are 'fake' objects (fake list of control points and fake list of weights). It is a commodity to handle some B-Spline data and to re-use the computeB member function of the BSpline class.

It provides some full constructors either control points and weights are given as vectors or as vectors or vectors (matrices), a copy constructor, a clone constructor, a destructor and related construction stuff:

```
Nurbs(SplineSubtype sbt, const std::vector<std::vector<Point> >& cpts,
      number_t degree_u=3,number_t degree_v=3,
      SplineBC bcs_u=_clampedBC, SplineBC bcs_v=_clampedBC,
      SplineBC bce_u=_undefBC, SplineBC bce_v=_undefBC,
      const std::vector<std::vector<real_t> >& w=std::vector<std::vector<real_t> >());
Nurbs(SplineSubtype sbt, const std::vector<Point>& cpts, number_t ncpu,
      number_t degree_u=3,number_t degree_v=3,
      SplineBC bcs_u=_clampedBC, SplineBC bcs_v=_clampedBC,
      SplineBC bce_u=_undefBC, SplineBC bce_v=_undefBC,
      const std::vector<real_t>& w=std::vector<real_t>());
void initMatrices(number_t ncpu, const std::vector<Point>& cpts, const std::vector<real_t>& w);
void init(number_t d_u,number_t d_v, SplineBC bs_u, SplineBC bs_v, SplineBC be_u, SplineBC be_v);
void initInterp();
Nurbs(const Nurbs&);
void copy(const Nurbs&);
Nurbs& operator=(const Nurbs&);
virtual Nurbs* clone() const;
virtual ~Nurbs();
```

The following accessors are available:

```
[const] Nurbs* nurbs() [const];
[const] std::vector<std::vector<Point> >& controlPointsM() [const];
[const] std::vector<std::vector<real_t> >& weightsM() [const];
const BSpline* bsu() const;
const BSpline* bsv() const;
const bool noWeight() const;
number_t nbcp() const;
number_t dim()const;
const Parametrization& parametrization() const;
RealPair uBounds() const;
RealPair vBounds() const;
```

The major function evaluate computes the nurbs at any admissible couple of parameters $(u, v)$. The overridden operator () is a user shortcut calling the function evaluate:

```
Point evaluate(real_t u, real_t v, DiffOpType d=_id) const;
Point operator()(real_t u,real_t v,DiffOpType d=_id) const;
```

In a same way as other spline classes, the `Nurbs` class provides an interface to a parametrization object that requires the two member functions:

```
Vector<real_t> funParametrization(const Point& pt, Parameters& pars, DiffOpType d=_id) const;
Vector<real_t> invParametrization(const Point& pt, Parameters& pars, DiffOpType d=_id) const;
```

and two additional external functions:

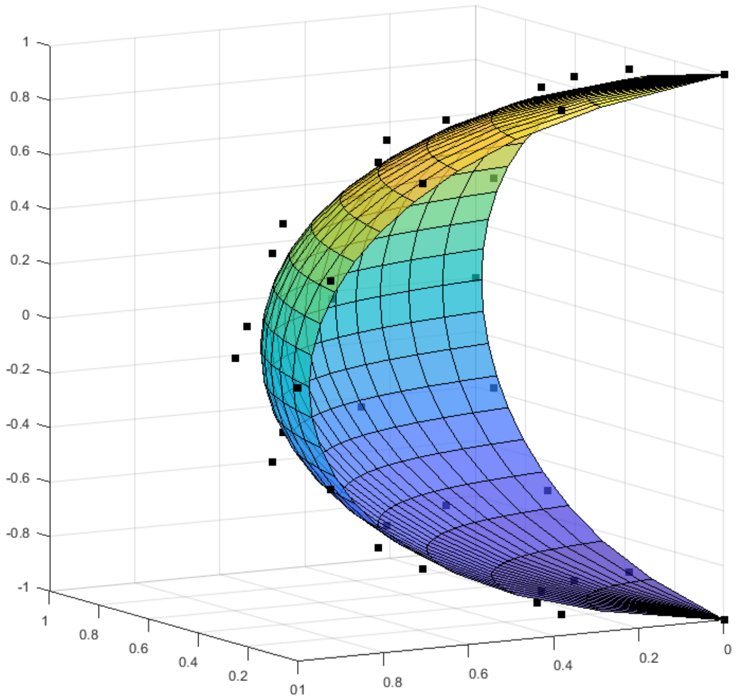
```
Vector<real_t> parametrization_Nurbs(const Point& pt, Parameters& pars, DiffOpType d=_id);
Vector<real_t> invParametrization_Nurbs(const Point& pt, Parameters& pars, DiffOpType d=_id);
```

Finally, some print facilities are provided:

```
void print(std::ostream&) const;
void print(PrintStream&   const;
ostream& operator<< (std::ostream&, const Nurbs&); //external
```

As an example, we give hereafter the code corresponding to the construction of the nurbs of degree 3 from 9x5 control points located on a quarter of the unity sphere:

```
Number ns=4; Real ds=pi_/(2*ns);
Real u=-pi_/2,v;
vector<vector<Point> > pts2(2*ns+1,vector<Point>(ns+1));
for(number_t i=0;i<=2*ns;i++,u+=ds)
  {v=0;
   for(number_t j=0;j<=ns;j++,v+=ds) pts2[i][j]=Point(cos(u)*cos(v),cos(u)*sin(v),sin(u));
  }
Nurbs nu(_splineApproximation,pts2);   //uniform nurbs of degree 3, clamped
Real du=1./20, dv=du;
ofstream of("nurbs.dat");
for(real_t u=0;u<=1;u+=du)
  for(real_t v=0;v<=1;v+=dv)
   {
    Point Q=nu(u,v);
    of<<Q[0]<<" "<<Q[1]<<" "<<Q[2]<<eol;
   }
of.close();
```


