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Ricerca di Sistema elettrico

Integration of the FELMORE Code in the Salome Platform

A. Cervone, D. Cerroni, R. Da Vià, F. Menghini, S. Manservizi, G. Pozzetti

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Il presente documento descrive le attività di ricerca svolte all’interno dell’Accordo di collaborazione "Sviluppo competenze scientifiche nel campo della sicurezza e collaborazione ai programmi internazionali per il nucleare di IV generazione"

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Titolo

INTEGRATION OF THE FEMLCORE CODE IN THE SALOME PLATFORM

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Sommario

In this report we describe the integration of the FEMLCORE code in the SALOME platform. The SALOME platform is an open source tool that has a CAD, a mesh generator and a visualization software integrated for model development. This integration represents a main step in the direction of coupling FEMLCORE with a nuclear system code like CATHARE, in order to drive three-dimensional simulation with boundary conditions obtained with the system code.
The CATHARE/SALOME interface is developed by CEA and EDF and it can be used only under private agreement. We substitute CATHARE with a mono dimensional code based on the SALOME integrated libMesh library which is open-source software. CEA and EDF originally developed the libMesh-SALOME interface for Laplacian and Linear Elastic two-dimensional solutions. Here we present 3D-CFD/3D-CFD coupling for energy and Navier Stokes with libMesh and FEMus libraries. Simulations with FEMLCORE (3D-porous) and the FEMUS interface are presented where the interface is used to transfer data for heat generation and pressure loss analytical distributions. Finally a 3D-porous/1D-porous coupling FEMLCORE/libMesh is presented.

Note

Il presente contributo è stato preparato con il contributo del personale ENEA e CIRTEN:
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Integration of the FEMLCORE code in the SALOME platform

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Introduction

Computational simulation of nuclear reactor is of great importance for design, safety and optimal use of fuel resources. Unfortunately a complete simulation of nuclear systems in three-dimensional geometries is not possible with the current available computational power and therefore it is necessary a multiscale approach where the global system is solved at a mono-dimensional level and only some components of interest are solved in great details.

In the previous reports the multiscale code FEMLCORE has been developed for LF reactor of generation IV in the framework of this multiscale approach. Mono-dimensional and three-dimensional modules have been created with appropriate interfaces [2, 3]. Porous modules have been developed for the reactor core where a detailed computation of all the reactor channels inside all the assemblies is not still possible [2, 3, 4]. Simplified freezing modules have been adapted to compute the thermal hydraulics of the reactor when solidification may occur [10, 5].

The mono-dimensional system code implemented in the FEMLCORE module is based on the balance equations [4, 5]. System codes cannot reproduce a multidimensional physical systems such as a nuclear reactor because they are based only on mono-dimensional physical principles and they need experimental data to add the missing information. One of the main goal of the FEMLCORE project is to include, as mono-dimensional modules, system codes validated with nuclear data. In order to do this we must integrate the FEMLCORE in the SALOME platform where several nuclear system codes are available.

SALOME is an open source generic platform for preprocessing and postprocessing of numerical simulations, developed by CEA and other institutions [32]. In the platform there are modules needed for multi-dimensional CFD computations and for system codes. There are tools for preprocessing CAD applications (GEOM) and for generating meshes (MESH). With the GEOM application one can create, modify, import, export (IGES, STEP and BREP format), repair and fix CAD models. With the MESH application one can edit, check, import and export meshes (in MED, UNV, DAT and STL formats). These modules are fully integrated in the SALOME platform. There are also postprocessing tools to analyze simulation data such as PARAVIS (PARAVIEW). PARAVIEW is an open-source, multi-platform data analysis and visualization application. The data analysis can be done interactively in three-dimension or using PARAVIEW's batch processing capabilities [28].

This platform has been conceived not only to collect a series of codes that have been extensively used in the field of thermal hydraulics of nuclear reactors but also to harmonize them with the aim of solving complex problems by exchanging information among different codes over a common platform and on large multiprocessor architectures. SA-

LOME can also be used as a platform for the integration of external third-party numerical codes to produce a new application with full pre and postprocessing management of CAD models.

The European NURESAFE (ex NURISP) project is planned to be based on the SALOME platform. The project has started with the CATHARE, NEPTUNE and TRIO_U codes as independent codes, with not compatible input and output formats [6, 7]. CATHARE is a Code for the Analysis of Thermal Hydraulics during an Accident of Reactor and safety Evaluation for LWR [22]. This system code is used mainly for PWR safety analysis, accident management and definition of plant operating procedures. It is also used to quantify conservative analysis margins and for nuclear reactor licensing [23, 24]. TRIO_U and NEPTUNE codes solve the flow equations in multidimensional geometries with particular attention to two-phase flow [26, 25]. CATHARE, NEPTUNE and TRIO_U are developed by CEA and EDF and they can be used only under NURESAFE project agreement. In particular we are interested in the CATHARE system code [22, 23, 24]. The CATHARE system code, like other important nuclear codes, have been developed with an interface on SALOME platform for coupling and integration [24, 27]. At the moment the platform is based on computational tools for light water reactors but many of the codes may be adapted to liquid metals simulations.

The integration of a code on the SALOME platform is obtained by generating an interface with functions available in the MEDMem library (provided in the SALOME platform) that allows the data transfer from the platform to the code and viceversa. Two different codes both with SALOME MEDMem interface can transfer data to the interface and then from the interface to the other code. All the data operations of the SALOME platform involve files in MED (Modèle d'Échange de Données) format. MED is a data storage format based upon the HDF library [35]. The HDF format is largely used and will probably become the standard in a short future. However the implementation in MED format is rare. In the SALOME platform a MED module is implemented. The MED module provides a library for storing and recovering computer data in MED format associating numerical meshes and fields, thus allowing the exchange between different codes and solvers. Inside SALOME these structures are exchanged between solvers at the communication level (CORBA or MPI) offering common read/write functions through MED files.

The MED data model defines the data structures exchanged by codes. The modeled data concern geometrical data and the resulting fields that can be defined on nodes. MED supports eight element shapes: point, line, triangle, quadrangle, tetrahedron, pyramid, hexahedron, polygon and polyhedron. Each element has a different number of nodes, depending on linear or quadratic interpolation. MED defines also numbering conventions and therefore a standard for data storage in HDF5 format. The MED libraries are divided into three groups of functions: MED File, MED Memory and MED CORBA. The first group (MED File) is a C and FORTRAN API that implements mesh and read/write functions into files with `.med` extension. These files are in HDF5 format. The MED Memory group, which is a C++ and Python API, creates mesh and field objects in memory. Mesh creation can be done using set functions, or by loading a file. Fields are also created loading files or by initialization with user-defined functions.

Finally the group of functions called MED CORBA allows distributed computation inside SALOME [32]. In order to have a working platform, common input and output formats should be harmonized between different codes. This can be achieved by using SALOME as the basic platform taking care of the data exchange between codes and of the distributed computation between different clusters.

In this report we describe the integration of the FEMLCORE code in the SALOME platform. This is the first step in the direction of coupling FEMLCORE with a system code, like CATHARE, to simulate the entire primary loop inside the SALOME platform. The CATHARE-SALOME interface is developed by CEA and EDF and it can be used only under agreement. Therefore in this report we developed a mono dimensional code with the libMesh library. The interface libMesh-SALOME was developed by CEA and EDF for Laplacian and Linear Elasticity solution but libMesh library is open-source software.

Chapter 1 is devoted to the integration of the libMesh and FEMLCORE (FEMus) libraries in SALOME platform. An interface class called FEMUS is developed following the construction of the interface class LIBMESH (developed originally by CEA and EDF) that allows the data transfer from/to FEMLCORE and any platform integrated code.

In Chapter 2 there is a description of many coupling tests carried on with LIBMESH and FEMUS interface. 3D-CFD/3D-CFD coupling for energy and Navier Stokes equations are presented with codes based both on libMesh and FEMus libraries. 3D-CFD/1D-CFD coupling for energy equation are also investigated. Simulations with FEMLCORE (3D-porous) and the FEMUS interface are presented where the interface is used to transfer data for heat generation and pressure drop analytical distributions. Finally a 3D-porous/1D-porous coupling FEMLCORE-libMesh is presented with the simulation of the core of the design reactor ELSY [13, 14, 15, 16, 17, 18]. The core of this reactor has been modeled and simulated with a 3D-porous model already implemented in FEMLCORE code, while the external primary loop has been simulated with a simple 1D-porous model implemented with libMesh library.

1 Code integration in SALOME platform

1.1 SALOME C++ library integration

In this section we describe the SALOME platform integration procedure with a generic code. Any code that can be reduced in the form of C or C++ libraries could be therefore integrated in the SALOME platform. The integration procedure ends with the generation of a code module that can run in the SALOME platform with or without GUI support and with or without graphical YACS support for code integration. This allows the user to couple the code at the desired level inside the platform.

We divide the procedure in three steps: **generation of the code library**, **generation of the SALOME module** and finally the **implementation of the module** inside the SALOME platform. The description procedure is based on the FEM-LCORE (FEMus) software, where the FEM-LCORE code is an application of the FEMus code. We assume that FEMus is installed in the directory

```
pathtoproj/femus
```

and its FEM-LCORE application in *pathtoproj/femus/USER_APPL/femlcore*. We use the directory *pathtoproj* as a main directory where all the software is supposed to be installed (SALOME, FEM-LCORE (FEMus), HDF5, MPI etc..). We assume that SALOME is installed in the directory

```
pathtoproj/salome
```

together with the MED libraries in *pathtoproj/salome/MED*. In order to use the SALOME platform the environment should be created by setting

```
cd pathtoproj/salome
source env_products.sh
```

where the *env_products.sh* script is available from the package itself in the binary release [32].

The compilation of the SALOME platform is needed to use MPI inside the platform. We remark that if the SALOME is not compiled with MPI then it cannot use MPI to pass MPI parallel information but the code can still run parallel and use MPI on its own [29, 30].

1.1.1 Generation of the C++ code library

In this section we generate a simple code by scratch in order to clarify the SALOME integration procedure. This integration procedure allows the user also to couple any code of the platform with a new one written by the user himself.

As a very simplified example we can consider the integration in the SALOME platform of this simple program: given x and y, the program computes $f = x + 3 * y + sin(x)$. In order to do this we can construct a set of function that can perform addition, multiplication, the operation *sin* and then a main program that combines them to obtain the desired results. The generation of a library code from a set of functions is simple and can be summarized in the following steps. We consider to write a set of functions that we call MATH. We set the application in the directory

```
pathtoproj/femus/contrib/Myapplication
```

where the *pathtoproj* is the directory where all the codes are installed. The application *MATH* must consist of the main directory MATHCPP and the sub-directories: *src*, *include*, *lib*. In the sub-directory *src* we have files *.cxx; in *include* directory we have files *.hxx; in *lib* we have dynamic libraries *.so

Inside the directory *include* one must write the header files for the C++ object oriented class. For example in order to build the MATH class (no MPI) we construct a class header MATH.hxx defined as

```
#ifndef _MATH_hxx
#define _MATH_hxx
#include <vector>

class MATH {
  // Simple class
  public:
   double sum(const std::vector<double>& tab);
   double squareroot(double x);
   double plus(double x, double y);
   double minus(double x, double y);
   double times(double x, double y);
   double sinx(double x);
 private:
   static const double epsilon;
   static const double pi;
 };
```

Inside the directory *src* one writes the source files. For example the MATH class can be defined by two constants

```
const double MATH::pi=3.1415926535897931;
const double MATH::epsilon=1.0E-12;
```

the default constructor and some functions

```
double MATH::squareroot(double x)     {return sqrt(x);}
double MATH::plus (double x, double y){return x+y;}
double MATH::minus(double x, double y){return x-y;}
double MATH::times(double x, double y){return x*y;}
double MATH::sinx(double x)           {return sin(x);}
```

The command to generate the dynamic library libMATHCPP.so in the *src* directory, if the program is parallel, is

```
 mpicxx -o libMATHCPP.so *.cxx -I/pathtoproj/femus/contrib/
             Myapplication/MATHCPP/include/ -lmpi -shared -fPIC
```

or

```
g++ -o libMATHCPP.so *.cxx -I/pathtoproj/femus/contrib/
             Myapplication/MATHCPP/include/ -lmpi -shared -fPIC
```

in the serial case. A file appears with name *libMATHCPP.so* which is the dynamic library just created. We move libMATHCPP.so in the *lib* directory with the name libMATHCXX.so.

Finally we should have in *src* the file MATH.cxx, in *include* the header MATH.hxx and in *lib* the dynamic library libMATHCXX.so. By starting from a set of functions we have now a library of functions.

1.1.2 Generation of the a SALOME module by using YACS-GEN

At this point we have the directory *Myapplication* which has MATH.cxx in *src* , MATH.hxx in *include* and libMATHCXX.so in *lib*. The environment for MATHCPP can be set by

```
export  MATHCPP_ROOT_DIR=/pathtoproj/femus/
                               contrib/Myapplication/MATHCPP/
```

In order to create a SALOME module with relative YACS functions one must run a python script by typing

```
python math_component.py
```

The script will use YACS-GEN module to generate the needed functions and modules and it can be written only in python language. This is the general form for the script:

```
#! /usr/bin/env python
import os
from module_generator import Generator,Module,Service,HXX2SALOMEComponent
# Generator python function generates the code
#
# grab from environment variables of interest (set by source env_products)
kernel_root_dir=os.environ["KERNEL_ROOT_DIR"]
gui_root_dir=os.environ["GUI_ROOT_DIR"]
yacs_root_dir=os.environ["YACS_ROOT_DIR"]
```

```
salome_env="pathtoproj/salome/env_products.sh"
#
# create a context, that provide environment information
context={'update':1,
         "makeflags":"-j2",
         "prerequisites":salome_env,
         "kernel":kernel_root_dir,
         "gui":gui_root_dir,
         "yacs":yacs_root_dir
        }
#
# specify a SALOME modules called MATHEMATICS, including one SALOME
# component called MATH
module="MATHEMATICS"
components_name=["MATH"]
components=[]
for compo_name in components_name:
  cpp_root_dir="pathtoproj/femus/contrib/Myapplication/MATHCPP"
  # print
  print compo_name,   components_name,    cpp_root_dir
  # generation of class components
  components.append(HXX2SALOMEComponent("MATH.hxx",
                                  "libMATHCXX.so",cpp_root_dir ) )

# we ask to install the module in pathtoproj/salome/MATHEMATICS
module_root_dir="pathtoproj/salome/MATHEMATICS"

# generate and compile the salome component with yacsgen
g=Generator(Module(module,components=components,prefix=module_root_dir),
                                                                context)
g.generate()
g.bootstrap()
g.configure()
g.make()
g.install()
#
# generate a SALOME application containing :
#   - the MATHEMATICS module,
#   - the native modules GUI, YACS
g.make_appli("appli_math", restrict=["KERNEL"],
                      altmodules={"GUI":yacs_root_dir,
                                  "YACS":yacs_root_dir})
```

The generated module is labeled MATH and it is installed in the SALOME module directory in a new directory called MATHEMATICS. Note that if SALOME is compiled with MPI (this is not the default) then the function *HXX2SALOMEParaComponent* should be used in the above script, replacing *HXX2SALOMEComponent*.

1.1.3 Running a SALOME module by using YACS

After running the script in the main directory *Myapplication* we have two new subdirectories, *MATHEMATICS_SRC* and *appli_math* and two files, *parse_result* and *parse_type_result*. The directory *MATHEMATICS_SRC* is the build directory. The *appli_math* is the directory where the application MATHEMATICS can be launched. A new directory named MATHEMATICS appears in the SALOME main directory *pathtoproj/SALOME*. This module consists of an *include*, *src*, *idl* and *lib* sub-directories.

The file *parse_result* contains the parsing of the function prototypes. In our case the *file parse_result* is

```
Function;double;sum
const std::vector<double>&;tab
Function;double;squareroot
double;x
Function;double;plus
double;x
double;y
Function;double;minus
double;x
double;y
Function;double;times
double;x
double;y
Function;double;sinx
double;x
```

This script generates the new directory *idl* in the module MATHEMATICS. Each function prototype is translated in a different language by parsing the return type and the type argument. For example the prototype *double sum(double x,double y)* gives double as a function return type and has two double input variables. These functions are used for YACS graphical representation. Before running the code one must set the environment for the module with

```
export MATHEMATICS_ROOT_DIR=pathtoproj/salome/MATHEMATICS/
```

From the directory *appli_math* one can start SALOME with this MATH module. Inside this directory two files are important: *config_appli.xml* and *SalomeAppli.xml*.

The file *config_appli.xml* contains

```
<application>
```

```
<prerequisites path="pathtoproj/salome/env_products.sh"/>

<modules>
<module name="KERNEL" path="pathtoproj/salome/KERNEL_7.3.0"/>
<module name="YACS" path="pathtoproj/salome/YACS_7.3.0"/>
<module name="GUI" path="pathtoproj/salome/YACS_7.3.0"/>
<module name="MATHEMATICS" path="pathtoproj/salome/MATHEMATICS"/>
</modules>
</application>
```

where one can see the modules loaded when starting the platform. By adding the location of the GEOM, SMESH, PARAVIS modules the platform can consider the loading of the GEOM, SMESH and PARAVIS modules too [28]. The file *SalomeAppli.xml* contains

```
<document>
  <section name="launch">
    <!-- SALOME launching parameters -->
    <parameter name="gui"        value="yes"/>
    <parameter name="splash"     value="yes"/>
    <parameter name="file"       value="no"/>
    <parameter name="key"        value="no"/>
    <parameter name="interp"     value="no"/>
    <parameter name="logger"     value="no"/>
    <parameter name="xterm"      value="no"/>
    <parameter name="portkill"   value="no"/>
    <parameter name="killall"    value="no"/>
    <parameter name="noexcepthandler"  value="no"/>
    <parameter name="modules"    value="YACS,MATHEMATICS"/>
    <parameter name="pyModules"  value=""/>
    <parameter name="embedded"   value="SalomeAppEngine,study,
                             cppContainer,registry,moduleCatalog"/>
    <parameter name="standalone" value=""/>
  </section>
</document>
```

By substituting YACS, MATHEMATICS with YACS, MATHEMATICS, GEOM, SMESH, PARAVIS the platform starts with GEOM, SMESH and PARAVIS modules too. Before starting SALOME the MATHCPP and MATHEMATICS libraries should be included in the *LD_LIBRARY_PATH* by typing

```
 export LD_LIBRARY_PATH=pathtoproj/femus/contrib/
                  Myapplication/MATHCPP/lib/:$LD_LIBRARY_PATH
 export LD_LIBRARY_PATH=pathtoproj/salome/MATHEMATICS/lib/
                                      salome:$LD_LIBRARY_PATH
```

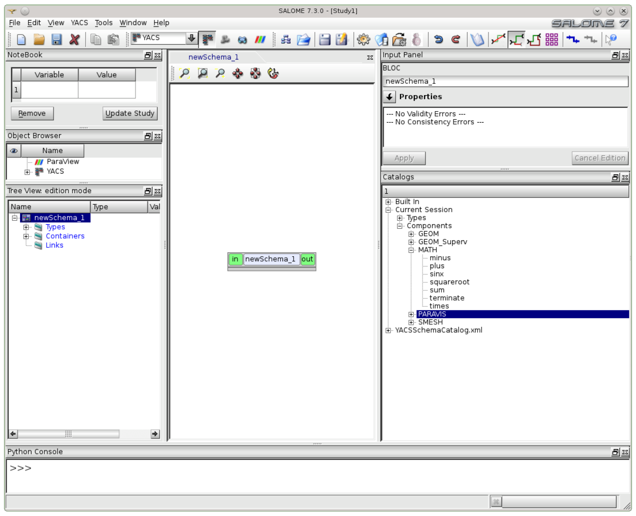


Figure 1.1: YACS with MATH module integration

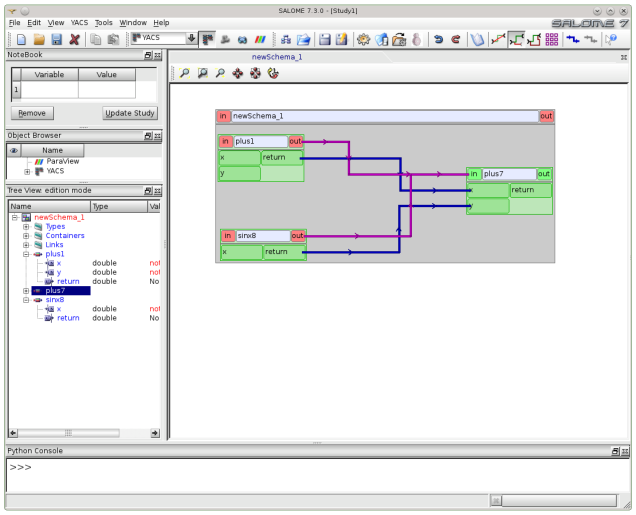


Figure 1.2: Building YACS schema for $f(x, y) = x + y + sin(x)$.

Now we start the YACS module by typing

```
cd appli_math
./runAppli
```

If only the YACS and MATHEMATICS modules are in the platform then SALOME starts with no active modules. One must select the *new* option from the menu to use the YACS module. If more than one module is loaded then a menu appears. We select YACS module and then *Create a new YACS schema*. From Figure 1.1 one can note

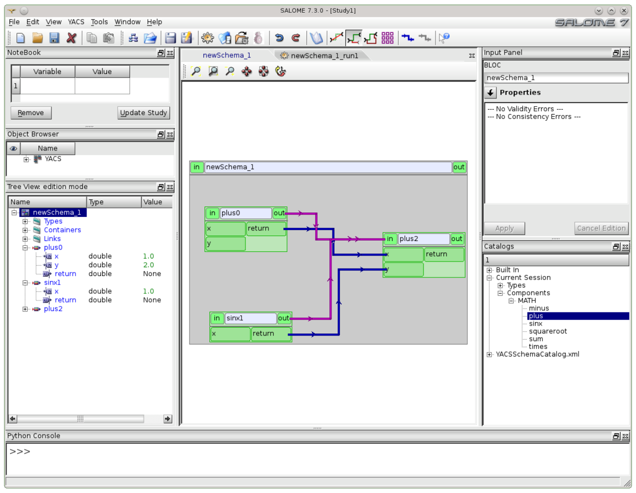


Figure 1.3: Running YACS schema for $f(x,y) = x + y + sin(x)$.

that the functions minus, plus, sum and sin(x) from the MATH module appear on the catalog panel. In order to construct the graphical YACS program that computes $f(x,y) = x+y+sin(x)$ we drag a sum, a sin and a sum function again from the catalog to the main schema. We connect the return of the *plus1* schema block to the x of the *plus7* block and the return of the *sin8* block to the y of the *plus7* block. After this we have a situation as depicted in Figure 1.2.

From the input panel we set the initial x and y value. Then from the menu at the top we choose *Prepare the schema for run* (gear button). A new schema appears which is not editable, from here the code can be run. The tree view on the left shows computation values and errors. It is important to note that an MPI code runs in the YACS schema only if SALOME is compiled with MPI. This may be a limitation in the use of the YACS module since not all MPI functions are implemented correctly in SALOME. However the program can be run in parallel without the use of the graphical environment YACS as it is explained in the next section.

1.1.4 Running directly with a main program

The same program can be run by using a simple main program. For example the same result of the YACS module can be obtained with the following simple program

```
#include "MATH.hxx"
#include <stdio.h>
#include <cmath>
int main(){
  MATH a;
  double x=1.;
  double y=2.;
  double t=a.plus(x,y);
  double s=a.plus(t,sin(x));
  printf(" %f", s);
 return 0;
}
```

This implies that in the SALOME platform a code can run both graphically (YACS) or through simple C or C++ programs. In order to compile this program we must include all the libraries and the paths to MATHCPP directory and MATHEMATICS module. Then the executable program can be launched directly by the YACS graphical interface with a *Pyscript* which can be found in the catalog in the elementary node section of the YACS module.

1.2 libMesh-SALOME integration

The integration of a stand-alone code is more complex but very similar. In this section we describe the integration of the libMesh library in SALOME platform with the aim of using computational modules generated with this library for multiscale coupling. In particular we are interested in coupling 1D modules written with libMesh library with the 3D FEM-LCORE applications using MEDMem library. The libMesh applications are open-source. The integration of an open-source code can be divided into three steps: **generation of the code-library** from the code, **generation of the MEDMem interface** and **SALOME-libMesh interface integration**. The source code is available and one can see how they are build. In non open-source code like CATHARE the source code is not available but we have the binary version of the library. In this case we can get over the first step of generation of the code-library and go directly to the second step.

1.2.1 Generation of the code-library

The generation of the dynamic library from a code is pretty straightforward for modern codes since they are already built as libraries. The main code is simply a collection of call functions to libraries where the algorithms are developed. For old codes, especially in FORTRAN, sometimes a monolithic main program is developed with a few functions in support with experimental data. In this case is straightforward, for developers, to rebuild the code using a library structure. The libMesh code is built using libraries and therefore, after the code installation, nothing should be done.

LibMesh is a parallel solver for PDE which uses the PETSC libraries as a main package solver. The open MPI is supposed to be installed in

```
pathtoproj/openmpi-1.4.5/
```

The version 1.4.5 is installed but the procedure should work also for any upgrade. The installation of the open-mpi libraries is really easy and standard. For details see [30]. The PETSC library is supposed to be installed in

```
pathtoproj/petsc-3.4.3
```

The version 3.4.3 is installed but the procedure should work also for others. We use the *opt* version and not the *dbg* version which one could use for debugging. For further details see [31].

We suppose that the libMesh code is installed in

```
pathtoproj/libmesh-0.9.2.2/
```

The installation can be easily obtained by following the standard procedure on [34]. The libMesh version is the 0.9-2.2. The integration described here does not work for library below version 0.9. The libMesh main directory must contain the *lib* and the *include* sub-directories. In the *lib* sub-directory the dynamic library *libmesh_opt.so.0* is located. The dynamic library *libmesh_opt.so.0* contains all the functions in binary form. In the *include* sub-directory the prototypes are available for obtaining the documentation and to compile.

1.2.2 libMesh-SALOME interface

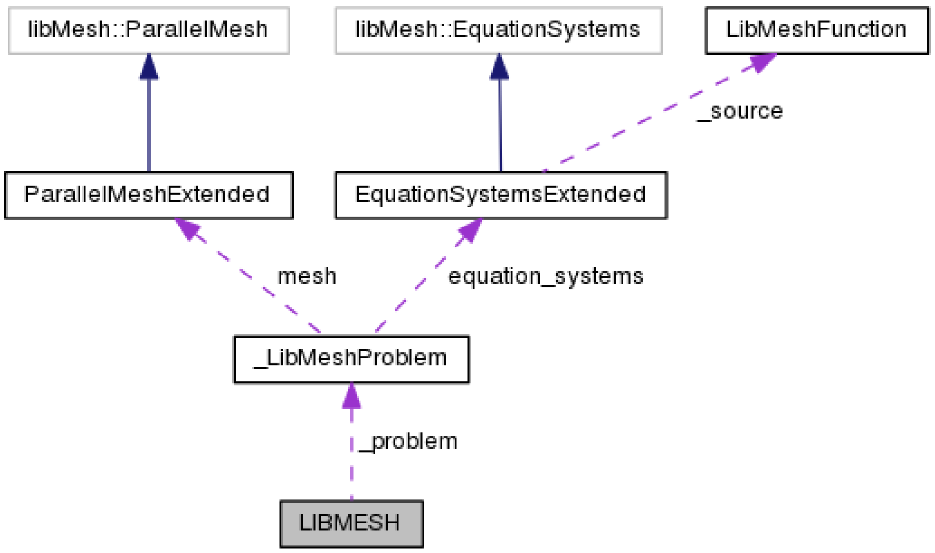


Figure 1.4: Collaboration diagram of the LIBMESH class inside the LibMeshCpp interface

Overview. The interface, called LibMeshCpp, between the MEDMem and the libMesh libraries consists basically of five classes: LIBMESH, LibMeshProblem, EquationSystemsExtended, ParallelMeshExtended and LibMeshFunction. All these classes are located in

```
pathtoproj/femus/contrib/Libmesh_cpp/
```

Each class has a file and a header with the class name and different extension. The LIBMESH class is the interface with the SALOME platform as it is shown in the collaboration diagram in Figure 1.4. This diagram illustrates how the LIBMESH class (interface to SALOME) transfers data to the LibMeshProblem class. In order to interact with the libMesh library two libMesh classes have been extended: the *libMesh::EquationSystems* and the *libMesh::ParalellMesh*.

The *EquationSystemsExtended* class, which uses only MEDMem functions, inherits the *libMesh::EquationSystems* which uses only libMesh functions as shown in Figure 1.5. The *libMesh::EquationSystems* contains the assembly and solver of the libMesh code. The data from the LIBMESH class can be transferred into the assembly routine which is user accessible. The data can also be transferred in the opposite direction from the *libMesh::EquationSystems* to the MEDMem interface. The data flow from *parent* to *son*

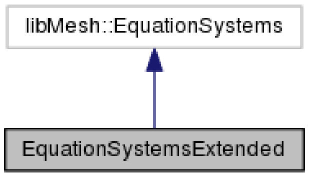


Figure 1.5: Inheritance diagram of the *EquationSystemsExtended* class

class is ensured by the C++ inheritance rules. The flow in opposite direction is defined by a *dynamic_cast* command that allows to use *son* class functions from the *parent* class. For this reason the *parent* class should be polymorphic with at least one virtual function.

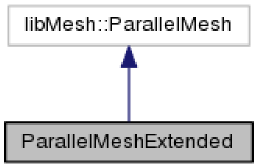
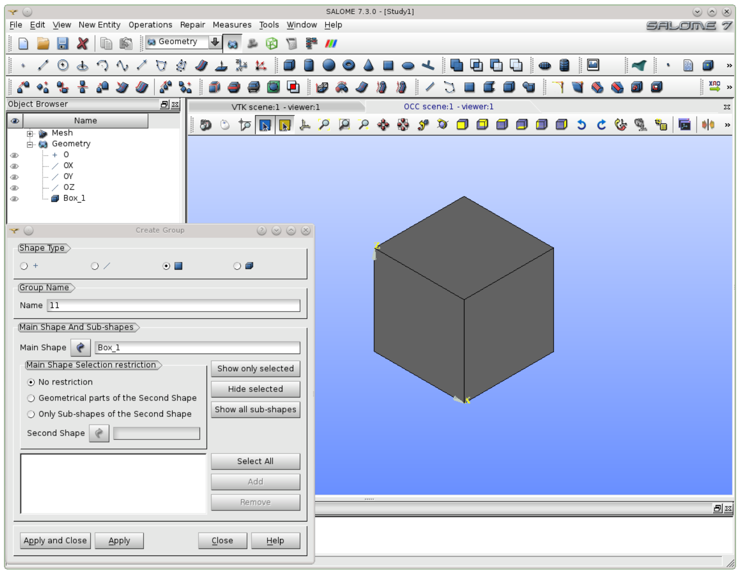


Figure 1.6: Inheritance diagram of the *ParallelMeshExtended* class

Also the mesh class has to be extended. As shown in Figure 1.6 the *ParallelMeshExtended* class, which uses only MEDMem functions, inherits the original class *libMesh::ParallelMesh* which uses only libMesh functions. As in the previous class, data from the LIBMESH class can be transferred, by using a *dynamic_cast* statement, into the assembly routine which is user accessible. Data can also be transferred in the opposite directions from the *libMesh::ParallelMesh* to the MEDMem interface through *parent* to *son* class inheritance rules. We recall again that the *parent* class should be polymorphic with at least one virtual function.

The *LIBMESH* interface class to SALOME. The LIBMESH class contains the SALOME platform commands. All the code interfaces must have similar commands to run the code from the same main program. Data in the LIBMESH class consist of a simple vector of string of boundary name. The boundary are defined by using the GEOM and the SMESH modules of the SALOME platform.

In order to generate a mesh with boundary we open the SALOME platform and the GEOM module as in Figure 1.7. From the menu we open the *Create a Box* button and select the box dimensions. Then we select *Create a Group* with option *face* and *no restriction* and click on the desired face. We label six different faces as *up*, *down*, *left*, *right*, *bottom* and *share*. We open the SMESH module and generate the mesh for the volume and the label for the boundary interfaces, see Figure 1.8. The boundary names and their flags are stored in the LIBMESH interface class. Over these boundaries and volume regions defined by using MEDMem functions we should be able to impose



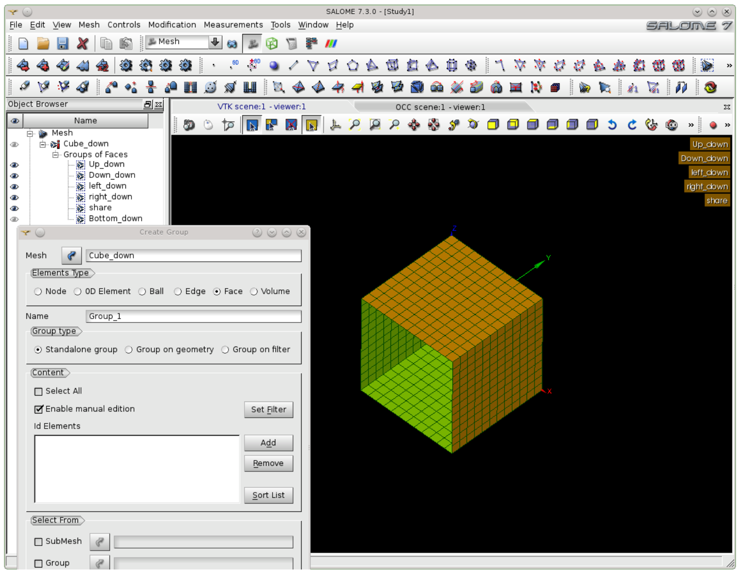
Name: 11

Main Shape: Box_1

[✓ No restriction] Geometrical parts of the Second Shape / Only Sub-shapes of the Second Shape

Second Shape

Figure 1.7: Generation of the boundary with the GEOM module



Mesh: Cube_down

Elements Type: Node / 0D Element / Ball / Edge / [✓ Face] / Volume

Name: Group_1

Group type: [✓ Standalone group] / Group on geometry / Group on filter

Content: ☐ Select All ☑ Enable manual edition

Id Elements

Select From: ☐ SubMesh ☐ Group

Figure 1.8: Generation of the boundary name in the SMESH module

values taken by other SALOME platform codes. The functions that start and stop the code are the constructor *LIBMESH(MPI_Comm comm)* and the function *terminate()*. These functions take into account the start and stop of all MPI parallel processes of the code. The commands

```
void  setType (const std::string &pbName)
void  setMesh (const std::string &meshFileName)
void  solve ()
```

are used to set the type of the problem (Navies-Stokes, energy, etc.) and the mesh. The mesh should be available in MED and libMesh format for data exchange. The MED format allows data transfer to other codes that use the same format. The solve command controls the solution of the discrete system.

The boundary should be controlled for input and output. For input we have the following interface functions

```
void  setSource (const ParaMEDMem::MEDCouplingFieldDouble *f)
void  setAnalyticSource (const std::string &f)
void  setAverageSources (int n, double val[])
void  setAnalyticBoundaryValues (const std::string &name,
                const std::string &typeBC, const std::string &f)
void  setFieldBoundaryValues (const std::string &name,
                                const std::string &bcType,
              const ParaMEDMem::MEDCouplingFieldDouble *bcField)
```

For output we have

```
std::string  getBoundaryName (int i)
std::vector< std::string >  getBoundaryNames ()
ParaMEDMem::MEDCouplingFieldDouble *  getOutputField
                                    (const std::string &vName) const
ParaMEDMem::MEDCouplingFieldDouble *  getValuesOnBoundary
           (const std::string &name, const std::string &vName) const
ParaMEDMem::MEDCouplingFieldDouble *  getValuesOnBoundary
        (const std::string &name, std::vector< char * > vName) const
ParaMEDMem::MEDCouplingFieldDouble *  getValuesOnBoundary_nodes
              (const std::string &name, std::vector< char * >) const
```

The solution values can be transfer on NODES or CELLS. In this SALOME interface the solution values are collected for CELLS or NODES but set only for CELLS.

***LibMeshProblem* class as interface class to libMesh code.** The interface to libMesh code is obtained through the LibMeshProblem class. Since the equation system has the mesh pointer of the original code the extended class is not available. For this reason the LibMeshProblem class should access to both ParallelMeshExtended and Equation-SystemsExtended classes as shown in the collaboration diagram of the *LibMeshProblem* class in Figure 1.9.

The *LibMeshProblem* class has been specialized for different physics. As one can see in Figure 1.10 this class is inherited by all the physical modules. We have constructed many modules for coupling. We have the energy equation in 1D, 2D and 3D and we call

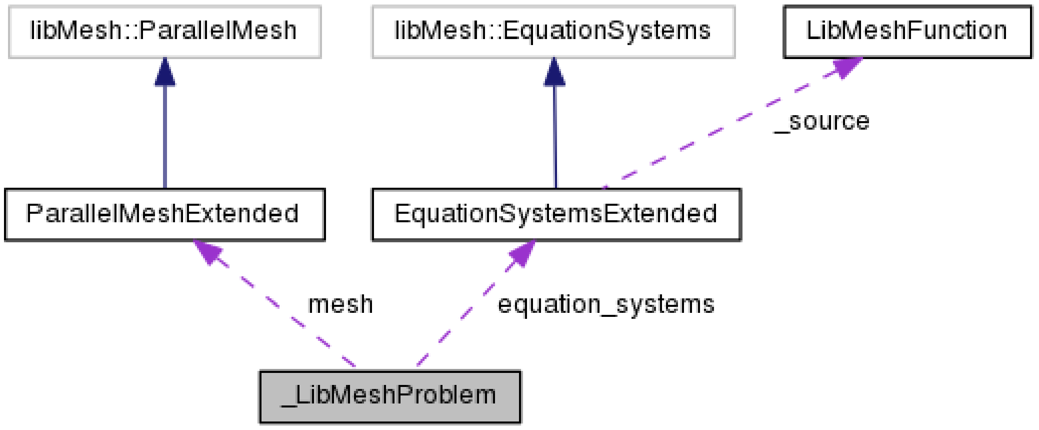


Figure 1.9: Collaboration diagram of the *LibMeshProblem* class.