1
0.8
0.6
0.4
0.2
0
-0.2
-0.4
-0.6
-0.8
-1
1
0.8
0.6
0.4
0.2
01
0.8
0.6
0.4
0.2
0

# 18 Multi-threading with OpenMP

OpenMP is a shared-memory application programming interface (API) whose features are based on prior efforts to facilitate shared-memory parallel programming. OpenMP is intended to be suitable for implementation on a broad range of SMP architectures, even for uniprocessor computers also. OpenMP can be added to a sequential program in Fortran, C, or C++ to describe how the work is to be shared among threads that will execute on different processors or cores and to order accesses to shared data as needed. The appropriate insertion of OpenMP features into a sequential program will allow applications to benefit from shared-memory parallel architectures with minimal modification to the code. Because of these advantages, OpenMP has been added to XLIFE++ in order to exploit its considerable parallelism in heavy computation parts. In a typical Finite Element package, assembling the stiffness matrices costs most of the total runtime then solving linear equation systems.

## 18.1 Sparse matrix-vector multiplication

In a Finite Element package, after repeatedly setting up the stiffness matrices, it needs to a solve linear equation system, which can be done either in two ways (1) by direct methods or (2) iterative methods. In direct methods, the factorization of matrix costs nearly most of the runtime, meanwhile, in iterative methods, matrix-vector multiplication plays an important role. Since the matrices arising from the discretisation are sparse, an appropriate matrix storage format, sparse format is used. XLIFE++ provides a plenty types of sparse matrix, which can serve for different purposes. Although all the sparse matrix can be taken for parallelized sparse-matrix-vector-multiplication (SpMV); among them, CSR (compressed storage row) seems to be the best candidate.
The form of SpMV is $y = Ax$, where $A$ is a sparse matrix, $x$ and $y$ are dense vectors. $x$ is source vector and $y$ is destination vector.
In the following, the algorithms of parallelization of matrix-vector multiplication for CSR and CSC (compressed storage column) are mentioned, on which parallelized matrix-vector multiplication of other sparse format (CSDual, CSSym, SkylineDual, SkylineSym) are based.

### 18.1.1 SpMV of CSR

Because CSR is a well-known format, only a small recall about its structure is presented.
A matrix $A$ is an $m \times n$ matrix, and the number of non-zero elements is $nz$, CSR format needs to store three arrays:

- values[nz] store the value of each non-zero element in matrix A
- colIndex[nz] stores the column index of each element in *val[nz]* array
- rowPointer[m+1] stores the index of the first non-zero element of each row and *rowPointer[m]* = *nz*

For instance, the following 5 × 6 matrix

$$A = \begin{bmatrix} 11 & 12 & 0 & 14 & 0 & 16 \\ 0 & 22 & 23 & 0 & 0 & 26 \\ 31 & 32 & 33 & 0 & 0 & 0 \\ 0 & 0 & 43 & 44 & 0 & 0 \\ 51 & 0 & 53 & 54 & 55 & 0 \end{bmatrix}$$

is stored as follow in XLIFE++ by the three following *std::vector*:
values = ( 0 11 12 14 16  22 23 26  31 32 33  43 44  51 53 54 55 )

colIndex = ( 0 1 3 5  1 2 5  0 1 2  2 3  0 2 3 4 )
rowPointer = ( 0 4 7 10 12 16)

In XLIFE++, different from "standard", the array *values* of CSR format contains one more element 0 at the first position.

Since it must store the location information explicitly as well as the value of each non-zero element, extra communication time is need to access these location data. As a matrix of CSR format is store row by row, the simplest way to parallelize the matrix-vector multiplication using OpenMP is to assign each thread of parallel region to work with one row. However, considering the problem of load balancing, scheduling overhead and synchronization overheads, it's bettr to apply the *row partitioning* scheme. The matrix will be partitioned into blocks of row by the number of threads.

```
// Assign each thread an approximately equal number of non-zero
Number nnzEachThread = std::floor(nnz/numThread);

// Index of non-zero in each range for each thread
Number nnzRangeIdx = nnzEachThread;

// Lower and upper bound position for each thread
std::vector<std::vector<Number>::const_iterator> itThreadLower(numThread);
std::vector<std::vector<Number>::const_iterator> itThreadUpper(numThread);

itp = itpb;
itThreadLower[0] = itpb;
for (int i = 0; i < numThread; i++) {
  itThreadLower[i] = itp;
  nnzRangeIdx = *itp + nnzEachThread;
  itpLower = std::lower_bound(itp, itpe, nnzRangeIdx);
  itpUpper = std::upper_bound(itpLower, itpe,nnzRangeIdx);
  itp = ((nnzRangeIdx - *(itpUpper -1))< (*itpUpper-nnzRangeIdx)) ? itpUpper-1 : itpUpper;
  itThreadUpper[i] = itp;
}
itThreadUpper[numThread-1] = itpe;
```

Each block is assigned to a thread and has an approximately equal number of non-zero elements. By partitioning this way, each thread operates on its own part of the *values, colIndex and rowPointer*. All threads access element of the source vector $x$. Since accesses on $x$ are read-only, there is no invalidation traffic. One advantage of *row partitioning* is that each thread works on its own part of destination vector $y$, therefore, there is no need of synchronization among threads.

```
#pragma omp parallel for default(none)\
                         private(i, itr, iti, itie, itim, itpLower, itpUpper) \
                         shared(numThread, itbLower, itbUpper, itpb, itib, itm, itvb, itrb) \
                         schedule(dynamic,1)
for(i = 0; i < numThread; i++) {
  itpLower = *(itbLower+i);
  itpUpper = *(itbUpper+i);
  for (;itpLower != itpUpper;itpLower++) {
    itr = itrb + (itpLower - itpb);
    *itr *=0;
    iti  = itib + *(itpLower);
    itie = itib + *(itpLower + 1);
    itim = itm + *(itpLower);

    while(iti != itie) {
      *itr += *(itim) * *(itvb + *iti);iti++; itim++;
    }
  }
}
```