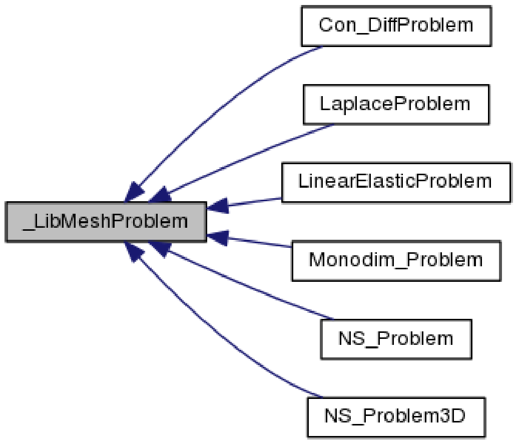


Figure 1.10: Inheritance diagram of the *LibMeshProblem* class.

it Convection-diffusion problem (*Con_DiffProblem*). We have the Laplace and Navier-Stokes problem in one, two and three dimensions. For the system scale we have a specific module called *Monodim_Problem* that can simulate pump, heat exchanger and source term for taking into account the whole loop of interest. Finally we have also a module for structural mechanics computations called *LinearElasticity_Problem*, available only for 2D computations like plates and sheets. In table 1.1 we have a summary of these modules and their relative scale of interest.

The *ParallelMeshExtended* class is an extension of the libMesh class *ParallelMesh*. This extension defines the map between the mesh nodes and elements in MEDMem and libMesh format. In particular the extension class contains the mesh in the ParaMEDMEM::MEDCouplingUMesh class format and all maps

Physics	Name module	scale
Energy equation	Con_DiffProblem	1D,2D,3D
Navier-Stokes equations	NS_Problem	2D
	NS_Problem3D	3D
System equation	Monodim_Problem	1D
Structural mechanics	LinearElasticity_Problem	2D
Laplace equation	LaplaceProblem	1D,2D,3D

Table 1.1: Multiphysics modules available in LibMesh for coupling.

```
_node_id: node MEDmem mesh      -> node libMesh mesh
_proc_id: processor MEDmem mesh -> processor libMesh mesh
_elem_id: element MEDmem mesh   -> element libMesh mesh
```

that allow the data transfer from one format to another.

The *EquationSystemsExtended* class is an extension of the libMesh class *EquationSystems*. The extension contains two standard maps

```
std::map< int,LibMeshFunction * > _bc
std::map< int, BCType >    _bc_type
```

that associate to any boundary a *LibmeshFunction* and a *BCType*. The BCType are the keywords *Neumann* or *Dirichlet* depending on the desired boundary condition. A database of these keywords can be updated by the user. The *LibmeshFunction* is a class object that completes the definition of the boundary conditions. The collaboration diagram of this class is shown in Figure 1.11. In the *EquationSystemsExtendedM* class

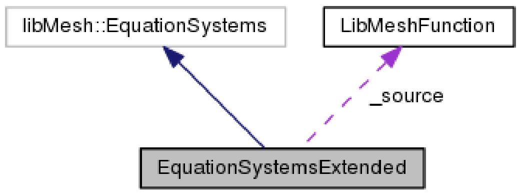


Figure 1.11: Collaboration diagram of the *EquationSystemsExtended* class

new functions are available in addition to the original EquationSystems functions. The following functions are used to set source fields computed by external codes

```
void setSource (const ParaMEDMEM::MEDCouplingUMesh *mesh,
                                                const char *s)
void eraseSource ()
LibMeshFunction * getSource ()
```

```
void setAverageSources (int n_AverageSources, double Average[])
double  getAverageSources (int i)
```

A coupling volumetric field can be transferred to a LibMesh computation by using *setSource* function. The field is defined over a ParaMEDMEM::MEDCouplingUMesh mesh which is a MEDMem mesh format. A volumetric field can be extracted from a libMesh solution and transferred to a LibMeshFunction with a MEDMem mesh format by using the *getSource* function. If the data transfer is between 3D and 1D the average source functions may be used.

The boundary conditions should be transferred from a code to another. Here we can use the following functions to add or erase a boundary coupling

```
int addBC (const ParaMEDMEM::MEDCouplingUMesh *b)
void  eraseBC (libMesh::boundary_id_type id)
```

or to set specific field and boundary condition type

```
void  setBCType (libMesh::boundary_id_type id, BCType type)
void  setBC (libMesh::boundary_id_type id, const char *s)
void  setBC (libMesh::boundary_id_type id,
                 const ParaMEDMEM::MEDCouplingFieldDouble *f)
void  setNodeBC (libMesh::boundary_id_type id,
                 const ParaMEDMEM::MEDCouplingFieldDouble *f)
LibMeshFunction * getBC (libMesh::boundary_id_type id)
BCType  getBCType (libMesh::boundary_id_type id)
```

The boundary labels and types can be imposed by using GEOM and SMESH modules in the SALOME platform, as already described.

The transfer data function. The data are transferred through an object class called LibmeshFunction. The data in these class are

```
const libMesh::MeshBase *                _mesh
const ParaMEDMEM::MEDCouplingUMesh *     _support
ParaMEDMEM::MEDCouplingFieldDouble *     _f
std::map< int, int >                     _nodeID
std::map< std::pair< int, int >, int >   _faceID
std::map< int, int >                     _elemID
```

The *_mesh* pointer points to the mesh in libMesh format while *_support* contains the mesh in MEDMem format. The solution of the internal or external problem in MEDMem format are stored in the field *_f*. The *_f* pointer may refer to the part of the mesh *(_support)* where the data are to be transferred. In fact if the function is associated with a part of the boundary, the mesh and its solution is relative only to this part. The *_nodeID*, *_faceID* and *_elemID* are the maps from the libMesh to the MEDMem mesh format for the nodes, faces and elements respectively.

The *LibmeshFunction* is used to evaluate the field at the boundary and to map the node and element connectivity between coupling codes. Each code has a MEDMem interface which is used to exchange data through the SALOME platform during execution.

1.2.3 Implementation of the SALOME-libMesh interface

In order to explain the code implementation of the data transfer we consider a simple example with the energy equation implemented in the LibMesh module *conv-diff*. We consider the domain $[0,1]\times[-1,0]\times[0,1]$ which is the same geometry generated in section 1.2.2. The mesh consists of $12 \times 12 \times 12$ HEX20 quadratic elements. By using GEOM and SMESH modules we have marked the boundary of the domain as *up* and *down* in the z direction, *left* and *right* in the x direction and *bottom* and *share* in the y direction as shown in Figure 1.12. We solve the energy equation that takes into account convection

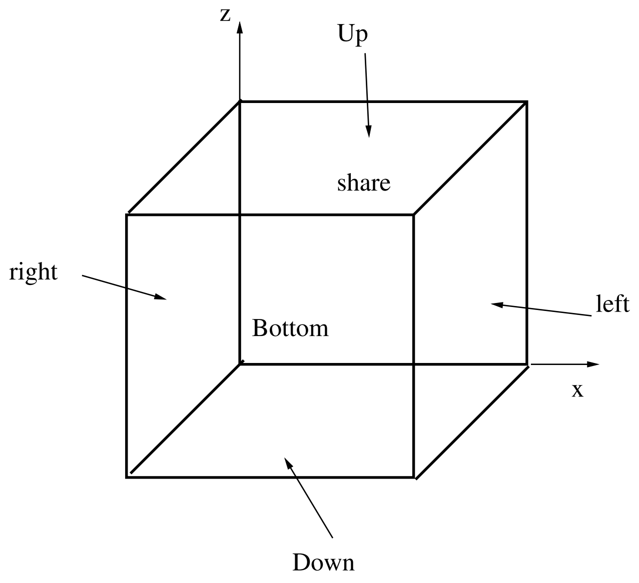


Figure 1.12: Geometry of the test case.

with constant velocity $\boldsymbol{v} = (0, 1, 0)$. The boundary has homogeneous Dirichlet boundary condition on the *up*, *down*, *left* and *right* faces. On the *share* face we set homogeneous Neumann boundary conditions while on the *bottom* we import a constant field from the MEDMem interface. The LibMesh code runs through the LIBMESH class in a few lines:

```
LIBMESH P;
P.setType("convdiff");
P.setMesh(dataFile);
getInput(P, boundary);

for(int itime=0;itime<60;itime++){
 for(int i=0; i<boundary.size(); i++) {
   sBC & b = boundary[i];
   if(b.isAnalytic)
   P.setAnalyticBoundaryValues(b.name,b.type,b.equation);
   else  P.setFieldBoundaryValues(b.name, b.type, b.field);
 }
 P.solve();
}
```

The interface P class is constructed in the first statement. The problem type (convdiff) is set with the *setType* function. The mesh in MED format is assigned with *setMesh* function which copy the mesh to the LibMesh program in LibMesh format. The interface conditions are set by *getInput* function which is set by the user.

In order to set the interface conditions the name of the different boundaries should be associated with the boundary conditions. The labels of the boundary regions are available calling the function *getBoundaryNames()* in the LIBMESH class. A simple statement as

```
std::vector<std::string> bcNames = P.getBoundaryNames();
```

returns the name of all the boundary regions. For each region a boundary structure *sBC* should be defined. This structure is defined as

```
 struct sBC {
  std::string name;
  std::string type;
  bool isAnalytic;
  std::string equation;
  MEDCouplingFieldDouble * field;
};
```

The *name* is the identity label of the boundary region. The *type* of boundary condition is “Dirichlet” or “ Neumann”. If the *isAnalitic* is true then an analytic condition is expected if false a numerical field is assigned. The analytical expression is defined in the string *equation* by using symbolic language. The numerical field is assigned through the pointer *field*. The solution computed from other codes can be transferred into this field pointer becoming available to the LibMesh code. In our case we build a vector of *sBC* structures called *boundary* and set the appropriate structure in the "Bottom" region which is the active interface. In this active face we set

```
  bcNames[0]=="Bottom";
  boundary[0].type = "Dirichlet";
  boundary[0].isAnalytic = true;
  boundary[0].field = NULL;
  boundary[0].equation = "1.";
```

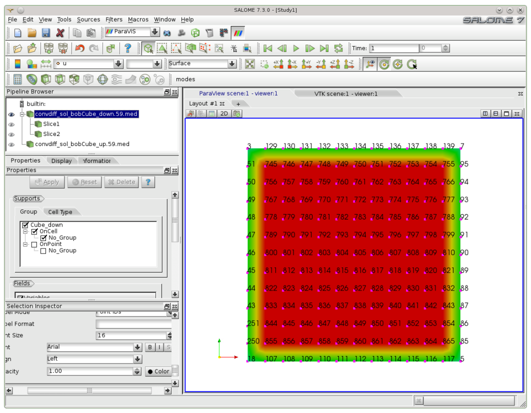


Figure 1.13: Common surface *Bottom* of the computation domain where the data transfer is allowed. Libmesh global numbering.

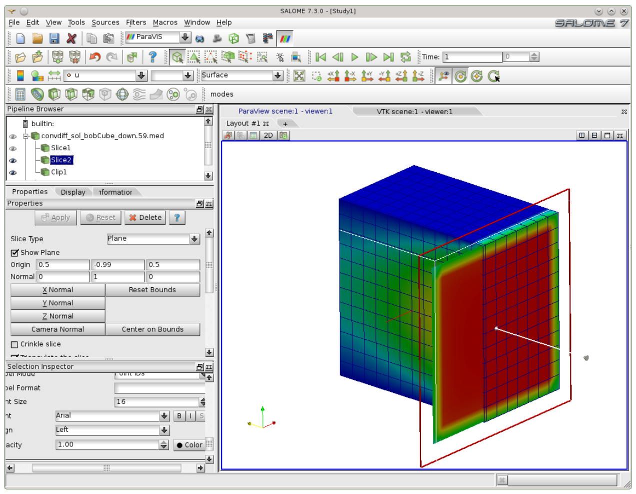


Figure 1.14: Solution when a surface allows a transfer of data.

Now at each time step the boundary condition defined by the external field *field* or any analytical expression *equation* is imposed. In Figure 1.13 one can see the surface (labeled as *Bottom*) of the computation domain where the data transfer is allowed with Libmesh global numbering. The LIBMESH interface creates a map to connect this global numbering to the surface mesh. The surface mesh in MEDMem representation has the same number of nodes but different numbering. It is necessary therefore to search point by point the correspondence. Once the map is computed all field values on the surface can be passed to the LibMesh surface and viceversa. When the interface condition is transferred then on the *Bottom* part of the boundary a constant field is applied as one can see from Figure 1.14.

1.3 FEMLCORE-SALOME integration

1.3.1 SALOME-FEMLCORE interface

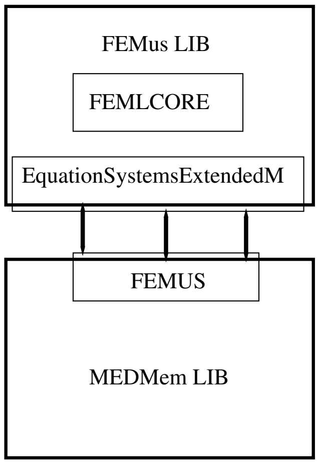


Figure 1.15: Diagram of the *FEMUS* class inside the MEDMem interface

Overview. FEMLCORE is an application of the FEMus library aimed at computation of 3D core thermal-hydraulics of a fast nuclear reactor. It is therefore interesting to integrate the FEMus library with SALOME platform by writing a MEDMem interface in order to be able to couple the 3D computation of the core obtained by FEMLCORE with a system code simulation, like CATHARE or RELAP. The interface between the MEDMem and the FEMus libraries consists basically of four classes: *FEMUS*, *EquationSystemsExtendedM*, *ParallelMeshExtendedM* and *LibMeshFunctionM*. All these classes are located in the *src* and *include* FEMus directories. As shown in the diagram of Figure 1.15, the *FEMUS* class is the interface between the library FEMus and the SALOME platform. The FEMUS interface allows to pass commands from MEDMem library to the *EquationSystemsExtendedM* class which is the problem solver core. This diagram illustrates as the *FEMUS* class (interface to SALOME) transfers the data to the *EquationSystemsExtendedM* class. In order to interact with the FEMus library two FEMus classes have been extended: the *MGEquationsSystem* and the *MGMesh*. The extensions are simply named as *EquationsSystemExtendedM* and *ParalellMeshExtendedM*, respectively.

The *EquationSystemsExtendedM* class, which uses only MEDMem functions, inherits the *EquationSystems* which uses only FEMus functions as shown in Figure 1.16. The *EquationSystems* contains the assembly and solver of the FEMus code. The data from the *FEMUS* class can be transferred into the assembly routine by a *dynamic_cast* operator. The *dynamic_cast* operator is a part of the run-time type information (RTTI) system that allows to use *son* class functions from the *parent* class. Data can also be transferred in the opposite direction from the *EquationSystems* to the MEDMem inter-

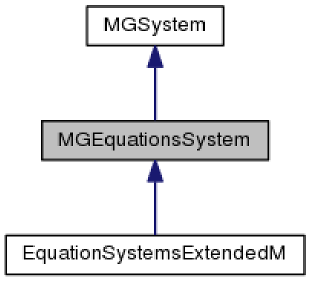


Figure 1.16: Inheritance diagram of the *EquationSystemsExtendedM* class

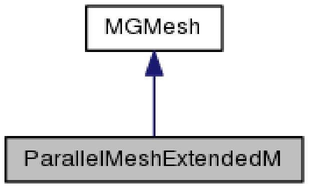


Figure 1.17: Inheritance diagram of the *ParallelMeshExtendedM* class

face by standard C++ inheritance rules. The *MGMesh* class contains the multilevel mesh in FEMus format. In order to interface FEMus with MEDMem library a new mesh format should be introduced and the mesh class should be extended. As shown in Figure 1.17 the *ParallelMeshExtendedM* class, which uses only MEDMem functions, inherits the *MGMesh* which uses only libMesh functions. In FEMus library, differently from LibMesh library, the mesh is known inside the *EquationSystemsExtendedM* class and therefore the interface *FEMUS* class does not need to communicate directly to the *ParallelMeshExtendedM* class. As in the class before the data from the *FEMUS* class can be transferred by using a *dynamic_cast* operator into the assembly routine which is user accessible.

The *FEMUS* interface class to SALOME platform. The *FEMUS* class is the unique interface class. It contains data from both FEMus and MEDMem libraries in order to transfer data from one mesh to another (MGMesh to MED). Therefore inside this class there are both pointers *_mg_mesh*, *_med_mesh* to their respective MGMesh and MED formats. The *FEMUS* class needs information to extract data from these different mesh structures. In particular, as shown in 1.18, the classes *MGUtils*, *MGGeomEL*, *MGFEMap* and *MGFemusinit* are available inside FEMus to transfer basic information such as file names, parameters, multigrid level, fem elements etc.. The *MGUtils* contains all the file names and input parameter values. The *MGGeomEL* and *MGFEMap* contain information about the finite element mesh structure and *MGFemusinit* class is the manager class for MPI and multigrid solvers.

The data needed to communicate with the MEDMem library consist of two structures:

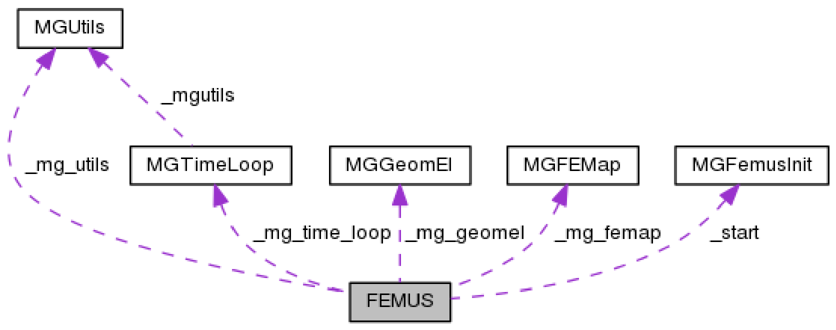


Figure 1.18: *FEMUS* class data to communicate with the FEMus library.

one for the mesh and another for the boundary conditions. The mesh structure is called *interface_mesh* and consists of

```
int id;
std::string name;
ParaMEDMEM::MEDCouplingUMesh * support;
```

where *id* is the integer number identity and *name* the name of the common interface. The *support* is the mesh in MED format. This in general is not the whole mesh but only the mesh for the interested interface region. Since this is a portion of the mesh numbering is different from the global one and a map is needed. There is one *interface_mesh* structure for each mesh interface of interest. The boundary conditions structure is called *UsersBC* and consists of

```
std::string name;
std::string type;
int from_cmp;
int n_cmp;
int order_cmp;
bool isAnalytic;
std::string equation;
ParaMEDMEM::MEDCouplingFieldDouble * field;
bool on_nodes;
```

The *name* is the name of the interface while *type* refers to the “Mark” or “UnMarked” flag that is used to construct the mesh map. If the interface is “Marked” the code prepares all the tools for the data exchange including an MGMesh-MED map for field exchange. The *from_cmp* and *n_cmp* define the first and the number of variables to be exchanged, respectively. The interpolation order is defined by *order_cmp*. A quadratic variable (on Hex27, Quad9, Tri6 or Tetra10, for example) should have *order_cmp*=2. If on the surface one desires to impose an analytic function then the Boolean variable *isAnalytic* should be set to “true” and the analytical expression should be defined in the string *equation*. For numerical fields the MED solution should be transfer through the *field* pointer as node or element values by setting the Boolean *on_nodes* of the *UsersBC* structure. There is one *UsersBC* structure for each mesh interface of interest and all of them are collected in the *std::vector*< $UsersBC$ > *_boundary*.

The *FEMUS* class contains the SALOME platform commands. All the code interfaces must have similar commands to run the code from the same main program. The functions that start and stop the code are the constructor *FEMUS(MPI_Comm comm)* and the function *terminate()*. These functions take into account the start and stop of all MPI parallel processes of the code. The initialization of the parameters and the FEM elements are obtained by the following functions

```
void init_param(MGUtils &mgutils);
void init_fem(MGGeomEl & mggeomel,MGFEMap & mgfemap);
```

The commands

```
void setSystem(const std::vector<NS_FIELDS> & pbName);
void setMesh();
void setMedMesh(const std::string & meshFile);
```

are used to set the type of the problem (Navies-Stokes, energy, etc.) and the mesh. The *NS_FIELDS* enumeration collects the name of some of the implemented modules as

```
 NS_F  =0,    // [0] -> Navier-Stokes (quadratic (2),NS_EQUATIONS)
 NSX_F =0,    // [0] -> Navier-Stokes (quadratic (2),NS_EQUATIONS)
 NSY_F =1,    // [1] -> Navier-Stokes (quadratic (2),NS_EQUATIONS)
 NSZ_F =2,    // [2] -> Navier-Stokes (quadratic (2),NS_EQUATIONS)
 P_F   =3,    // [3] -> Pressure (linear (1),NS_EQUATIONS==0 or 2)
 T_F   =4,    // [4] -> Temperature   (quadratic (2),T_EQUATIONS)
 K_F   =5,    // [5] -> Turbulence K  (quadratic (2),TB K_EQUATIONS)
 EW_F  =6,    // [6] -> Turbulence W  (quadratic (2),TB W_EQUATIONS)
 KTT_F =7,    // [7] -> Turbulence K  (quadratic (2),TB K_EQUATIONS)
 EWTT_F=8,    // [8] -> Turbulence W  (quadratic (2),TB W_EQUATIONS)
 SDSX_F=9,    // [9] -> Displacement (quadratic (2), DS_EQUATIONS)
 SDSY_F=10,   // [10] -> Displacement (quadratic (2), DS_EQUATIONS)
 SDSZ_F=11,   // [11]-> Displacement (quadratic (2), DS_EQUATIONS)
 DA_F  =12,   // [12]-> DA solver (quadratic (2), DA_EQUATIONS)
 DA_P  =13,   //[13]-> DA solver (piecewise, DA_EQUATIONS)
 TA_F  =14,   // [13]-> Temp adjoint
 FS_F  =15    // [13]-> Temp adjoint
```

For example, a vector pbName defined as pbName[0]=NS_F, pbName[1]=T_F defines a problem which consists of the Navier-Stokes and energy equations. The solution of the system is obtained by using these commands

```
void solve ()
void solve_setup (int &t_in, double &time)
void  solve_onestep (const int &t_in, const int &t_step,
              const int &print_step, double &time, double &dt)
```

The *solve_setup* initializes system at $t = 0$. The *solve_onestep* function controls a single time step of the problem while *solve()* can be used to solve more time steps at once.

The boundary should be controlled for input and output. For input we have the following interface functions

```
setSource (const ParaMEDMEM::MEDCouplingFieldDouble *f)
void setAnalyticSource (const std::string &f)
void setAverageSources (int n, double val[])
void setAnalyticBoundaryValues (const std::string &name,  int n_cmp,
                    const std::string &typeBC, const std::string &f)
void setFieldBoundaryValues (const std::string &name, int n_cmp,
                             const std::string &bcType,
                 const ParaMEDMEM::MEDCouplingFieldDouble *bcField)
```

For output we have

```
std::string                  getBoundaryName (int i)
std::vector< std::string >  getBoundaryNames ()
ParaMEDMEM::MEDCouplingFieldDouble getValuesOnBoundary (
                             const std::string &nameBC,
                             const std::string &systemName)
ParaMEDMEM::MEDCouplingFieldDouble *getValuesOnBoundary(
                             const std::string &nameBC,
                             const std::string &systemName, int iCmp)
ParaMEDMEM::MEDCouplingFieldDouble *  getValuesOnBoundary (
                             const std::string &nameBC,
                             const std::string &systemName,
                             int Cmp0, int nCmp)
```

The solution values can be transferred only on nodes.

The interface in this library must be used in different step. They must be initialized, marked and then used. For this reason we have different interface functions

```
void  init_interfaces (const std::string &medfilename,
                               const int index_mgmesh=0,
                               const int index_medmesh=0)
void  init_interfaces (const std::string &medfilename,
       const std::string &medfile_namePold,const FEMUS &P_old,
       const int index_mgmesh=0, const int index_medmesh=0)
void  set_param_BCzone ()
void  set_param_BCzone (FEMUS &P1)
void  init_BCzone (std::vector< std::string > &bcNames)
void  set_interface_userbc ()
```

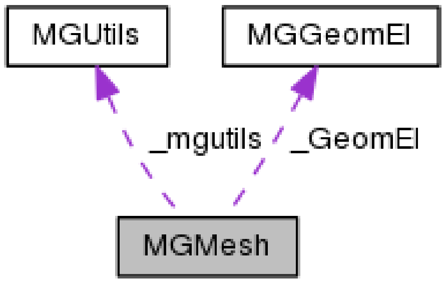


Figure 1.19: Collaboration diagram of the *ParallelMeshExtendedM* class

The *ParallelMeshExtendedM* class. The *ParallelMeshExtendedM* class is an extension of the FEMus class *MGMesh*. This extension defines the map between the mesh nodes and elements in MEDMem and libMesh format. In particular the extension class contains the mesh in the ParaMEDMEM::MEDCouplingUMesh class format and all the maps

```
_node_id: node MEDmem mesh      -> node libMesh mesh
_proc_id: processor MEDmem mesh -> processor libMesh mesh
_elem_id: element MEDmem mesh   -> element libMesh mesh
```

that allow the data transfer from one format to another.

Moreover this class contains one standard map and two vector flags

```
 std::map< int, int >  _bd_group
 std::vector< int >  _bc_id
 std::vector< int >  _mat_id
```

The first associates the integer names to an integer. We recall that the names for the boundary and volume zones must be integer number in the range $[10, 10000]$ and $[1, 9]$, respectively. The vector *_bc_id* contains the boundary flag at each node of the integer name ($[10-10000]$) of the surface/interface . The vector *_mat_id* contains the boundary flag with the integer name ($[1-9]$) of the volume/material at each node. The collaboration diagram is shown in Figure 1.19.

The *EquationSystemsExtendedM* class. As shown in Figure 1.20 the *EquationSystemsExtendedM* can access to the mesh classes and to the *FEMUSFunction* class. In order to transfer data from MEDMem and FEMus library new functions are available in addition to the original EquationSystems functions.

The following functions are available to set source fields computed by external codes

```
void setSource (const ParaMEDMEM::MEDCouplingUMesh *mesh,
                                                const char *s)
```

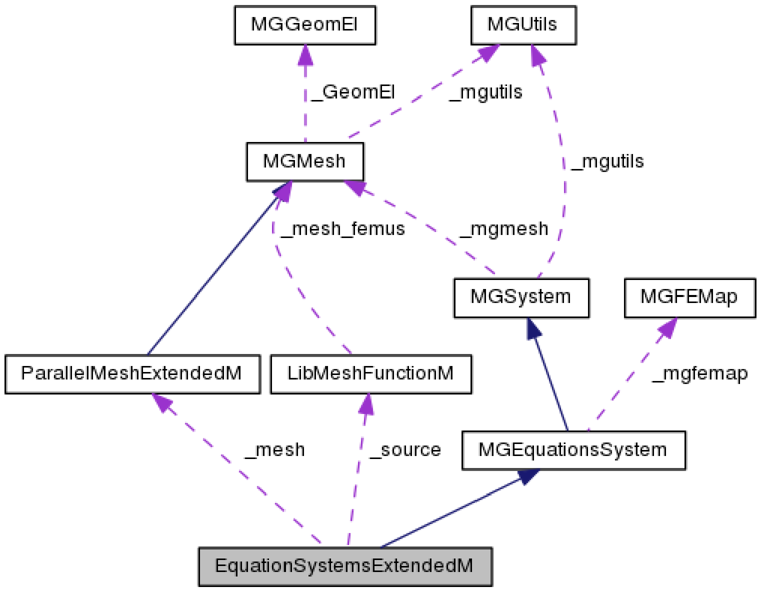


Figure 1.20: Collaboration diagram of the *EquationSystemsExtendedM* class

```
void eraseSource ()
FEMUSFunction * getSource ()
void setAverageSources (int n_AverageSources, double Average[])
double  getAverageSources (int i)
```

As for the LibMesh library coupling volumetric field can be achieved by using *setSource* function. The field is defined over a ParaMEDMEM::MEDCouplingUMesh mesh which is a MEDMem mesh format. A volumetric field can be extracted from a FEMus solution and transferred to a FEMUSFunction with a MEDMem mesh format by using the *getSource* function. If the data transfer is between 3D and 1D the average source functions may be used.

The boundary conditions should be transferred from a code to another. Here we can use the following functions to add or erase a boundary coupling

```
FEMUSFunctionM *get_interface_function_BC (boundary_id_type id)
void  erase_interface_function_BC (boundary_id_type id)
```

The boundary labels and types can be imposed by using GEOM and SMESH modules in the SALOME platform.

The *FEMUSFunctionM* transfer data class. The data are transferred through an object class called *FEMUSFunctionM*. In Figure 1.21 the collaboration diagram for this class is reported, while its data are

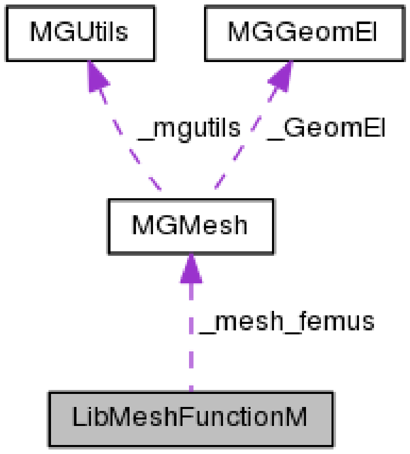


Figure 1.21: Collaboration diagram of the *FEMUSFunctionM* class

```
const MGMesh *                                _mesh
const ParaMEDMEM::MEDCouplingUMesh *          _support
ParaMEDMEM::MEDCouplingFieldDouble *          _f
std::map< int, int >                          _nodeID
std::map< std::pair< int, int >, int >        _faceID
std::map< int, int >                          _elemID
```

The *_mesh* pointer points to the mesh in FEMus format while *_support* contains the mesh in MEDMem format. The solution of the internal or external problem in MEDMem format are stored in the field *_f*. The *_f* pointer may refer to the part of the mesh (*_support*) where the data are to be transferred. In fact if the function is associated with a part of the boundary, the MED mesh and the solution is relative only to this part. The *_nodeID*, *_faceID* and *_elemID* are the maps from the FEMus to the MEDMem mesh format for the nodes, faces and elements respectively.

The *FEMUSFunction* is used to evaluate the field at the boundary and to map the node and element connectivity between coupling codes. Each code has a MEDMem interface which is used to exchange data through the SALOME platform during execution.

1.3.2 Implementation of the SALOME-FEMLCORE interface

In order to explain the code implementation of the data transfer we consider a simple example with the Navier-Stokes equations implemented in the FEMus module *Navier-Stokes*. We consider a rectangular domain with inlet labeled “50” and outlet “111”. The sides are labeled “100” and “11”. We recall that over common points the higher number prevails.

The boundary condition in the FEMUs library can be set in the file *User_NS.C* located in SRC directory. We set

```
void MGSolNS::bc_read(int bc_gam,int bc_mat,
     double xp[],int bc_Neum[],int bc_flag[]) {
   int imesh=atoi(_mgutils.get_file("MESHNUMBER").c_str());
   bc_Neum[0]=1; bc_Neum[1]=1;  bc_Neum[2]=1; bc_Neum[3]=1;
   bc_flag[0]=0; bc_flag[1]=0;  bc_flag[2]=0; bc_flag[2]=0;

   // mesh1 simple_hex27.med
   if( bc_gam==100){
     bc_Neum[0]=0; bc_Neum[1]=0;  bc_Neum[2]=0;
     bc_flag[0]=0; bc_flag[1]=0;  bc_flag[2]=0;
  }   // lateral
   if( bc_gam==50){
     bc_Neum[0]=0; bc_Neum[1]=0;  bc_Neum[2]=0;
     bc_flag[0]=0; bc_flag[1]=0;  bc_flag[2]=0;
  }   // inlet
    if( bc_gam==11){
     bc_Neum[0]=0; bc_Neum[1]=0;  bc_Neum[2]=0;
     bc_flag[0]=0; bc_flag[1]=0;  bc_flag[2]=0;
  }   // lateral
   if( bc_gam==111){
     bc_Neum[0]=0; bc_Neum[1]=0;  bc_Neum[2]=1;
     bc_flag[0]=0; bc_flag[1]=0;  bc_flag[2]=0;
  }   // outlet
```

in order to have Dirichlet boundary at the inlet in the vertical direction and no slip boundary condition on the walls. For details see [1, 2, 3, 4, 5]. The FEMus code runs by using only FEMUS class functions as

```
  FEMUS P;                            // constructor
  P.init_param(*mgutils[0]);          // init parameter
  P.init_fem(*mggeomel,*mgfemap);     // init fem
  // setting mesh --------------------------------------
  P.setMedMesh(osfilenameP[0].str().c_str());// med-mesh
  P.setMesh();                                // MGmesh
  // setting system -------------------------------------
  P.setSystem(myproblemP);        // set system
  P.init_interfaces(filenameP[0].str().c_str());
  P.set_param_BCzone();           // define param bc
  P.set_interface_userbc();       // set bc conditions

  // time loop initialization ---------------------------
  int    n_steps = mgutils[0]->get_par("nsteps");
  double      dt = mgutils[0]->get_par("dt");
  int print_step = mgutils[0]->get_par("printstep");
  int    itime_0  = mgutils[0]->get_par("itime");
  double time    = 0.;
  P.solve_setup(itime_0,time); // initial time loop (t=0)

  // transient loop (i0time ->i0time+ n_steps) ----------
  for(int itime=itime_0; itime< itime_0 + n_steps;
      itime++) {
    P.solve_onestep(itime_0,itime,print_step,time,dt);
  }
  P.terminate();
```

The interface P class is constructed in the first statement. The physical, geometrical and FEM parameters are set by the $P.init\_param(*mgutils[0])$ where the *mgutils* vector may contain several mesh domains. In order to initialize the finite element environment we use the $P.init\_fem(*mggeomel, *mgfemap)$ functions. The *mgutils*, *mggeomel* and *mgfemap* are objects of the classes *MGUtils*, *MGGeomEL* and *MGFEMap* respectively. These classes form a mandatory computational environment for setting a Navier-Stokes problem. The problem type (myproblemP) is set with the *setSystem* function. In this case the first unique component of the vector myproblemP is set to $myproblemP[0] =$ “NS_F“ which is the Navier-Stokes problem. For Navier-Stokes and energy equation problem one must set $myproblemP[0] =$ “NS_F“ and $myproblemP[1] =$ “T_F“.

The mesh in med format is assigned with *setMesh* function which transfers automatically the mesh to the FEMus program. The interface conditions are set by *getInput* function which is set by the user.

We construct a vector of interface where the data should be transferred and we call it *_boundary*. In this case we want to set only an analytic field on the interface ”50“. The interface where we like to have data transfer must be marked in the file *FEMUS_BC.C* in the function *init_BCzone(std::vector< std :: string > &bcNames)* of the *FEMUS* class as

```
   _boundary[0]=="50";
   _boundary[0].type = "Mark";
   _boundary[0].on_nodes = true;
```

Once the interface is marked the boundary condition and the data transfer should be specified in the *set_param_BCzone* function as

```
    _boundary[0]=="50";
    _boundary[0].from_cmp = 0;       // UsersBC initial cmp
    _boundary[0].n_cmp = 3;          // UsersBC n of cmp
    _boundary[0].order_cmp = 2;      // UsersBC order cmp
    _boundary[0].isAnalytic = true; // sBC struct flag
    _boundary[0].equation = "IVec*0.0+JVec*0.0+KVec*0.1";
    _boundary[0].field = NULL;      // sBC struct num field
    _boundary[0].on_nodes = true;   // UsersBC node field (true)
```

Finally the function

```
P.set_interface_userbc();
```

sets the desired field computing and evaluates the field at the interface nodes.

In the next chapter several examples of computations using this SALOME-FEMLCORE interface are reported in order to better describe the potentials of the SALOME platform integration tool presented in this report.

1.4 Deployment of the SALOME platform on the CRESCO cluster

In this section we illustrate the steps that are required in order to deploy the SALOME platform on the CRESCO cluster. The CRESCO infrastructure at ENEA is made up of different clusters that are managed with a unified access control system based on SSH and AFS [36].

The SALOME platform has been installed along with the other codes belonging to the *fissicu* project, in order to ease the interaction with them. In particular, the code is available at the address

`/afs/enea.it/project/fissicu/soft/salome/`

Different version are available in this folder:

- `v7.2.0`, precompiled from the SALOME team. This version in available in the `v7.2.0` sub-directory.
- `v6.6.0`, compiled in place from sources. This version has been compiled using the `SAlomeTools` (`sat`) and it is available in the `sat-install` sub-directory.

The installation of two different version has been necessary since in the framework of the NURESAFE project only `v6.6.0` is officially supported. This version is the only one for which the interfaces to couple codes to the platform are tested and developed, and widely used by many European partners of the project.

`v7.2.0` was the latest available from the SALOME website [33] and it was selected since it offered updated sources with an easier and more tested API for code coupling, that has been exploited for the development of the FEMLCORE interface.

The installation from sources of the whole SALOME platform requires a lot of effort, since it depends on a huge number of third-party libraries that have to be installed with the correct version. For this reason the SALOME development team has introduced the `SAlomeTools` (`sat`) in order to simplify the installation procedure. With this tool, the user can automate the installation of all the components that are required for SALOME. Anyway, a certain degree of experience with installation procedures and the specific SALOME installation scripts is required to properly complete the installation procedure. Many details are left to the user, that has to check the proper installation of the third-party libraries and be sure to avoid mix-ups between `sat`-installed and system-wide installed libraries. The advantage of doing a complete build from sources is that it is possible to enable more features and disable others with respect to the pre-compiled binaries that are available on the website. In particular, all pre-compiled binaries do not have MPI capabilities enabled, so it is possible to use it only compiling the platform from sources.

A list of the prerequisite third-party libraries that are used with `v6.6.0` (developed specifically for the NURESAFE partners) is shown in Table 1.2.

Library	Version
Python	2.6.6
qt	4.6.3
sip	4.13.2
PyQt	4.9.1
boost	1.49.0
swig	2.0.4
tcl	8.5.9
tk	8.5.9
freetype	2.3.7
ftgl	2.1.3-rc5
cmake	2.8.7
gl2ps	1.3.5
freeimage	3.14.1
CAS	6.5.4
qwt	5.2.1
omniORB	4.1.6
omniORBpy	3.6
omniNotify	2.1
expat	2.0.1
hdf5	1.8.8
med	3.0.6
metis	4.0patched
scotch	5.1.11
libxml2	native
netgen	4.9.13
graphviz	2.28.0
numpy	1.5.1
doxygen	1.8.0
setuptools	0.6c11
docutils	0.8.1
Pygments	1.5
Jinja2	2.6
Sphinx	1.1.3
QScintilla	2.6.1
ParaViewData	3.14.0
ParaView	3.14.0
cppunit	1.12.1
openmpi	1.4.5
Homard	10.5
MeshGems	1.0

Table 1.2: SALOME `v6.6.0` third-party libraries.