However, the coarse-grained approach sometimes can not assure the load balancing of SpMV of a very large matrix (e.g with million non-zero elements), and a **granularity factor** is a solution to make it more fine-grained. Each block of row of a thread is divided into smaller pieces, which not only make SpMv more fine-grained but also allow a thread to take work from each other.

```
const Number GRANULARITY = 16;
numThread *= GRANULARITY;
```

| | |
|---:|---|
| library : | **largeMatrix** |
| header : | **RowCsStorage.hpp** |
| implementation : | **RowCsStorage.cpp** |
| unitary tests : | **test_OpenMP.cpp** |
| header dependences : | **CsStorage.hpp, config.h, utils.h** |

### 18.1.2 SpMV of CSC

A matrix $A$ is an $m \times n$ matrix, and the number of non-zero elements is $nz$, CSC format needs to store three arrays:

- values[nz] store the value of each non-zero element in matrix A
- rowIndex[nz] stores the row index of each element in *val[nz]* array
- colPointer[m+1] stores the index of the first non-zero element of each column and *colPointer[m]* = *nz*

For instance, the following 5 × 6 matrix

$$A = \begin{bmatrix} 11 & 12 & 0 & 14 & 0 & 16 \\ 0 & 22 & 23 & 0 & 0 & 26 \\ 31 & 32 & 33 & 0 & 0 & 0 \\ 0 & 0 & 43 & 44 & 0 & 0 \\ 51 & 0 & 53 & 54 & 55 & 0 \end{bmatrix}$$

is stored as follow in XLiFE++ by the three following *std::vector*:
values = ( 0 11 31 51 12 22 32 23 33 43 53 14 44 54 55 16 26 )
rowIndex = ( 0 2 4 0 1 2 1 2 3 4 0 3 4 4 0 1)
colPointer = ( 0 3 6 10 13 14 16)
In XLiFE++, different from "standard", the array *values* of CSC format contains one more element 0 at the first position
Because the "column-like" storage of CSC is contrast to the natural manner of "row-processing" matrix-vector multiplication, the approach using OpenMP to parallelize matrix-vector multiplication of CSC is to limit the affect of this "column-like" characteristic.
Since a CSC matrix is stored in column by column, the simplest way to parallelize the matrix-vector multiplication using OpenMP is to use each thread to process a column, one by one; then the result of each thread is contributed to the destination vector by a "reduction-like" operation. Obviously, this approach is not efficient. Not only each thread processes non-adjacent column, which causes cache misses in cases of many threads; but also the problem of load-balancing can happen because of the difference in the number of non-zero elements in each column. An improved approach is to divide the matrix into groups of column, each of which has an approximately equal number of non-zero elements. Because all the columns in each group are adjacent, it limits the effect of cache miss. Moreover, load-balancing hardly happens thanks to equal number of non-zero elements processed by each thread.
The following code implements the approach described above.

```
// Lower and upper bound position for each thread
std::vector<std::vector<Number>::const_iterator> itThreadLower(numThread);
std::vector<std::vector<Number>::const_iterator> itThreadUpper(numThread);

std::vector<Number>::const_iterator itpLower, itpUpper;
// Find the smallest and largest rowIndexs corresponding to each thread
std::vector<Number> sRowIdx(numThread);
std::vector<Number> lRowIdx(numThread);

itp = itpb;
itThreadLower[0] = itpb;
for (int i = 0; i < numThread; i++) {
  itThreadLower[i] = itp;
  nnzRangeIdx = *itp + nnzEachThread;
  itpLower = std::lower_bound(itp, itpe, nnzRangeIdx);
  itpUpper = std::upper_bound(itpLower, itpe,nnzRangeIdx);
  itp = ((nnzRangeIdx - *(itpUpper -1))< (*itpUpper-nnzRangeIdx)) ? itpUpper-1 : itpUpper;
  itThreadUpper[i] = itp;
}
itThreadUpper[numThread-1] = itpe;

std::vector<std::vector<Number>::const_iterator >::const_iterator itbLower, itbUpper;
itbLower = itThreadLower.begin();
itbUpper = itThreadUpper.begin();
```

The serial codes above split a CSC matrix into blocks of column, each of which has nearly the same number of non-zero elements. After that, each of thread will process a block of column, store the result into its temporary vector and write this vector into the destination vector by a "reduction-like" operation. One remark is that temporary vector of each thread have necessarily the same size as the destination vector. It's is the trade-off of this method.

After finishing its own matrix-vector multiplication, each thread writes its result into the destination vector. Since array reduction isn't supported in OpenMP C++ (some projects have tried to make this feature available but it seems not to be ready in the near future!!). The only way, at the moment, is to use critical section. And we can easily realize that it is coarse-grained.

```
typedef typename IterationVectorTrait<ResIterator>::Type ResType;
#pragma omp parallel  \
                      private(i, tid, itr, iti, itie, itim, itpLower, itpUpper, itv) \
                      shared(numThread, itbLower, itbUpper, itpb, itib, itm, itvb, itrb, nRows)
{
    tid = omp_get_thread_num();
    std::vector<ResType> resTemp(nRows);
    typename std::vector<ResType>::iterator itbResTemp = resTemp.begin(), iteResTemp =
        resTemp.end(), itResTemp = itbResTemp;

    #pragma omp for nowait schedule(dynamic,1)
    for(i = 0; i < numThread; i++) {
         itpLower = *(itbLower+i);
         itpUpper = *(itbUpper+i);
         for (;itpLower != itpUpper;itpLower++) {
             itv = itvb + (itpLower - itpb);
             iti  = itib + *(itpLower);
             itie = itib + *(itpLower + 1);
             itim = itm + *(itpLower);

             while(iti != itie) {
                 itResTemp   = itbResTemp + (*iti);
                 *itResTemp += *itim * *(itv);
                 iti++; itim++;
             }
         }
    }
    #pragma omp critical (updateResult)
    {
        for (itResTemp = itbResTemp;itResTemp != iteResTemp; itResTemp++) {
            itr = (itrb + (itResTemp - itbResTemp));
            *itr += *itResTemp;
        }
    }
}
```

| | |
|---:|---|
| library : | **largeMatrix** |
| header : | **ColCsStorage.hpp** |
| implementation : | **ColCsStorage.cpp** |
| unitary tests : | **test_OpenMP.cpp** |
| header dependences : | **CsStorage.hpp, config.h, utils.h** |

## 18.2 Sparse matrix factorization

As mentioned above, one way to solve a linear equation system is to use direct methods, which heavily depends on matrix factorization. Firstly, the costly runtime factorization is done, secondly, the factorized matrix is used to solve the linear equation system $Ax = b$. Till now, XLIFE++ has supported some popular factorization methods: LU, LDLt and LDL*; all of them have a parallelized version with OpenMP. Because of factorization algorithm, only skyline storage is suitable to be factorized.

Because LDLt can be considered to be a special case of LU, the following only mentions the parallelized LU factorization.

The idea behind multi-threaded factorization is simple: Instead of implementing the factorization element by element as in the serial version, we make the algorithm work on block by block. For each iteration, block on diagonal is processed then block on the row and column corresponding to this diagonal block.

First of all, the diagonal block is calculated

```
#pragma omp single
      diagBlockSolverParallel(k*blockSize, blockSizeRow[k], it_rownx,
                              k*blockSize, blockSizeCol[k], it_colnx,
                              it_fd, it_fl, it_fu,
                              it_md, it_ml, it_mu);
```

After that, the block of row and column can be computed in the same time

```
#pragma omp for nowait
      for (jj = k+1; jj < nbBlockCol; jj++) {
          #pragma omp task untied firstprivate(k, jj) \
                      shared(blockSize, blockSizeRow, blockSizeCol, it_rownx, it_colnx, it_fl,
                          it_fu, it_mu)
          upperBlockSolverParallel(k*blockSize, blockSizeRow[k],it_rownx,
                              jj*blockSize, blockSizeCol[jj], it_colnx,
                              it_fl, it_fu, it_mu);
      }

#pragma omp for
      for (ii = k+1; ii < nbBlockRow; ii++) {
          #pragma omp task untied firstprivate(k, ii) \
                      shared(blockSize, blockSizeRow, blockSizeCol, it_rownx, it_colnx, it_fd,
                          it_fl, it_fu, it_ml)
          lowerBlockSolverParallel(ii*blockSize, blockSizeRow[ii], it_rownx,
                              k*blockSize, blockSizeCol[k], it_colnx,
                              it_fd, it_fl, it_fu, it_ml);
```

```
        }
    }
```

In these code, we use one of the latest feature of OpenMP, directive task, which has been only supported since OpenMP 3.0. By using this directive, we can take advantage of taskification of the code and prevent the potential of load balancing problem.
One common problem on working with blocking-algorithm is the block size. It is impossible to find out a optimal value for the blockSize that is able to change the performance of program largely. After some experiments with typical sparse matrices of XLIFE++, one simple formula is provided to specify blockSize.

```
const Number BLOCKFACTOR = 0.05*std::min(nbOfRows(),nbOfColumns());
Number numBlockMin = BLOCKFACTOR;
Number blockSize   = std::floor(diagonalSize()/numBlockMin);
Number nbBlockRow = std::ceil(nbOfRows()/blockSize);
Number nbBlockCol = std::ceil(nbOfColumns()/blockSize);
Number numBlock = std::min(nbBlockRow, nbBlockCol);

std::vector<Number> blockSizeRow(nbBlockRow, blockSize), blockSizeCol(nbBlockCol, blockSize);
blockSizeRow[nbBlockRow-1] = nbRows_ - (nbBlockRow-1)*blockSize;
blockSizeCol[nbBlockCol-1] = nbCols_ - (nbBlockCol-1)*blockSize;
```

Again, this value is only "good" for a certain group of sparse matrices. It maybe needs changing in the future.

# A External libraries

## A.1 Installation and use of Blas and Lapack libraries

Using UmfPack or Arpack means using Blas and Lapack libraries. XLiFE++ offers the ability to choose your Blas/Lapack installation :

- Using Blas/Lapack installed with UmfPack or Arpack
- Using default Blas/Lapack installed on your computer
- Using standard Blas/Lapack libraries, such as OpenBlas.

To do so, you juste have to use XLIFEPP_LAPACK_LIB_DIR and/or XLIFEPP_BLAS_LIB_DIR to set the directory containing Lapack and Blas libraries:

```
cmake [...] -DXLIFEPP_BLAS_LIB_DIR=path/to/Blas/library/directory
    -DXLIFEPP_LAPACK_LIB_DIR=path/to/Lapack/library/directory path/to/CMakeLists.txt
```

**XLIFEPP_LAPACK_LIB_DIR** and/or **XLIFEPP_BLAS_LIB_DIR** options are useless if you do not activate configuration with UmfPack or Arpack

## A.2 Installation and use of UmfPack library

The prerequisite to make use of UmfPack is to have it installed or at least its libraries are compiled. The *umfpackSupport* can be linked with or without UmfPack in case of none of its functions is invoked. Otherwise, any try to use its provided functions can lead to a linkage error. Details to compile and install UmfPack can be found at `http://www.cise.ufl.edu/research/sparse/umfpack/`. All the steps will be described below supposing UmfPack**already installed or compiled** in the user's system.