2 FEMLCORE coupling on SALOME

In the previous chapter we have seen the integration of the libMesh and the FEMus libraries on the SALOME platform. We have constructed interface classes (named *LIBMESH* and *FEMUS*, respectively) that allow us to transfer data to and from the code library to the SALOME MEDMem library. In this way by using a common computational platform a solution computed from a code can be transferred to another code through these interfaces. This is an ideal situation for multiscale analysis of LF reactors. The main idea is to use mono-dimensional codes to compute the primary loop evolution and three-dimensional codes to simulate in details parts of the nuclear plant. In order to do this the three-dimensional modules developed in the FEMLCORE project are therefore coupled with mono-dimensional module created in libMesh or with any other code available on the SALOME platform. Since high specialized system codes for nuclear reactor are not open-source in this report we describe the coupling with libMesh codes in order to reach the final purpose to couple FEMLCORE with CATHARE when this code will be available on SALOME platform with an appropriate license.

In this chapter we report coupling simulations on SALOME platform based on the integration described in the previous chapter. The first section introduces libMesh coupling and the second section FEMus coupling. Finally, in the third section, examples of FEMLCORE coupling with a mono-dimensional code developed with libMesh library are reported.

2.1 Coupling libMesh modules on SALOME

2.1.1 LibMesh energy problem coupling (3D-3D)

In order to verify the data transfer during the coupling with libMesh codes we consider a first simple example with the energy equation over the geometry shown in Figure 2.1. The domain consists of two cubes: one in the region $[0,1] \times [0,1] \times [-1,0]$ (Ω_1) and another in $[0,1] \times [0,1] \times [0,1]$ (Ω_2). The two meshes are created in a separate way and the common face has the same number of points but different numbering. Each mesh consists of $12 \times 12 \times 12$ HEX20 quadratic elements. By using GEOM and SMESH modules we have marked the boundary of the domain as *up_down* and *down_down* in the z direction, *left_down* and *right_down* in the x direction and *bottom_down* and *share* in the y direction for the down region Ω_1. The same labels is used for the up-region (Ω_2) by substituting *down* with *up*. The share region which is the common interface is labeled *share* in both domains.

Over this domain we consider a problem described by the energy equation with constant velocity field of $\boldsymbol{v} = (0, 1., 0)$. The boundary has homogeneous Dirichlet boundary

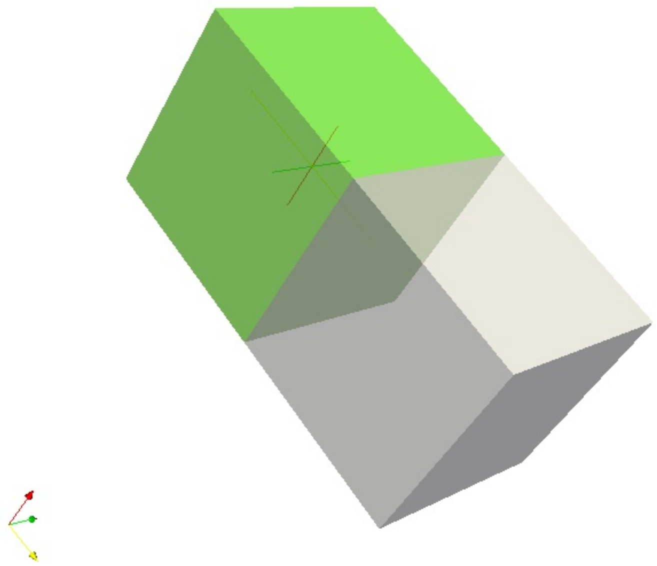


Figure 2.1: Coupling 3D-3D geometry. Domain $\Omega_1 \cup \Omega_2$.

condition on the *up*, *down*, *left* and *right* faces. On the *share* face we set homogeneous Neumann boundary conditions in the down problem and non homogeneous boundary conditions in the up region which transfers the field computed in the down problem. The *Bottom_down* gets a constant field from the MEDMem interface while the top up has homogeneous Neumann boundary conditions. We start in parallel two different problems: one in the down-region and another in the up-region and continuously transfer data from the down to the top region. The LibMesh code runs through the LIBMESH class with the following code lines

```
LIBMESH P;                    LIBMESH P1;
P.setType("convdiff");       P1.setType("convdiff");
P.setMesh(dataFile);         P1.setMesh(dataFile1);
P.setAnalyticSource("0."); P1.setAnalyticSource("0.");
getInput(P, boundary);

for(int itime=0;itime<60;itime++){
  for(int i=0; i<boundary.size(); i++) { // boundary problem P
   sBC & b = boundary[i];
   if(b.isAnalytic)
     P.setAnalyticBoundaryValues(b.name, b.type, b.equation);
   else
```

```
      P.setFieldBoundaryValues(b.name, b.type, b.field);
   }
   P.solve();
   getInput1(P1, P,  boundary1);

   for(int i=0; i<boundary1.size(); i++) { // boundary problem P1
     sBC & b1 = boundary1[i];
     if(b1.isAnalytic)
       P1.setAnalyticBoundaryValues(b1.name, b1.type, b1.equation);
     else
       P1.setFieldBoundaryValues(b1.name, b1.type, b1.field);
    }
    P1.solve();
    sol = P.getOutputField("u");
    sol1 = P1.getOutputField("u");
  }
  P.terminate();
  P1.terminate();
```

The LibMesh problems P and P1 are constructed in the first line. Each constructor starts its MPI boot. The problem type (convdiff) is set with *setType* function. The mesh with med format is assigned with *setMesh* function which transfers automatically the mesh to the LibMesh program. We have two meshes inside which are read from *dataFile* and *datafile1* respectively. The interface condition of the problem P are set by the *getInput* function which is set by the user.

In order to set the interface condition the name of the different boundaries should be associated with the boundary conditions. The labels of the boundary regions are available with the function *getBoundaryNames()* in the LIBMESH class. The boundary conditions for the problem P are set as

```
boundary[0].name="right_down"
boundary[0].type = "Dirichlet";
boundary[0].isAnalytic = true;
boundary[0].field = NULL;
boundary[0].equation = "0.";
....
....
boundary[4].name="Bottom_down"
boundary[4].type = "Dirichlet";
boundary[4].isAnalytic = true;
boundary[4].field = NULL;
boundary[4].equation = "1.";

boundary[5].name="share"
boundary[5].type = "Neumann";
```

```
boundary[5].isAnalytic = true;
boundary[5].field = NULL;
boundary[5].equation = "";
bcNames[5]="share"
```

The boundary conditions for the problem P1, in the upper part of the domain are set as

```
boundary[0].name="right_up"
boundary[0].type = "Dirichlet";
boundary[0].isAnalytic = true;
boundary[0].field = NULL;
boundary[0].equation = "0.";
....
....
boundary[4].name="share"
boundary[4].type = "Dirichlet";
boundary[4].isAnalytic = false;
boundary[4].field = bdy;
boundary[4].equation = "";

boundary[5].name="top_up"
boundary[5].type = "Neumann";
boundary[5].isAnalytic = true;
boundary[5].field = NULL;
boundary[5].equation = "";
bcNames[5]="share"
```

In this case on the interface *share* of the problem P1 we set a Dirichlet boundary condition imposing the boundary field of the problem P. The boundary field is obtained from the problem P simply by using the following commands

```
MEDCouplingFieldDouble *bdy= P.getValuesOnBoundary("share", "u");
```

where the pointer P is passed to the problem P1 in the *getInput1* function.

At each time step the boundary conditions defined by the external field *field* are imposed on the common *share* cube face. In Figure 2.2 one can see the surface (labeled as *share*) of the computational domain where the data transfer is allowed with Libmesh global numbering. The LIBMESH interface creates a map to connect this global numbering to the surface mesh *share* of the region Ω_1 and another surface map *share* of the region Ω_2. The surface mesh in MEDMem representation has the same number of nodes but different numbering. It is necessary therefore at the beginning of the computation to search point by point the correspondence to build the map. Once the map is computed all field values on the surface can be passed to the LibMesh surface and viceversa.

The solution over the coupled interface on the region Ω_1 and Ω_2 can be seen on the left and right of Figure 2.3, respectively. The solution over the coupled domain is shown in Figure 2.4. In this figure the solid is cut along the common interface *share*. Finally in

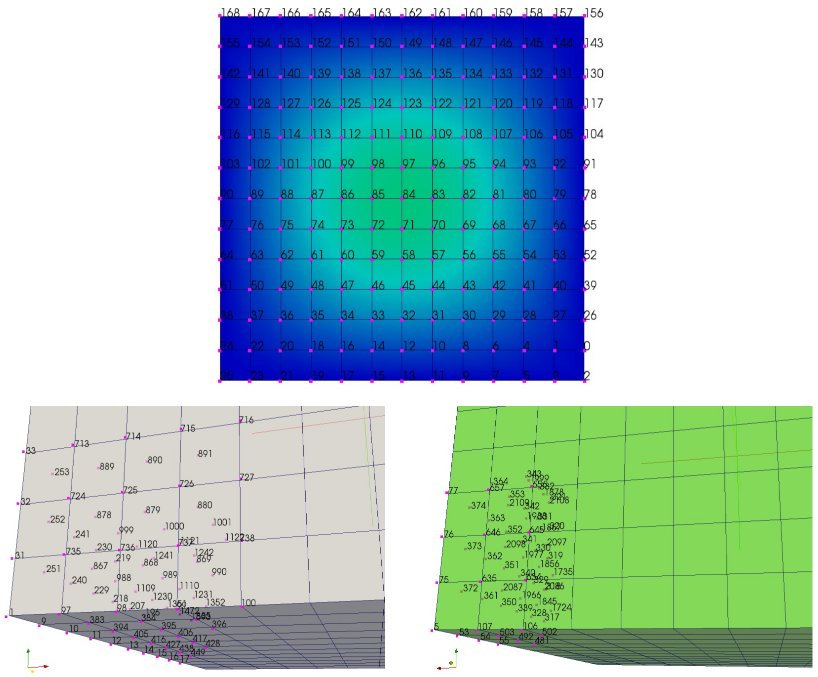


Figure 2.2: Numbering of the same surface in MEDMem mesh (top) and in libMesh as Ω_1 (left bottom) and as Ω_2 (right bottom).

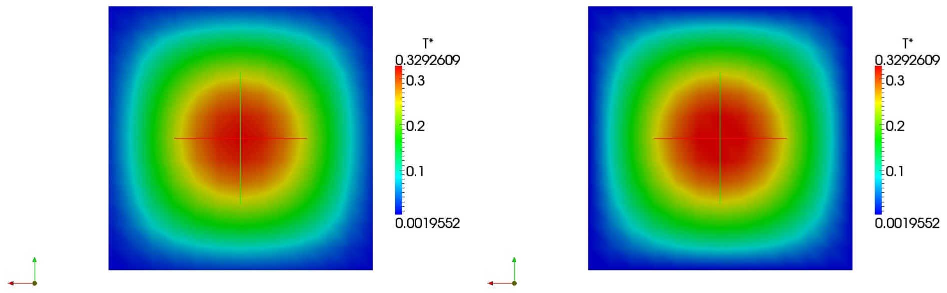


Figure 2.3: Solution over the coupled interface as Ω_1 (left) and as Ω_2 (right).

Figure 2.5 the evolution of the solution over the coupled domain is reported. For high resolutions and small time steps the solution is continuous. The interface discontinuity in the derivative can be seen at the initial time steps. The data transfer from the nodes of the common face of the domain Ω_1 to Ω_2 seems efficient and reliable.

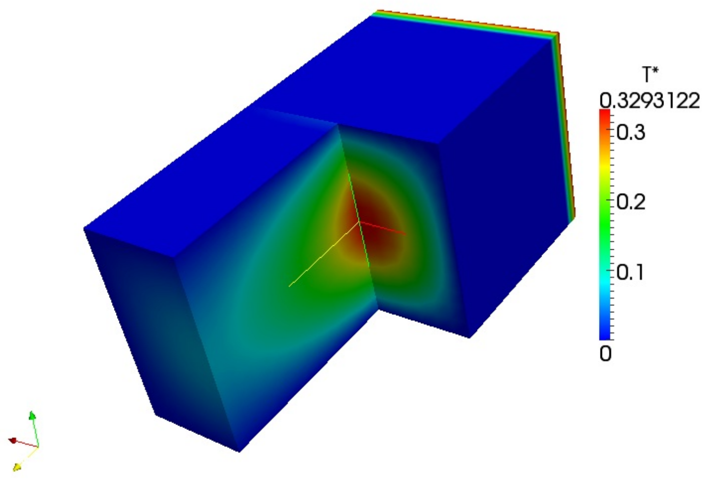


Figure 2.4: Solution over the coupled domain.

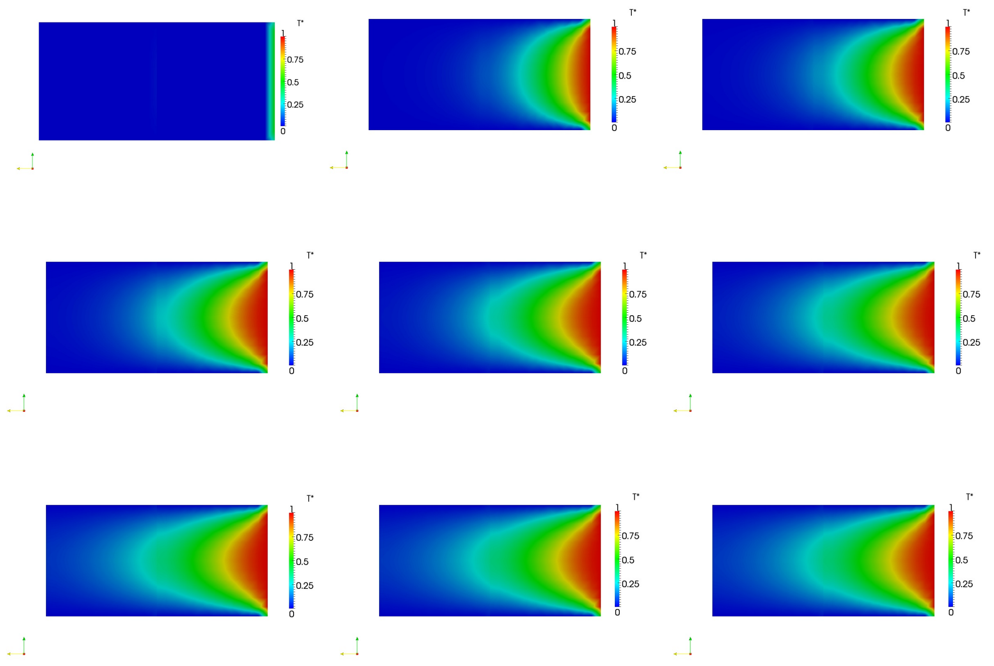


Figure 2.5: Solution evolution over the coupled domain.

2.1.2 LibMesh Navier-Stokes coupling (3D-3D)

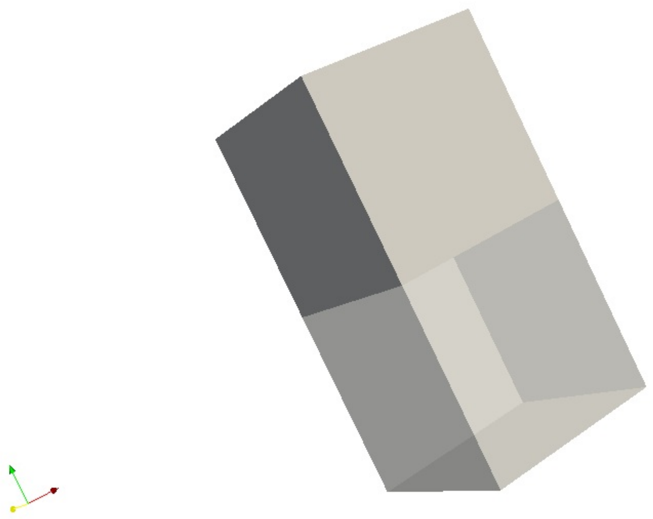


Figure 2.6: Coupling 3D-3D geometry. Domain $\Omega_1 \cup \Omega_2$.

The coupling of a scalar over a surface common region between two codes has been shown in the previous section. Now we consider a data transfer for a vector in the Navier-Stokes equation. We consider the geometry shown in Figure 2.6 which is similar to the geometry presented in the previous section. This time the motion is along the z-axis. The boundary has no slip boundary condition on the *up*, *down*, *left* and *right* faces. On the *share* face we set outlet conditions in the down problem and non homogeneous Dirichlet boundary conditions in the up problem imposing the continuity of velocity field computed in the down problem. In the inlet *bottom_down* we impose standard velocity boundary conditions with a constant field. In the *top_up* outflow conditions are imposed. Again we start in parallel two different problems on multiprocessor machines, one in the down-region and another in the up-region. The LibMesh code runs two coupled Navier-Stokes problems through the LIBMESH class with the following code lines

```
LIBMESH P;                    LIBMESH P1;
P.setType("navierstokes3D"); P1.setType("navierstokes3D");
P.setMesh(dataFile);          P1.setMesh(dataFile1);
getInput(P, boundary);

for(int itime=0;itime<60;itime++){
  for(int i=0; i<boundary.size(); i++) { // boundary problem P
```

```
      sBC & b = boundary[i];
      if(b.isAnalytic)
        P.setAnalyticBoundaryValues(b.name, b.type, b.equation);
      else
        P.setFieldBoundaryValues(b.name, b.type, b.field);
    }
    P.solve();
    getInput1(P1, P,  boundary1);

    for(int i=0; i<boundary1.size(); i++) { // boundary problem P1
      sBC & b1 = boundary1[i];
      if(b1.isAnalytic)
        P1.setAnalyticBoundaryValues(b1.name, b1.type, b1.equation);
      else
        P1.setFieldBoundaryValues(b1.name, b1.type, b1.field);
    }
    P1.solve();
    vsol[0] =  P.getOutputField("u");
    vsol[1] =  P.getOutputField("v");
    vsol[2] =  P.getOutputField("w");

    vsol1[0] =  P1.getOutputField("u");
    vsol1[1] =  P1.getOutputField("v");
    vsol1[2] =  P1.getOutputField("w");
  }
  P.terminate();
  P1.terminate();
```

The LibMesh problems P and P1 are constructed with the empty interface constructor LIBMESH P and LIBMESH P1. The problem type (navierstokes3D) is set with the *setType* function. The mesh with med format is assigned with the *setMesh* function which transfers automatically the mesh to the libMesh program. We have two meshes, one for the top mesh and another from the bottom one. The file is read with the *setMesh* function from the *dataFile* and *dataFile1* file respectively. The interface conditions of the problem P are set by the *getInput* function. The *getInput* function is defined in the main file and it is available to the user.