In order to make use of UmfPack routines, user must configure CMake with options: XLIFEPP_ENABLE_UMFPACK, XLIFEPP_UMFPACK_INCLUDE_DIR and XLIFEPP_UMFPACK_LIB_DIR.

```
cmake -DXLIFEPP_ENABLE_UMFPACK=ON
    -DXLIFEPP_UMFPACK_INCLUDE_DIR=path/to/UMFPACK/include/directory
    -DXLIFEPP_UMFPACK_LIB_DIR=path/to/UMFPACK/library/directory path/to/CMakeLists.txt
```

Theoretically, UmfPack does not need to use Blas/Lapack, but as it is highly recommended by UmfPack (for accuracy reasons), XLiFE++ demand that you use Blas/Lapack.

UmfPack is provided by SuiteSparse. When looking how UmfPack is compiled, it seems that it can depend (maybe in the same way as Blas/Lapack) from other libraries provided by SuiteSparse.

In this case, you have a simpler way to define paths: by using XLIFEPP_SUITESPARSE_HOME_DIR. When given alone, it consider the given directory as the home directory containing every library provided by SuiteSparse with a specific tree structure. If it is not the case, you can use more specific options of the form XLIFEPP_XXX_INCLUDE_DIR and XLIFEPP_XXX_LIB_DIR, where XXX can be AMD, COLAMD, CAMD, CCOLAMD, CHOLMOD, SUITESPARSECONFIG or UMFPACK.

## A.3 Installation and use of ARPACK++ library

ARPACK++ distribution can be obtained from the following URL: http://www.ime.unicamp.br/~chico/arpack++/. However, because of the deprecation of this version, a patch at http://reuter.mit.edu/index.php/software/arpackpatch/ needs applied to make sure a correct compilation. Users of Unix-like system can follow the instructions on https://help.ubuntu.com/community/Arpack%2B%2B to make the patch. And this patch is often not enough to compile correctly with recent compilers.
So XLIFE++ contains its own patched release of ARPACK++, used by default.

Because ARPACK++ is an interface to the original ARPACKFORTRAN library, this library must be available when installing the C++ code. Although FORTRAN files are not distributed along with ARPACK++, they can be easily downloaded from Netlib and are even available under some Unix-like systems.
The BLAS and LAPACK routines are required by the ARPACKFORTRAN, so make sure these two libraries are installed in the system. Like ARPACK, these two libraries are available under some Unix-like systems.
By default, the intern eigensolver of XLIFE++ is used for calculating eigenvalues and eigenvectors. To make use of ARPACK++, users must configure CMAKE with options : XLIFEPP_ENABLE_ARPACK and XLIFEPP_ARPACK_LIB_DIR. The current directory is the root directory containing XLIFE++ source code. To enable ARPACK, we use the command:

```
cmake -DXLIFEPP_ENABLE_ARPACK=ON -DXLIFEPP_ARPACK_LIB_DIR=path/to/arpack/libraries/directory
    path/to/CMakeLists.txt
```

After configuring, we can make the library

```
make
```

Now, there is additional options. Indeed, the default behavior of XLIFE++ installation process is to compile and use a provided distribution of ARPACK. If you want to configure XLIFE++ with another distribution, you may set the option XLIFEPP_SYSTEM_ARPACK to ON.
At last, when a system distribution of ARPACK is such that the name of the library file contains the version number, the standard detection process of CMAKE will not find it. In this case, instead of setting XLIFEPP_ARPACK_LIB_DIR, you will use XLIFEPP_ARPACK_LIB.

# B Documentation policy

The documentation policy of the library is based on three complementary documentations:

- a online documentation compliant with DOXYGEN syntax,
- a user documentation describing main features of the library with some examples,
- a developer documentation describing as possible all the features and given additional explanations.

It is the responsibility and the duty of the developers to write these documentations **in English**.

## B.1 Inline documentation

The inline documentation is compliant with DOXYGEN syntax and the html documentation is automatically generated with majors updates by the source control manager.
This inline documentation follows a documentation convention available on the development page of the XLIFE++ website: http://uma.ensta-paristech.fr/soft/XLiFE++/ . We will sum it up now in the following:

### B.1.1 General points

1. The reference language of the documentation is English.
2. Function or operation declarations are documented with brief (one-line, one-sentence) comments and only brief comments.
3. Function or operation definitions (inline or not) are documented by detailed comments.

### B.1.2 Documentation of a file

Here is the structure of the comment you have to write to document a file (header or source) :

```
/*!
    brief comment

    \file Parameter.hpp
    \author T. Anderson
    \date 25 jan 2011
    \since 3 mar 2007

    next part of detailed comment
 */
```

This comment is dedicated to present the content of the file: list of classes, list of external functions, ... It is written at the top of the file before everything else.

Some additional remarks:

- Thanks to the QT_AUTOBRIEF = YES parameter, the first line of the comment is interpreted as the brief comment. Therefore, the brief comment has to be placed before everything else. There is another solution with the macro \brief:

```
/*!
    \file Parameter.hpp
    \author T. Anderson
    \date 25 jan 2011
    \since 3 mar 2007

    \brief brief comment

    next part of detailed comment
 */
```

- The \date macro is the last modification date.
- The \since macro is the file creation date.
- When there are several authors, you will use the \authors macro:

```
/*!
    brief comment

    \file Parameter.hpp
    \authors T. Anderson, R. Cypher
    \date 25 jan 2011
    \since 3 mar 2007

    next part of detailed comment
 */
```

In this case, authors are separated by commas.

The file documentation rules are:

1. The file documentation is written at the top of the file, before everything else,
2. The file documentation follows one of the previous syntaxes, with the 4 pieces of information file name, author(s), creation date and last modification date.

### B.1.3 Documentation of a class, a typedef, an enum or a struct

1. A class documentation is written just before the class declaration/definition in the header file.
2. The structure of the class documentation is as follows:

```
/*!
    \class A
    brief comment associated to A

    next part of detailed comment associated to A
 */
class A {
...
};
```

3. To document a typedef, you will use the \typedef macro instead of the \class macro.
4. To document a struct, you will use the \struct macro instead of the \class macro.
5. To document an enum, you will use the \enum macro instead of the \class macro.

### B.1.4 Documentation of attributes

1. Attributes can be documented according to one of the following syntax:

```
class A {
  public :
    //! comment associated to i
    int i;
    double j; //!< comment associated to j
    /*!
      comment associated to k
     */
    B k;
    ...
```

### B.1.5 Documentation of functions and constructors

1. Functions and operations declarations are documented with a brief comment, and only a brief comment. The syntax, shown here for operations but valid for external functions, is one of the following :

```
class A {
  public :
    ...
   //! brief comment associated to declaration of f
   void f();

   /*!
       brief comment associated to declaration of g
    */
   void g();

   void h(); //!< comment associated to declaration of h
};
```

2. Functions and operations definitions (inline or not) are documented with detailed comments. If the declaration has not been commented first, the first line of the comment will be the brief comment, as seen in previous sections. The syntax, shown here for inline operations but valid for the others types, is one of the following:

```
class A {
  public :
    B b;
    ...
   //! comment associated to definition of f
   void f() {
   ...
   }
   void g() //! comment associated to definition of g
   {
   ...
   }
   A() //! comment associated to definition of composite constructor
   : B()
   {
   ...
   }

   /*!
      comment associated to definition of h
    */
   void h() {
   ...
   }
};
```

You may notice that for the function g, the comment marking is //! and not //!< and that for the constructor in the same case, the comment is placed before components constructor calls.

Let's see how to document function arguments.

### B.1.6 Documentation of arguments

1. In the case only of a function definition (or an operation definition), you may want to document arguments and return value. The syntax is one of the following :

```
/*!
    comment of function f
 */
int f (double d, //!< comment of d
       int i //!< comment of i
      ) {
...
}
/*!
    comment of function g
    \param d comment of d
    \param i comment of i
    \return comment of return value
 */
int g (double d, int i) {
...
}
```

## B.2 User and developer documentation

User documentation as well developer documentation have to be written **in LaTeX format**. Each tex file concerns a package of files of the library, namely a topics of the library, for instance Parameters. For each package *xxx*, two files have to be written: the user documentation file, named *xxx.tex* placed in subdirectory `doc/pdf/inputs/dev/` and the developer documentation file, also named *xxx.tex*, but placed in the subdirectory `doc/pdf/inputs/usr/`. In these files, there are only latex section items (one or fewer) and subsection items, no chapter items. All these files are collected in the main tex files: *user_documentation.tex* and *dev_documentation.tex* in chapter environment, each chapter corresponding to a folder of the library.

For instance, the Parameters user documentation (*Parameters.tex*) looks like:

```
\section{Parameters classes}

In order to attached some user's data to anything (in particular functions), two classes
(Parameter and Parameters) are proposed. The \class{Parameter} class handles a single data
of type \emph{integer, real, complex, string} or \emph{void *} with the possibility to name
the parameter. The \class{Parameters} class handles a list of \class{Parameter} objects.\\

\subsection{The \class{Parameter} object}

It is easy to define a parameter by its constructor or the assignment operation:
...
\subsection{The \class{Parameters} object: List of parameters}
...
```

The Parameters developer documentation (*Parameters.tex*) looks like:

```
\section{Parameters}

It may be useful to have a data structure to store freely any kind of parameters (values,
string, ...) with a very simple interface for the end user. In particular, such structure
could be attached to user functions (see chap. \ref{chapfunctions}). This is achieved with
two classes: the \class{Parameter} class which define one parameter and the
\class{Parameters} class which manages a list of \class{Parameter} objects.

\subsection{The \class{Parameter} class}

The aim of the \class{Parameter} class is to encapsulate in the same structure, a data of
integer type, real type, complex type, string type and pointer type (void pointer) with the
capability to name the parameter. Thus, this class proposes as private members:
...
\subsection{The \class{Parameters} class}
...

\displayInfos{library=utils, header=Parameters.hpp, implementation=Parameters.cpp,
 test=test\_Parameters.cpp, header dep={config.h, String.hpp}, stl dep={map, iostream,
sstream}}
```

- The end of a file has to be exposed the file dependences with the following form:

| | |
|---:|:---|
| library : | **utils** |
| header : | **Parameters.hpp** |
| implementation : | **Parameters.cpp** |
| unitary tests : | **test_Parameters.cpp** |
| header dependences : | **config.h, String.hpp** |

For this purpose, you have to use the \**displayInfos** macro.

- To handle some C++ lines, you have to use the environment *lstlisting*:

```
\begin{lstlisting}
class Parameter
{...};
\end{lstlisting}
```

```
class Parameter
{...};
```

or if you want to ignore language colors:

```
\begin{lstlisting}[language={}]
class Parameter
{...};
\end{lstlisting}
```

```
class Parameter
{...};
```

The language coloring is automatic. You can add words in the language coloring database in the file *xlifepp-listings-style.sty*.

- When you name a class, for example `Messages`, you have to use the \**class** macro:

```
The \class{Messages} class
```

- When you name a sublibrary of XLiFE++ (a subdirectory of src), you have to use the **\lib** macro:

  ```
  The \lib{utils} library
  ```

- When you name a function, you have to use the **\cmd** macro:

  ```
  The \cmd{findDomain} function
  ```

- When you name the library XLiFE++, you have to use the **\xlifepp** macro. For external libraries of softwares, such as Gmsh or Arpack++, you have to use **\gmsh** or **\arpackpp** macros. The full available list is : **\xlifepp**, **\gmsh**, **\arpack**, **\arpackpp**, **\blas**, **\lapack**, **\umfpack**, **\eispack**, **\melina**, **\melinapp**, **\montjoie**, **\paraview**, **\freefem**, **\doxygen**, **\cmake**, **\git** and **\convmesh**.