In order to set the interface conditions the name of the different boundaries should be associated with the boundary conditions. The labels of the boundary regions are available with the function *getBoundaryNames()* in the *LIBMESH* class. The boundary conditions for the problem P are set as

```
boundary[0].name="right_down"
boundary[0].type = "Dirichlet";
boundary[0].isAnalytic = true;
boundary[0].field = NULL;
```

```
boundary[0].equation = "IVec*0.0 + JVec*0.0+ KVec*0.0";
....
....
boundary[4].name="Bottom_down"
boundary[4].type = "Dirichlet";
boundary[4].isAnalytic = true;
boundary[4].field = NULL;
boundary[4].equation = "IVec*0.0 + JVec*0.0+ KVec*1.0";

boundary[5].name="share"
boundary[5].type = "Neumann";
boundary[5].isAnalytic = true;
boundary[5].field = NULL;
boundary[5].equation = "0.";
bcNames[5]="share"
```

The boundary conditions for the problem P1, in the upper part of the domain are set as

```
boundary[0].name="right_up"
boundary[0].type = "Dirichlet";
boundary[0].isAnalytic = true;
boundary[0].field = NULL;
boundary[0].equation = "IVec*0.0 + JVec*0.0+ KVec*0.0";
....
....
boundary[4].name="share"
boundary[4].type = "Dirichlet";
boundary[4].isAnalytic = false;
boundary[4].field = bdy;
boundary[4].equation = "";

boundary[5].name="top_up"
boundary[5].type = "Neumann";
boundary[5].isAnalytic = true;
boundary[5].field = NULL;
boundary[5].equation = "";
bcNames[5]="share"
```

It is easy to note that vectors are written in the vectorial form as "IVec*u + JVec*v+ KVec*w", where an expression for each velocity component u, v and w should be appropriately written. In this case on the interface *share* of the problem P1 we set a Dirichlet boundary condition imposing the boundary field of the problem P. The boundary field $\boldsymbol{v}$ is obtained from the problem P by using the following functions

```
MEDCouplingFieldDouble *bdy=P.getValuesOnBoundary
```

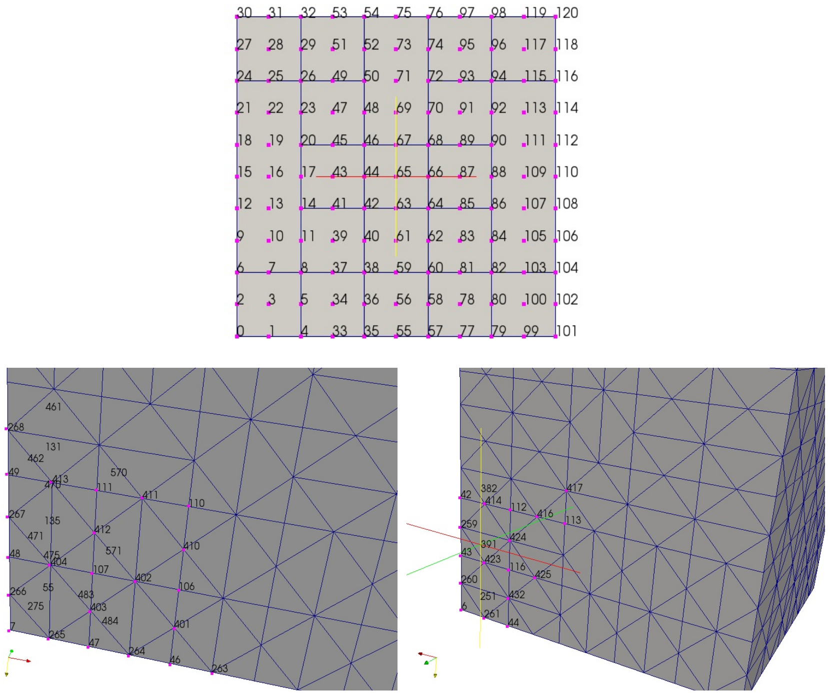


Figure 2.7: Numbering of the same surface in MEDMem mesh (top) and in libMesh as Ω_1 (left bottom) and as Ω_2 (right bottom).

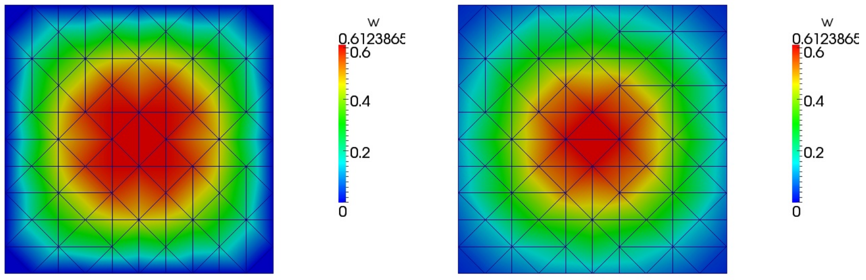


Figure 2.8: Solution over the coupled interface as Ω_1 (left) and as Ω_2 (right).

```
                    ("share","IVec* u + JVec* v + KVec* w");
P.getValuesOnBoundary("share", "w");
```

where the pointer P is passed to the problem P1 in the *getInput1* function.

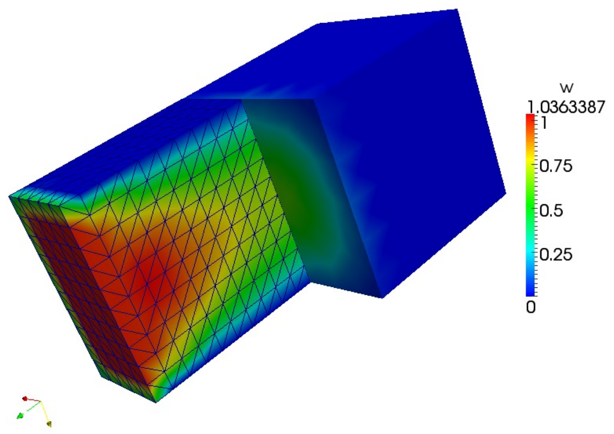


Figure 2.9: Solution over the coupled domain.

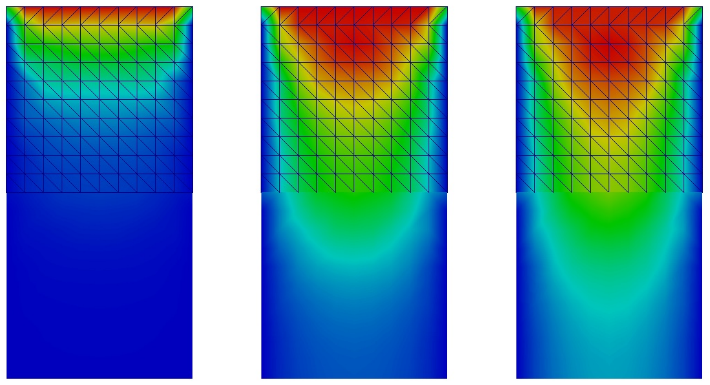


Figure 2.10: Solution evolution over the coupled domain.

At each time step the boundary conditions defined by the external field *field* are imposed on the common *share* cube face. In Figure 2.7 one can see the surface (labeled as *share*) of the computation domain where the data transfer is allowed with libMesh global numbering. The *LIBMESH* interface creates a map to connect this global numbering to the surface mesh *share* of the region Ω_1 and another surface map *share* of the region Ω_2. The surface mesh in MEDMem representation has the same number of nodes but different numbering. It is necessary therefore to search point by point the correspondence. Once the map is computed all field values on the surface can be passed to the libMesh surface and viceversa.

The solution over the coupled interface on the region Ω_1 and Ω_2 can be seen on the left and right of Figure 2.8, respectively. Some differences can be noted. The solution, as explained before, is not passed by NODES but by CELLS. The computation of the values over the CELL implies averaging and for large mesh the difference is not negligible. In Figures 2.9- 2.10 one can see the solution over the coupled interface on the region Ω_1 and Ω_2. The solution over the coupled domain is shown in Figure 2.9. Finally in Figure 2.10 the evolution of the solution over the coupled domain is reported. For high resolutions and small time steps the solution seems continuous. The interface discontinuity in the derivative can be seen clearly due to large meshes used.

2.1.3 LibMesh energy coupling 3D-module/1D-module

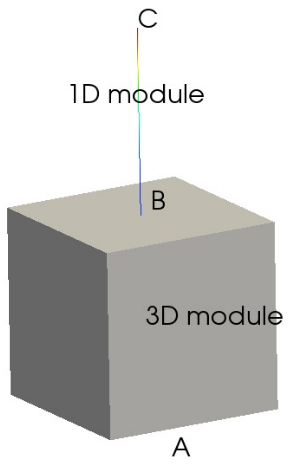


Figure 2.11: Coupling 3D-1D geometry. Domain $\Omega_1 \cup \Gamma_2$ (BC line).

The multiscale coupling of a scalar over a 2D surface connecting a 3D module and 1D module can be done easily by using averaging operator on boundary. We consider the geometry shown in Figure 2.11 which is similar to the geometry presented in the previous section for the three-dimensional domain. The equations considered here are the energy libMesh modules in 3D and 1D respectively. The motion in the 3D domain is along the z-axis from A to B. The 1D region is attached to the three-dimensional region at the point B. The mono-dimensional domain goes from B to C.

The 3D domain has Dirichlet boundary condition on the *up*, *down*, *left* and *right* faces. On the *share* face (B) we set Neumann in the down problem and non homogeneous Dirichlet boundary conditions at the point B of the 1D problem, imposing the average temperature computed in the 3D problem. In the inlet (face (A)) we impose constant Dirichlet boundary conditions with a constant field as at the end of the line (C) closing the loop. Again we start in parallel two different problems on multiprocessor clusters: one in the down-region and another in the line region. The LibMesh code runs through the LIBMESH class with the following code lines

```
LIBMESH P;  LIBMESH P1;
P.setType("convdiff");      P1.setType("monodim");
P.setMesh(dataFile);        P1.setMesh(dataFile1);
P.setAnalyticSource("1.");  P1.setAnalyticSource("0.");
double source[1]={1};
P1.setAverageSources(1,source);
std::vector<sBC> boundary;  std::vector<sBC> boundary1;
getInput(P, boundary);
// time loop
```

```
  for(int itime=0; itime<=15; itime++) {
    for(int i=0; i<boundary.size(); i++) {
      sBC & b = boundary[i];
      if(b.isAnalytic)
        P.setAnalyticBoundaryValues(b.name, b.type, b.equation);
      else
        P.setFieldBoundaryValues(b.name, b.type, b.field);
    }

    P.solve();
    // for constant average value from P
    MEDCouplingFieldDouble *bdy=NULL;
    std::vector<char*> name;  name.push_back("u0");
    bdy = P.getValuesOnBoundary("share", "u");
    double average[1]; average[0] = bdy-> getAverageValue();
    P1.setAverageSources(1,average);
    P1.solve();
 }

  P.terminate();  P1.terminate();
```

In this case on the interface *share* of the problem P1 we set a Dirichlet boundary condition imposing the boundary field of the problem P. The boundary field u is obtained from the problem P by using the following commands

```
 bdy = P.getValuesOnBoundary("share", "u");
```

where the pointer P is passed to the problem P1 in the *getInput1* function. Since the point B is a single point we need to take the average of the surface values using the MEDMem function

```
  bdy-> getAverageValue();
```

before imposing the Dirichlet boundary condition over the first point of the line domain. In Figure 2.12 the evolution of the solution over the coupled domain is reported. The 1D solution follows the 3D dimensional solution as expected. From the left top to the bottom right the solution is reported for different time steps. In each Figure on the left it is reported the three-dimensional domain while on the right the temperature along the central axis of the cube domain (segment A-B) and along the mono-dimensional domain (B-C). The temperature at B in the mono-dimensional domain is always below the central point temperature of the coupling surface.

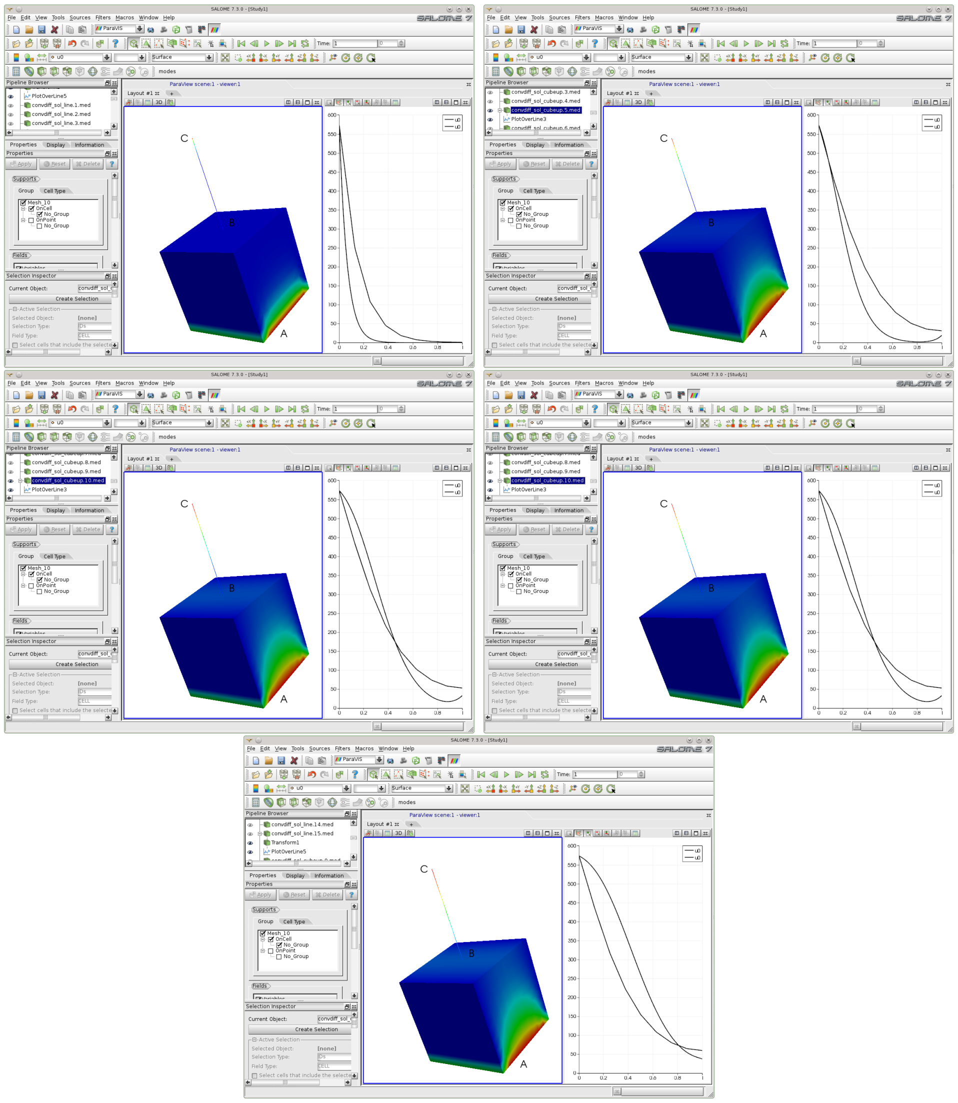


Figure 2.12: Solution evolution over the coupled domain.

2.2 Coupling FEMLCORE modules

The FEMLCORE code is build by using FEMus library and it has been integrated in SALOME platform as already described in the previous chapter. In the first section we test the coupling for the single 3D-CFD module of the library in order to combine this code in the next section with 3D-porous module.

2.2.1 FEMus Navier-Stokes 3D-CFD module coupling

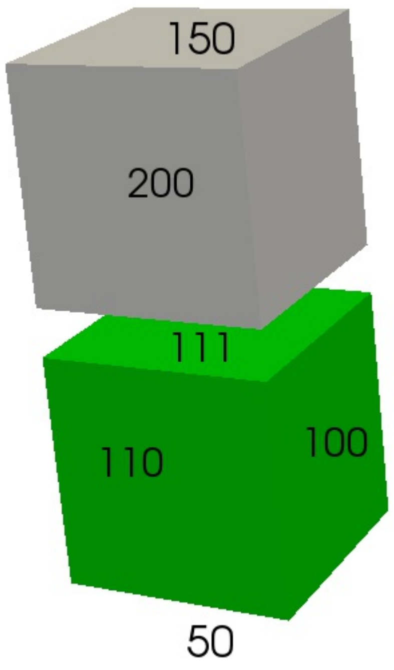


Figure 2.13: Coupling 3D-3D geometry for Navier-Stokes equation. Domain $\Omega_1 \cup \Omega_2$.

We consider the geometry shown in Figure 2.13 with motion along the vertical z-axis. The boundary has no slip boundary condition on the *110*, *100* and *200* face. On the *111* face we set outlet conditions in the down problem and non-homogeneous Dirichlet boundary conditions in the up problem imposing the continuity of velocity field computed in the down problem. In the inlet *50* we impose standard velocity boundary conditions with a constant field. In the surface *150* outflow conditions are imposed. Again we start in parallel two different problems on multiprocessor machines. We run two coupled Navier-Stokes problems through the LIBMESH class with the following code

```
// system 1
FEMUS P;                            // constructor
P.init_param(*mgutils[0]);          // init parameter
P.init_fem(*mggeomel,*mgfemap);     // init fem
// setting mesh --------------------------------------
P.setMedMesh(osfilenameP[0].str().c_str()); // MEDmesh
P.setMesh();                                // MGmesh
// setting system -------------------------------------
P.setSystem(myproblemP);        // set system
P.init_interfaces(filenameP[0].str().c_str()); // init
P.set_param_BCzone();           // def bc conditions
P.set_interface_userbc();       // set bc conditions

// system 2
FEMUS P1;                         // constructor
P1.init_param(*mgutils[1]);      // init parameter
P1.init_fem(*mggeomel,*mgfemap); // init fem
 // setting mesh -------------------------------------
P1.setMedMesh(osfilenameP[1].str().c_str());// MED-mesh
P1.setMesh();                               // MGmesh
 // setting system -----------------------------------
P1.setSystem(myproblemP);            // set system
P1.init_interfaces(filenameP[1].str().c_str()); // init

// solving ---------------------------------------------
int    n_steps = mgutils[0]->get_par("nsteps");
double      dt = mgutils[0]->get_par("dt");
int print_step = mgutils[0]->get_par("printstep");
int    itime_0 = mgutils[0]->get_par("itime");
double time    = 0.;
P.solve_setup(itime_0,time); // initial time loop (t=0)
P1.solve_setup(itime_0,time);// initial time loop (t=0)

// transient loop  (i0time ->i0time+ n_steps)
for(int itime=itime_0; itime<
                       itime_0 + n_steps; itime++) {
  P.solve_onestep(itime_0,itime,print_step,time,dt);
   P1.set_param_BCzone(P);   // define param bc conditions
   P1.set_interface_userbc();// set bc conditions
   P1.solve_onestep(itime_0,itime,print_step,time,dt);
}   // end time loop
P.terminate();   P1.terminate();
```

The LibMesh problem P and P1 are constructed with the empty interface constructor

FEMUS P and FEMUS P1. The problem type ("NS_F") is set with the *setSystem* function. The mesh with med format is assigned with the *setMedMesh* function which transfers automatically the mesh to the FEMUS program. Now we have two meshes, one for the top cube and another from the bottom one. The file is read with the *setMesh* function from the *utils class*. The interface mesh of the problem P are generated by the *init_interfaces* function. The *set_param_BCzone* function defines the boundary conditions. This function is available to the user since it is in the *FEMUS_BC.C*.