- When you add a package documentation in *user_documentation.tex* or *dev_documentation.tex*, you have to use the **\inputDoc** with the basename of the file in argument, and to add it in the main itemize of the library:

```
\chapter{The \lib{utils} library}

The \lib{utils} library collects all the general useful classes and functionalities of the
\xlifepp library. It is an independent library. It addresses:

\begin{itemize}
\item \class{String} capabilities (mainly additional functions to the
\class{std::string} class)
\item \class{Point} class to deal with point of any dimension
\item \class{Vector} class to deal with numerical vectors (say real or complex vectors)
\item \class{Matrix} class to deal with numerical matrices with dense storage (small
matrices)
\item \class{Parameter} classes to deal with general set of user parameters
\item \class{Function} class encapsulating user functions
\item \class{Messages} classes to handle error, warning and info messages
\end{itemize}

\inputDoc{String}
\inputDoc{Point}
\inputDoc{Vector}
\inputDoc{Matrix}
\inputDoc{Parameters}
\inputDoc{Functions}
\inputDoc{Messages}
```

- When you add a general documentation in *user_documentation.tex* or *dev_documentation.tex*, you have to use the **\inputDoc*** with the basename of the file in argument, and to add it in the main itemize of the library:

```
\chapter{Tests policy}

In order to maintain backward compatibility of the code during its development, it is
mandatory to have various test functions. Some of them are local test functions, says
low level tests, and concerns "exhaustive" tests of functionalities of a class or a
collection of classes or utilities. Others are global test functions, say high level test
functions, involving a lot of classes of the library, for instance, solving a physical
problem from the mesh up to the results.

\inputDoc*{tests_policy}
```

# C Tests policy

In order to maintain backward compatibility of the code during its development, it is mandatory to have various test functions. Some of them are local test functions, says low level tests, and concerns "exhaustive" tests of functionalities of a class or a collection of classes or utilities. Others are global test functions, say high level test functions, involving a lot of classes of the library, for instance, solving a physical problem from the mesh up to the results.

## C.1 Test families and test functions

### C.1.1 Tree structure

#### Root directory

Tests are hosted in the `XLIFEPP_HOME/tests` directory. Here, there are `XLIFEPP_HOME/tests/testUtils.hpp` and `XLIFEPP_HOME/tests/testUtils.cpp`, defining a wide range of utility functions.
`XLIFEPP_HOME/tests/testUtils.hpp` has to be included by every test file.

#### Reference Data and log

Reference data are stored in `XLIFEPP_HOME/tests/inputs`. They are organised in subdirectories whose names are the name of the test they are about. For instance, `XLIFEPP_HOME/tests/unit_Domain`.
Log files are stored in `XLIFEPP_HOME/tests/res`. Their names are the same as the test they are about. For instance, `XLIFEPP_HOME/tests/res/unit_Domain.res`.

#### About test families

There are several families of tests:

**unit** Unitary tests are aimed to test each function of each class separately. In fact, it is easier to say it than to do it. But with a very large set of unitary tests, one can avoid most of bugs.

**sys** System tests are aimed to test some user applications but with size of the linear systems not too big.

**dev** Developer tests are aimed to test new functionalities someone is developing. These tests are often like system tests, but are supposed to be deleted as soon as functionalities are fully developped. This family can also be used to check error convergence and cputime for larger problems.

**ext** External tests are aimed to test wrappers to external libraries, such as ARPACK and UMFPACK. These tests will be integrated in the **unit** family in the end.

Each family correspond to a subdirectory of *XLIFEPP_HOME/tests*.

### C.1.2 Definition of a test function

A test function is a usual c++ function with a meaningful name **prefixed by the family name it belongs to** defined in a file with the same name. The test function takes an optional boolean as input argument and returns a string (String class). For instance, for the unitary tests of the class `GeomDomain`, the file *unit_Domain.cpp* in the *unit* directory looks like:

```
/*! \file unit_Domain.cpp
    \author XXX
    \since YYY
    \date  ZZZ
*/
#include "xlife++-libs.h"
#include "testUtils.h"

namespace unit_Domain {

...

void unit_Domain(bool check)
{
  String rootname = "unit_Domain";
  trace_p->push(rootname);

  Number nbErrors = 0;
  String errors;

  ...

  if (check)
  {
    if (nbErrors == 0 ){ theCout << message("test_report", rootname, 0, ""); }
    else { error("test_report", rootname, nbErrors, ":\n"+errors); }
  }
  else { theCout << "Data updated " << eol; }

  trace_p->pop();
}

}
```

The `String` `errors` has to contain information about the errors occuring during the test in order to easily locate them. When errors occurs, an error message with format `test_report` displays the number of errors (computed and stored in the `Number` `nberrors` variable) and every error, by specifying which part of the tests and which line of the generated data are concerned.
**It is up to developers to write meaningful tests and as many exhaustive tests of the class functionalities as possible.**

### C.1.3 Development of a test function

There are mainly two approaches to make a test:

- internal value testing: compare results to expected results inside the function (value comparison),
- external value testing: comparing results to reference results get previously and stored in a file (ascii comparison).

Both of them works with a wide range of `checkValues` or `checkValue` available functions, overloaded for quite every kind of datatype to be tested. These functions are defined in `XLIFEPP_HOME/tests/testUtils.hpp` and `XLIFEPP_HOME/tests/testUtils.cpp`.

For instance, the following internal value testing comes from `unit_HMatrix` (the computed norm is tested to be equal to 9.03223055164e-17 with a tolerance or 1e-6.) :

```
nbErrors+=checkValue(norm(Bx-B0x), 9.03223055164e-17, 1e-6, errors, "exact HM/LM  |Bx-B0x|");
```

and the following external value testing comes from `unit_Geometry` (the string to be tested contains a range of unitary tests of member functions of class `BoundingBox`:

```
nbErrors += checkValue(theCout, rootname+"/BoundingBox.in", errors, "Test of BoundingBox class",
    check);
```

Here, you have the general case of external value testing. By using the stream `theCout` in tests, you fill the log file and a string. The content of this string will be compared with the content of a reference file (.in extension). The external value testing is rather dedicated to the tests of classes and functionalities which involve a lot of basic tests.

> ⚠ `checkvalue(s)` routines clears the internal string of variable `theCout`. If you intend to write a "test" whose output is not meant to be tested but only printed in the log file, you have to use `thePrintStream` instead of `theCout`.

### C.1.4 Includes

As you may have noticed in previous listings, a test file, whatever its family always includes 2 headers: `xlife++-libs.h` and `testUtils.hpp`.

## C.2 Test of a new version of the library

This section addresses the process of global test involved before a minor or major upgrade of the library. It concerns the administrators of the library.

### C.2.1 Compilation of tests

When compiling tests, each individual test is compiled, but also one global test per family. There is also a specific global test running both unit and sys test families. When compiling a global test, CMAKE sources all files in the corresponding directory prefixed by the family. If a source file does not respect this naming convention, it is ignored.

### C.2.2 Running tests

The administrators have a special tool to run a lot of tests, *xlifepp_test_runner.rb*. This is a `Ruby` script that runs one executable without compiling it if it does not exist.

```
xlifepp_test_runner.rb deals with all automatic tasks such as updating doxygen, generating
    commit history and generating snapshots and releases

SYNOPSIS:
    xlifepp_test_runner.rb -c [-n] <test>
    xlifepp_test_runner.rb -e [-n] <test>
    xlifepp_test_runner.rb -h

DESCRIPTION:
    XLiFE++ is a C++ library with a large set of tests. Each test can be launched in 2 modes :
      - the edit mode (default in XLiFE++ executables) makes tests generating results file, so
          called res file
      - the check mode (default in xlifepp_test_runner.rb) makes tests comparing results to the
          current res file

    As XLiFE++ compilation is based on CMake, it is not a good way to define running targets,
        because
    of generators (to Eclipse, XCode, Visual Studio, CodeBlocks, ...). On the one hand, the
        lesser targets
    there are the easier XLiFE++ is to compile and run, on the other hand targets in generators
        are not just
    compilation targets: you can run them, and pass parameters to them.
    However, XLiFE++ developers using cmake in command-line mode must have an easy way to run
        tests.
    That's what xlifepp_test_runner.rb is for !!!

OPTIONS:
    -h, --help                      shows the current help
    -c, --check                     test will be run in check mode (default)
    -cxx, --cxx-compiler            sets the compiler to use
    -e, --edit                      test will be run in edit mode
    <test>                          name of the test (Examples: all, unit_Mesh_gmsh, sys_1d, ...)
    -n                              activates dry-run mode
    -v                              activates verbose level (same as --verbose-level 1)
    --verbose-level <num>           allows to set the verbose level. Default is 0, none.
```

# D Compiling and linking policy

## D.1 General purpose

With XLiFE++, we want to develop a C++ library, that we can use easily and at list on Windows, Unix and Mac OS platforms. The last two are very similar, whereas the Windows platform is a very different working environment as far as compiling is concerned. Generally, developing code on Windows means the use of an IDE, such as Visual Dev C++, Eclipse, CodeBlocks, ... On Unix and Mac OS, you can use a "basic" text editor and Gnu Makefile. You can also use IDE, such as XCode on Mac OS.
As we do not want to impose an IDE, the multi-platform solution comes with CMake!!!

## D.2 CMake and IDE generators

### D.2.1 CMake and Windows

It is very easy to have a IDE generator with CMake. The GUI was very well thought. The most important part is to give the path to the CMakeLists.txt file.

### D.2.2 CMake and Unix or Mac OS

If you does not want to use an IDE, you just have to execute the following command :

```
cmake PATH_TO_CMakeLists.txt
```

### D.2.3 New files and IDE generators

When you change the name of some source files or delete some source files or create source files, you have to rerun CMake to take them into account. If you modify file contents, it is unnecessary.
This means you have to rebuild the IDE generator you use. A new file will not be detected and compiled.

## D.3 CMake and XLiFE++

Whatever your OS or IDE choice, you may have to go to the `build` directory to launch CMake. As a result, every file generated by CMake will be in this directory, even for a IDE generator. The `CMakeLists.txt` file is in the XLiFE++ root directory.

How does the `CMakeLists.txt` work ?

### D.3.1 Building libraries

First, it lists all files in the `src` directory with extension .hpp or .cpp and extracts the names of the direct sub-directories of `src`. This list is the list of the libraries to compile.
Then, for each library, it lists all files with extension .hpp or .cpp and builds targets for the library generation. The name of the lib is libXXX.a where XXX is the name of the directory in the lib list and is supposed to be placed in the `lib` directory. More precisely, it will be in subdirectories of `lib` whose names are built according to the compiler used (version included), the architecture of the computer, and the build type (debug, release, ...).

### D.3.2 Building and linking test executables

CMAKE lists all files in the `tests` directory with pattern XXX/XXX_YYY.cpp. Each of these files correspond to a function having the same name. CMAKE uses a template file to build the test main program : main_XXX_YYY.cpp. The main function will take an argument, edit or check, to define the value of the boolean check.
These files are placed in the sub-directory `build` of the directory `tests` are are linked to an executable. Furthermore, one additional file is generated : main_test.cpp to launch all tests.