In order to set the interface conditions the name of the different boundaries should be associated with the boundary conditions. The labels of the boundary regions are available with the function *getBoundaryNames()* in the *LIBMESH* class. The boundary conditions for the problem P are set as

```
boundary[0].name="110"
boundary[0].type = "Dirichlet";
boundary[0].isAnalytic = true;
boundary[0].n_cmp = 3;
boundary[0].field = NULL;
boundary[0].equation = "IVec*0.0 + JVec*0.0+ KVec*0.0";
....
....
boundary[4].name="50"
boundary[4].type = "Dirichlet";
boundary[4].isAnalytic = true;
boundary[0].n_cmp = 3;
boundary[4].field = NULL;
boundary[4].equation = "IVec*0.0 + JVec*0.0+ KVec*1.0";

boundary[5].name="111"
boundary[5].type = "Neumann";
boundary[5].isAnalytic = true;
boundary[5].field = NULL;
boundary[5].equation = "0.";
bcNames[5]="share"
```

The boundary conditions for the problem P1, in the upper part of the domain, are set as

```
boundary[0].name="200"
boundary[0].type = "Dirichlet";
boundary[0].isAnalytic = true;
boundary[0].n_cmp = 3;
boundary[0].field = NULL;
boundary[0].equation = "IVec*0.0 + JVec*0.0+ KVec*0.0";
....
....
```

```
boundary[4].name=""111"
boundary[4].type = "Dirichlet";
boundary[4].isAnalytic = false;
boundary[0].n_cmp = 3;
boundary[4].field = bdy;
boundary[4].equation = "";
```

It is easy to note that vectors are written in the vector form as *"IVec*u + JVec*v+ KVec*w"*, where an expression for each velocity component u, v, w should be appropriately written. In this case on the interface *111* of the problem P1 we set a Dirichlet

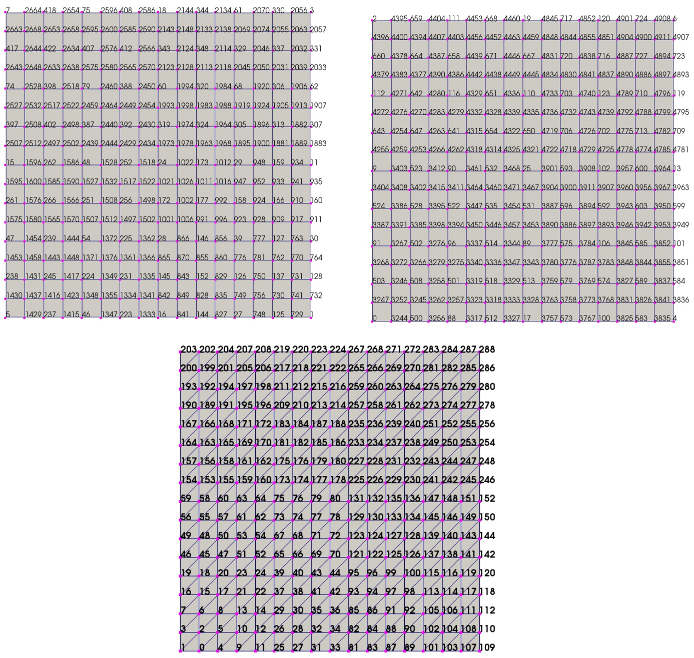


Figure 2.14: Numbering of the same surface in MEDmesh (bottom) and in MGMesh as Ω_1 (left top) and as Ω_2 (right top).

boundary condition imposing the boundary field of the problem P. The boundary field $\boldsymbol{v}$ is obtained from the problem P by using the following functions

```
MEDCouplingFieldDouble *bdy=P.getValuesOnBoundary
                       ("111","NS0",0,3);
```

where the pointer P is passed to the problem P1 in the *set_param_BCzone* function.

At each time step the boundary conditions defined by the external field *field* are imposed on the common *111* cube face. In Figure 2.14 one can see the surface (labeled as *111*) of the computation domain where the data transfer is allowed with FEMus global

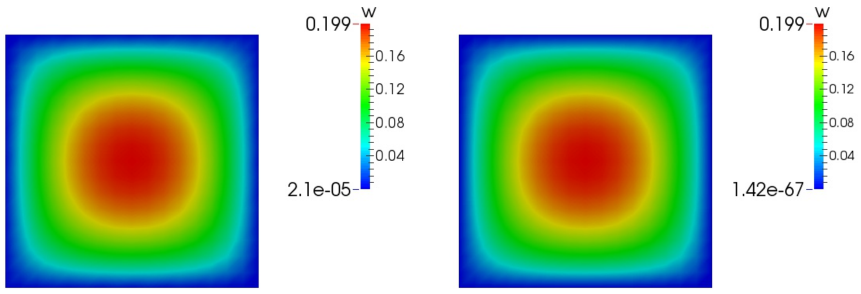


Figure 2.15: Solution over the coupled interface as Ω_1 (left) and Ω_2 (right).

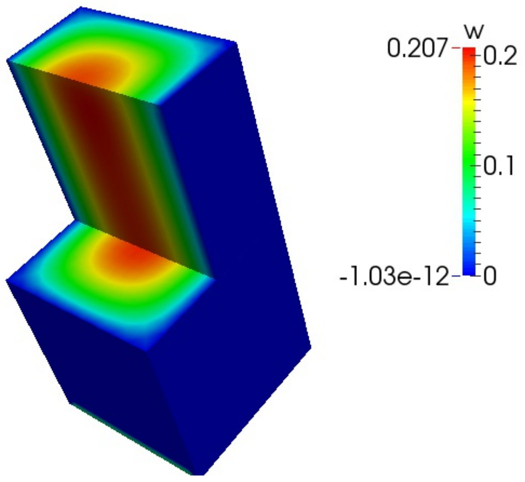


Figure 2.16: Solution over the coupled domain.

numbering. The *FEMus* interface creates a map to connect this global numbering to the surface mesh *111* of the region Ω_1 and another surface map *111* of the region Ω_2. The surface mesh in MEDMem representation has the same number of nodes but different numbering. It is necessary therefore to search point by point the correspondence. Once the map is computed all field values on the surface can be passed to the FEMus surface and viceversa.

The solution over the coupled interface on the region Ω_1 and Ω_2 can be seen on the left and right of Figure 2.15, respectively. No differences can be noted in this case. We remark the difference with the libMesh case where the data exchange was for CELLS. In this case (FEMus) the data are transferred points by points and differences are negligible.

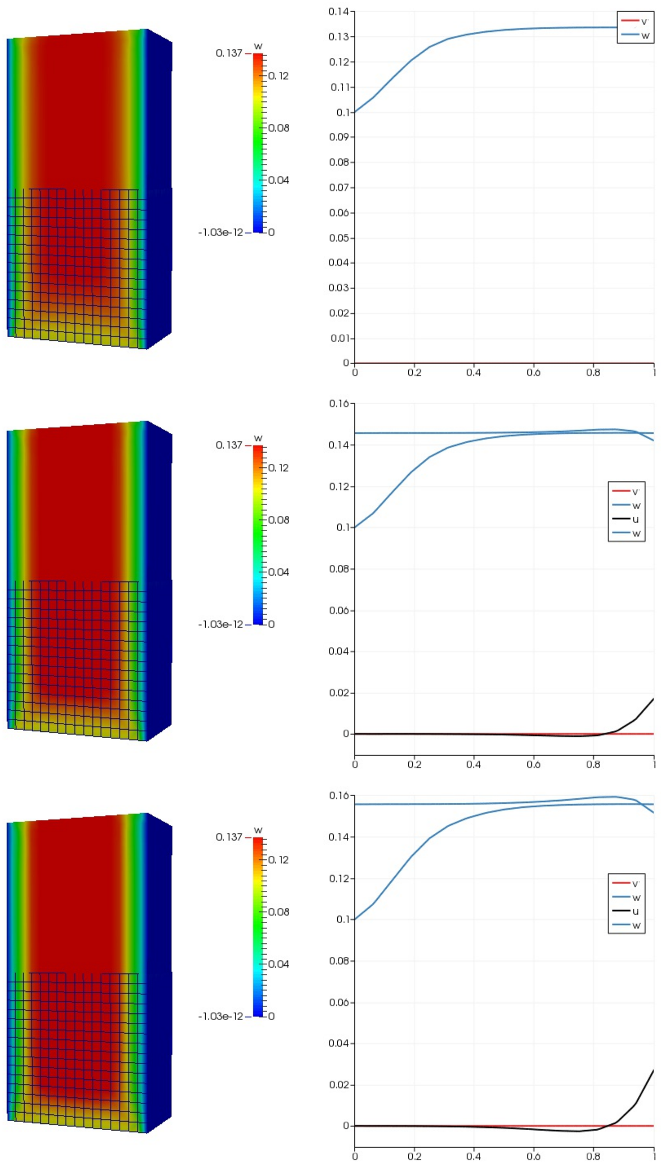


Figure 2.17: Solution evolution over the coupled domain in 3D (left) and over the center line (right).

In Figure 2.16 one can see the solution over the coupled domain $\Omega_1 \cup \Omega_2$, while in Figures 2.17 the solution evolution is reported in the three-dimensional domain (left) and over the center line (right).

2.2.2 FEMus-libMesh coupling (3D-1D)

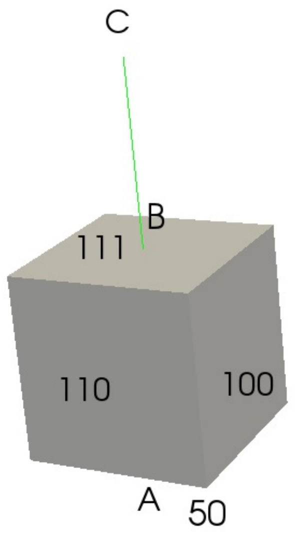


Figure 2.18: Coupling 3D-1D geometry. Domain $\Omega_1 \cup \Gamma_2(BCline)$.

The multiscale coupling of the temperature over a 2D surface connecting a 3D module and 1D module can be done easily by using SALOME MEDMem library. In this library many functions are available for averaging, finding maximum or minimum of any field over a surface. We consider the geometry shown in Figure 2.18. The equations considered here are the energy FEMus module in 3D and the monodim module of libMesh for the 1D mesh. The motion in the 3D domain is along the z-axis from A to B. The 1D region is attached to the three-dimensional region at the point B. The mono-dimensional domain goes from B to C over a unitary length.

The boundary has Dirichlet boundary condition on the *100*, *50* and *110* faces. On the *110* face (B) we set Neumann in the down problem and non-homogeneous Dirichlet boundary conditions at the point B problem imposing the average temperature computed in the down problem. In the inlet *50* we impose constant Dirichlet boundary conditions with a constant field. At the end of the line (C) Dirichlet boundary condition are imposed as at the face (A). We start in parallel two different problems on multiprocessor machines: a FEMus problem is solved in the down-region and a libMesh problem in the line region. The FEMus and the libMesh problems are coupled. The LibMesh and FEMus code coupling runs with the following code lines

```
// system1 ----------------------------------------
FEMUS P;
P.init_param(*mgutils[0]);
```

```
  P.init_fem(*mggeomel,*mgfemap);
  // setting mesh ---------------------------------
  P.setMedMesh(osfilenameP.str().c_str());// MEDmesh
  P.setMesh();                            // MGMesh
  // setting system -------------------------------
  std::vector<NS_FIELDS> myproblem; myproblem.resize(1);
  myproblem[0]=T_F;
  P.setSystem(myproblem);
  P.init_interfaces(filenameP.str().c_str());

  // system 2
  LIBMESH P1;
  P1.setType("monodim");
  P1.setMesh(dataFile1);
  P1.setAnalyticSource("1.");
  std::vector<sBC> boundary1;

  // solving
  int    n_steps = mgutils[0]->get_par("nsteps");
  double      dt = mgutils[0]->get_par("dt");
  int print_step = mgutils[0]->get_par("printstep");
  int    i0time = mgutils[0]->get_par("itime");
  double time =0.;
   P.set_param_BCzone();
   P.set_interface_userbc();
   P.solve_setup(i0time,time);
   MEDCouplingFieldDouble *bdy=NULL;

  // transient loop  (i0time ->i0time+ n_steps)
  for(int itime=i0time; itime<
                  i0time +n_steps; itime++) {
  P.solve_onestep(i0time,itime,print_step,time,dt);
  bdy = P.getValuesOnBoundary("111","T",0);
  double average[1];
  average[0] =bdy-> getAverageValue();
  P1.setAverageSources(1,average);
  P1.solve();
 }
 P.terminate();
 P1.terminate();
```

In this case on the point B of the problem P1 we set a Dirichlet boundary condition imposing the boundary field of the problem P. The boundary field T is obtained from

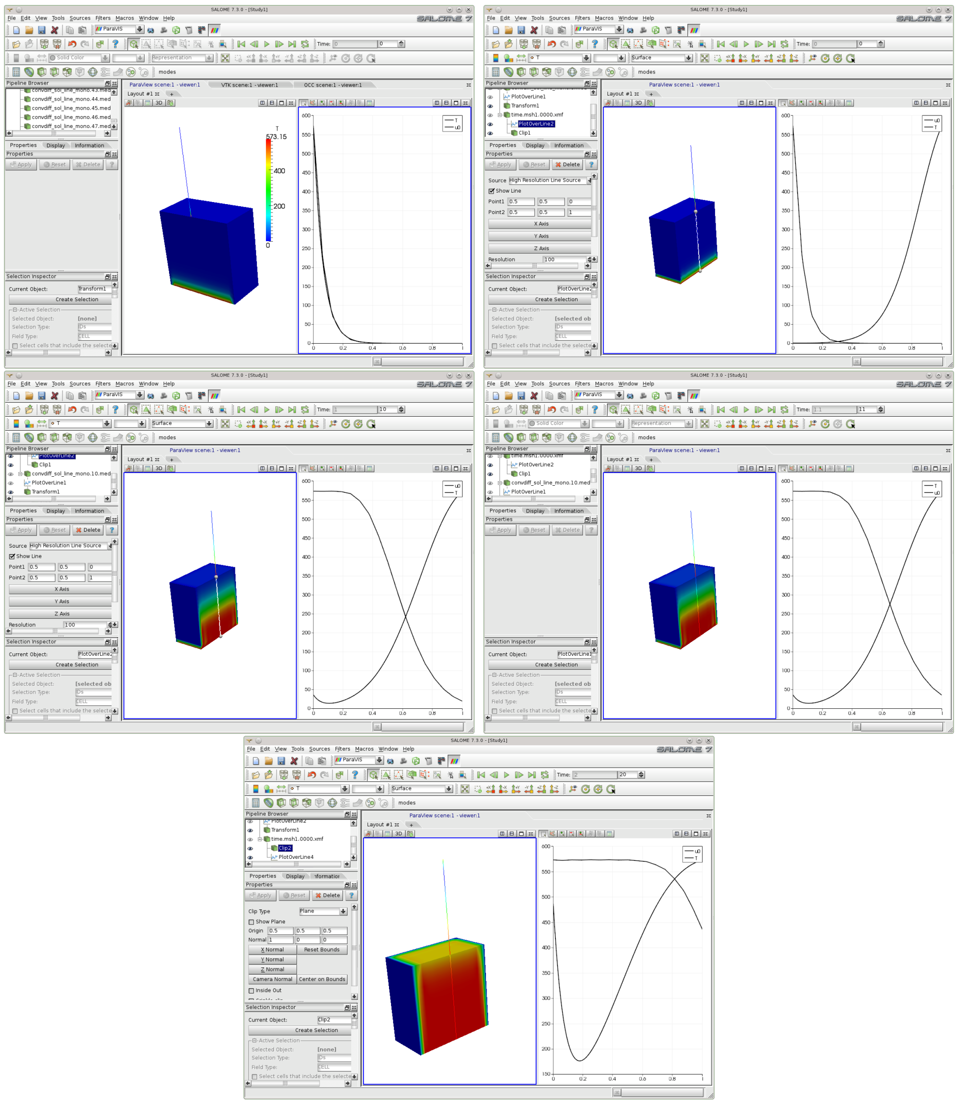


Figure 2.19: Evolution over the coupled domain at different time steps. On the left the three-dimensional solution and on the right the solution over the mono-dimensional line BC.

the problem P by using the following commands

```
bdy =P.getValuesOnBoundary("111","T",0);
```

Since the point B is a single point we need to take the average of the surface using the MEDMem function

```
bdy-> getAverageValue();
```

before imposing the Dirichlet boundary condition over the first point of the line domain.

In Figure 2.19 the evolution of the solution over the coupled domain is reported. The 1D solution follows the 3D dimensional solution as expected. From left top to bottom right the solution is reported for different time steps. In each figure on the left is reported the three-dimensional domain while on the right the temperature along the central axis of the cube domain (segment A-B) and along the mono-dimensional domain (B-C). The temperature at B in the mono-dimensional domain is always below the central point temperature of the coupling surface.

2.3 Coupling FEM-LCORE on SALOME platform

2.3.1 Introduction

GEOMETRICAL PARAMETERS	
side	$1\ m$
height	$4.485\ m$
C_{in}	$1.3\ m$
C_{out}	$3.245\ m$
H_{in}	$2.25\ m$
H_{out}	$3.15\ m$
D_{eq}	$0.0129\ m$
r	0.5408
H_c	$1.945\ m$
H_a	$0.9\ m$

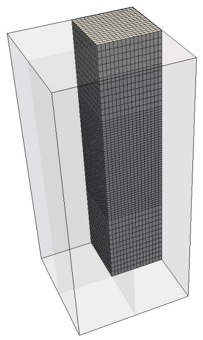


Figure 2.20: Geometrical parameters, physical and computational domain.

In this section we perform some tests to verify the integration on the SALOME platform of the FEM-LCORE module on a simple domain defined in Figure 2.20. In this test analytical functions are constructed through MEDMem interface in order to define the heat source distribution and the pressure losses. In a more complex coupling these functions can be computed by external codes and the data transferred through the FEMUS interface classes. As clearly shown it is possible to consider, given the particular symmetry of the problem, only a quarter of the physical domain.

The model implemented for temperature, pressure and velocity field inside the domain is the same used for the geometry of LF reactors described in previous reports. The interested reader can see details in [5, 3, 4]. We recall briefly that, while for the lower and upper plenum geometry we solve the standard three-dimensional CFD system of equations, within the core region we instead use a porous medium model. The domain has a square cross section of side 1 m and an overall height of 4.485 m. The reactor, along the z direction, is divided into three zones that model the upper, the lower plenum and the core, respectively. The lower plenum extends between the horizontal plane with $z = 0$ and $z = C_{in}$ while the upper plenum bounds between $z = C_{out}$ and $z = 4.485$. The core extends between the plane $z = C_{in}$ and $z = C_{out}$ in the central part of the reactor. The other geometrical dimensions are defined in Figure 2.20.

As it is well known, the core houses fuel elements and assembly channels used for control rod motion. This must be taken into account in developing the core porous model. In fact both bundles of fuel and control rods reduce the section available for the fluid decreasing the dimension of the coolant sub-channels. In this region of the domain where the porous medium model is implemented, distributed pressure losses due to viscous friction and accidental ones due to grid spacers must be taken into account. We set both the source of thermal power and the distributed pressure losses due to spacer grids of fuel elements at the top of the core, between $z = H_{in}$ and $z = H_{out}$.

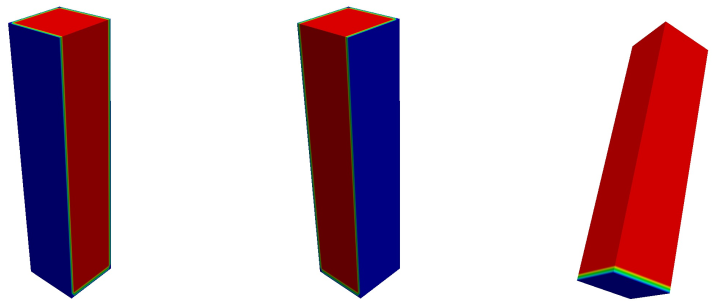


Figure 2.21: Boundary conditions for the velocity components u, v (center and left) and w and temperature field (T) (both in right). The blue color indicates the type of boundary conditions *Dirichlet*; the red boundary conditions of type *Neumann*.

The input and output sections of the core reactor are modeled by appropriate pressure losses as defined in Table 2.2. The core inlet and outlet pressure losses are automatically taken into account by solving three-dimensional modules. The physical properties of

Physical properties Lead at $673.15\ K$	
ρ	$10562.99\ kg/m^3$
μ	$0.002227\ Pa\,s$
c_p	$147.3\ J/kg\,K$
κ	$16.58\ W/m\,K$

Operating parameters in nominal conditions	
T_{in}	$673.15\ K$
ΔT	$80\ K$
$\overline{q}_g$	$1.1761715 \cdot 10^8\ W/m^3$

Table 2.1: Physical properties and operating parameters in nominal conditions

the fluid and the operating conditions are reported in Table 2.1. In Figure 2.20 the values of all the geometric parameters of interest are reported, while in Figure 2.21 the boundary conditions used for the calculations are shown. The blue color indicates the *Dirichlet* type of boundary conditions; the red boundary conditions of type *Neumann*. Boundary condition of *Dirichlet* type means that the value of the variable is fixed on the boundary surface considered. Boundary conditions of homogeneous Neumann type

Accidental Pressure loss	
β_{in}	0.5
β_{out}	1
β_{grids}	0.52

Table 2.2: Computational parameters for Accidental Pressure losses.

means that the value of the derivative of the variable along the normal direction is equal to zero. The vertical component w of the velocity field is fixed to the input section at $z = 0$ (condition of *Dirichlet* type) and it is free to take any value on both side surfaces and on the outlet at $z = 4.485$ (*Neumann* conditions). The temperature is fixed on the input surface while on the lateral surfaces and on the output surface an adiabatic condition is imposed. Either the velocity component u and v are fixed on the two outer surfaces (surface $x = 1$ and $y = 1$) while they are to be computed on the exit surface. Furthermore, the component u is fixed on the inner surface $x = 0$ and free on the inner surface $y = 0$ while, on the contrary, the component v is fixed on the inner surface $y = 0$ and free on the inner surface $x = 0$. The symmetry of the problem allows us to solve the equations only over a quarter of the domain and therefore symmetry conditions are imposed on the internal surfaces both for u and v, ensuring that there is no mass exchange between the four subdomains in which the physical domain is divided.

2.3.2 Exact solution and benchmark cases

The particular geometry considered, similar to a simple horizontal duct, and the simple boundary conditions imply that the problem can be solved along the one-dimensional coordinate z obtaining the exact analytical solution. In fact, in steady state conditions, assuming the constant physical properties in Table 2.1, the equations assume the following simplified form

a) Continuity equation

$$\frac{\partial w^*}{\partial z} = 0 \tag{2.1}$$

b) Momentum equation

$$\frac{\partial p}{\partial z} = -\frac{2\,\rho\,(w^*)^2}{D_{eq}}\,\lambda(w^*) \tag{2.2}$$

c) Energy equation

$$\rho\, c_p\, w^* \,\frac{\partial T}{\partial z} = \kappa\,\frac{\partial^2 T}{\partial z^2} + \frac{q_g}{r} \tag{2.3}$$

where r is the constant filtration coefficient defined as $r = A_{eff}/A_{core}$. The problem (2.1-2.3) can be further simplified when the convective heat transfer term prevails over the diffusion transfer term. With this assumption, the energy diffusion term can be neglected by assigning the thermal conductivity of the fluid $\kappa \to 0$. With this assumption and integrating along the axis z we have

$$w^* = \text{const.} \tag{2.4}$$

$$p_{in} - p_{out} = \frac{2\,\rho\,(w^*)^2}{D_{eq}}\,\lambda(w^*)\,H_c \tag{2.5}$$

$$\rho\,c_p\,w^*\,(T_{out} - T_{in}) = \frac{\overline{q}_g}{r}\,H_a \tag{2.6}$$

where H_c is the height of the core and H_a is the height of the part of core where the source term $q_g \neq 0$.

By using the equations (2.4)-(2.6) we can validate the solution of the FEM code-LCORE in momentum and energy. This implies the possibility to compare the distributed load losses due to viscous friction and the temperature field, calculating the temperature output in stationary conditions at nominal power.

Pressure. By setting the filtration rate w equal to 0.85 m/s we have that the velocity is equal to

$$w^* = \frac{w}{r} = \frac{0.85}{0.5408} = 1.572\ m/s\,. \tag{2.7}$$

We recall that while the real velocity is the one of the fluid actually crossing the sub-channels within the core, the filtration velocity is a fictitious velocity that the coolant would have if it had access to the entire section of the core. The link between these velocities is determined by the velocity ratio between the two sections

$$W/w^* = A_{eff}/A_{core} = r = 0.5408\,.$$

For the Reynolds number we have

$$Re = \frac{\rho\,w^*\,D_{eq}}{\mu} = \frac{10562.99 \times 1.572 \times 0.0129}{0.002227} = 96185\,. \tag{2.8}$$

When the Reynolds number is known the Fanning friction coefficient can be calculated directly for the case of turbulent motion. In this case we have

$$\lambda = \frac{0.0791}{Re^{0.25}} = \frac{0.0791}{96185^{0.25}} = 0.0044916\,. \tag{2.9}$$

Finally, we calculate the total pressure losses resulting solely from the losses distributed on the crossing of the sub-channels as

$$\begin{aligned} \Delta P_{dist} = p_{in} - p_{out} &= \frac{2\,\rho\,(w^*)^2}{D_{eq}}\,\lambda\,H_c = \\ &= \frac{2 \times 10562.99 \times 1.572^2 \times 0.0044916}{0.0129}\,1.945 = \\ &= 35355\ Pa\,. \end{aligned} \tag{2.10}$$

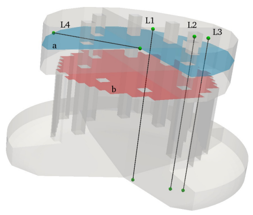


Figure 2.22: Positioning of graphics and images.

The accidental pressure drop, due to abrupt changes of the core inlet and due to the presence of the grids spacing, can be calculated as follows

$$\begin{aligned}\Delta P_{acc} &= \frac{1}{2}\rho\,(w^*)^2 \sum_i \beta_i = \\ &= 0.5\times 10562.99\times 1.572^2\times(1+0.5+0.52\times 5) = \\ &= 53511\ Pa\end{aligned} \tag{2.11}$$

w m/s	**w*** m/s	**Re**	$\mathbf{\Delta P_{dist}}$ Pa	$\mathbf{\Delta P_{in\&out}}$ Pa	$\mathbf{\Delta P_{grids}}$ Pa	$\mathbf{T_{out}}$ K
0.1	0.184	11314.09	835.3047	270.8786	469.5229	1353.57
0.2	0.369	22628.18	2809.6191	1083.5145	1878.0919	1013.41
0.5	0.924	56570.45	13965.0490	6771.9660	11738.0745	809.31
0.85	1.571	96169.77	35345.0074	19570.9820	33923.0354	753.28

Table 2.3: Analytical results for benchmark.

Temperature. In order to estimate the outlet temperature we use the simplified energy equation in (2.6) as

$$\begin{aligned}T_{out} &= T_{in} + \frac{q_g\,H_a}{\rho\,c_p\,w} = \\ &= 673.15 + \frac{1.1761715\cdot 10^8\times 0.9}{10562.99\times 147.3\times 0.85} = 753.15\ K\,.\end{aligned} \tag{2.12}$$

The analytical procedure just shown, useful for the evaluation of pressure drops and outlet temperature, was repeated for the other values of the vertical velocity. The calculations were carried out with the aid of a spreadsheet calculation and the results obtained are shown in Table 2.3.

2.3.3 Benchmarks on FEM-LCORE integration.

In order to validate the functionality of the MEDMem interface created for the FEM-LCORE code we perform three test cases, A, B and C. In case A-B we perform eight numerical tests with the heat source term uniform in space. In case C a test with variable heat source distribution is performed.

$\mathbf{w}\ m/s$	$\mathbf{\Delta P_{dist}}\ Pa$		$\mathbf{T_{out}}\ K$	
	Exact	*FEM – LCORE*	*Exact*	*FEM – LCORE*
0.1	835.3047	835.3047	1353.57	1353.52
0.2	2809.6191	2809.6190	1013.41	1013.37
0.5	13965.0490	13965.0483	809.31	809.25
0.85	35345.0074	35345.0046	753.28	753.19

Table 2.4: Case A. Comparison between analytical results and the code: ΔP_{dist} and T_{out}.

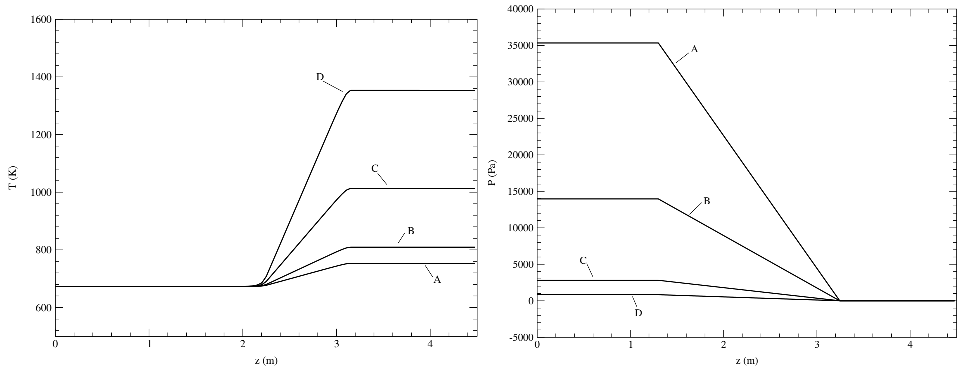


Figure 2.23: Case A. Temperature (left) and pressure (right) profiles along the segment $\overline{ST}$. Line A: inlet velocity $w = 0.85\ m/s$; Line B: inlet velocity $w = 0.5\ m/s$; Line C: inlet velocity $w = 0.2\ m/s$; Line D: inlet velocity $w = 0.1\ m/s$.

Case A The physical properties of the refrigerant are considered constant with temperature equal to the value of the inlet temperature ($673.15\,K$).

In these four tests we consider only pressure drops distributed along the entire length of the core (H_c) while the accidental pressure drops are neglected. We consider four values of filtration velocity w in the range w = 0.1 - 0.85 fixed on the interface of the input section.

In Table 2.4, for the four cases listed above, they are reported both the pressure drop and the outlet temperature together with the comparison between the numerical results provided by the code and the corresponding analytical results. As one can see from the table, the results provided by the FEM-LCORE code reproduce the analytical ones with remarkable precision.

In Figures 2.23 and 2.24 the profiles of temperature, pressure and filtration velocity w

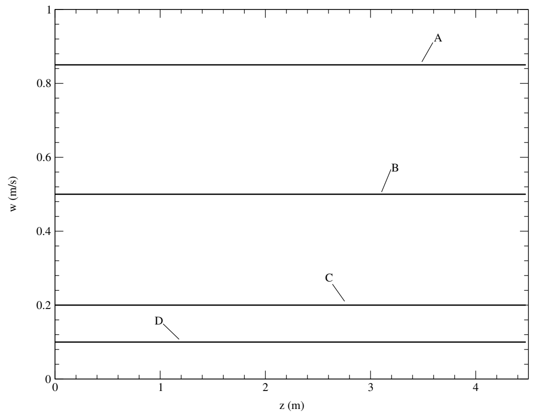


Figure 2.24: Case A. Profile of the filtration velocity w along the segment $\overline{ST}$. Line A: inlet velocity $w = 0.85\ m/s$; Line B: inlet velocity $w = 0.5\ m/s$; Line C: inlet velocity $w = 0.2\ m/s$; Line D: inlet velocity $w = 0.1\ m/s$

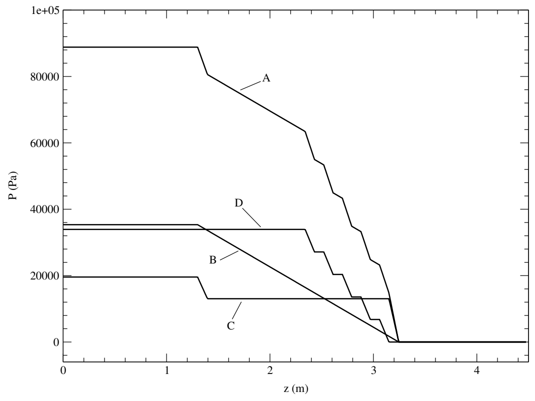


Figure 2.25: Case A. Profile of pressure drop along the segment $\overline{ST}$. Line A: total pressure drop; Line B: contribution of distributed drop; Line C: contribution to energy losses due to abrupt changes of section at the entrance and exit of the core; Line D: contribution due to spacer grids.

along the segment $\overline{ST}$ of coordinates $S = (0.5,\ 0.5\,0)$ and $T = (0.5,\ 0.5\,4485)$ are shown for the first four tests, respectively.

Case B In the other four tests we set the same inlet velocity of $w = 0.85\ m/s$ for all cases, while for each test we consider different pressure drop cases:

- total pressure drop;
- only distributed;

$\mathbf{w}\ m/s$	$\mathbf{\Delta P_{dist}}\ Pa$		$\mathbf{\Delta P_{in \cdot out}}\ Pa$	
	Exact	*FEM − LCORE*	*Exact*	*FEM − LCORE*
0.85	35345.0074	35345.0046	19570.9820	19570.9807

Table 2.5: Case B. Comparison between analytical results and the FEM-LCORE code: ΔP_{dist} and ΔP_{acc}.

$\mathbf{w}\ m/s$	$\mathbf{\Delta P_{grids}}\ Pa$	
	Exact	*FEM − LCORE*
0.85	33923.0354	33923.0316

Table 2.6: Case B. Comparison between analytical results and the FEM-LCORE code: ΔP_{dist} and ΔP_{acc}.

$\mathbf{w}\ m/s$	$\mathbf{\Delta P_{tot}}\ Pa$	
	Exact	*FEM − LCORE*
0.85	88839.0249	88839.0058

Table 2.7: Case B. Comparison between analytical results and the results of the code: ΔP_{tot}.

- only accidental due to sudden changes in section;
- only accidental due to spacer grids.

These different conditions are imposed by using the volume interface from the MEDMem library. For this test we use

```
setAnalyticSource("analitic expression");
```

where different analytical expressions are taken for different cases. Figure 2.25 shows the pressure profile along the segment $\overline{ST}$ for the four cases described above. In Figure 2.26 on the right it can be seen where the accidental pressure losses are located within the core: the grids are labeled 1, 2 3 4 and 5, while with *inlet* and *outlet* we label the pressure drop due to changes of section.

Tables (2.5-2.7) show the comparison between the numerical results of the FEM-LCORE code and the exact analytical results for these last four tests. Once again the Tables show the excellent accuracy of the numerical code FEM-LCORE.

Case C As a final test we want to make a comparison between solutions considering the physical properties of the fluid constants with temperature and power generation uniform in space and the solutions with variable physical properties with temperature and power

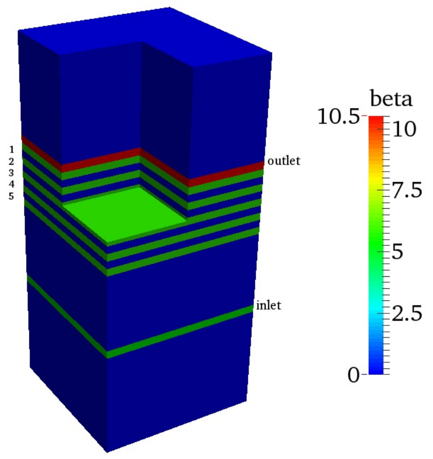


Figure 2.26: Case B. Spatial distribution of the pressure drop coefficient *beta*.

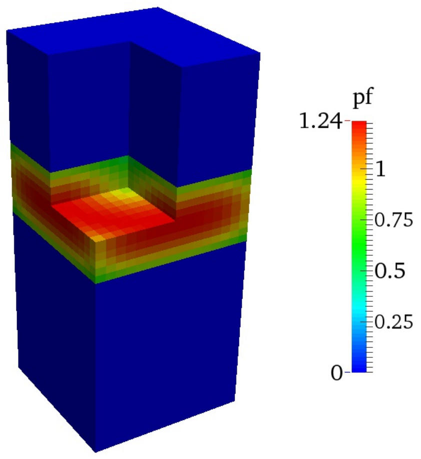


Figure 2.27: Case C. Spatial distribution of the power factor pf.

generation variable in space. In this test we set all the pressure drops previously discussed and vertical velocity w to the value $0.85\ m/s$. The variable distribution of the peak factor is assigned by using a volume interface of the MEDMem library.

The correlations used to describe the dependence of the lead temperature physical

Physical property	Temperature dependence
Density	$\rho = 11367 - (1.1944 \times T) \quad kg/m^3$
Viscosity	$\mu = 4.55 \cdot 10^{-4} \exp(1069/T) \quad Pa\, s$
Thermal conductivity	$\kappa = 9.3 + (0.0108 \times T) \quad W/m\, K$
Specific heat	$c_p = 147.3 \quad kJ/kg\, K$

Table 2.8: Case C. Temperature dependence of the lead physical properties.

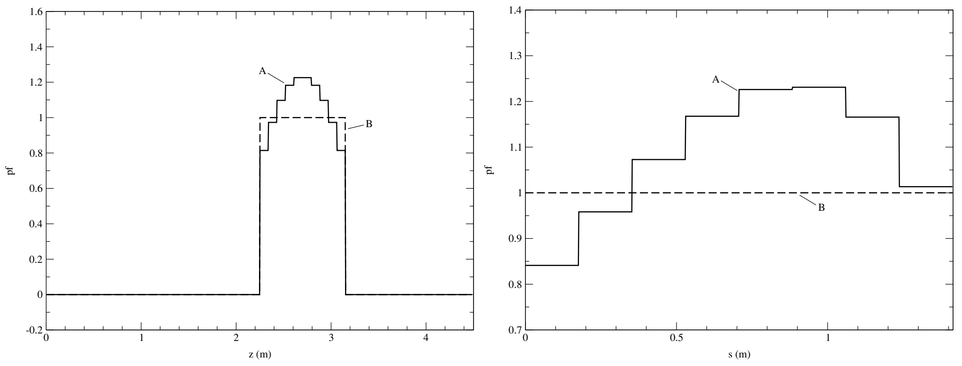


Figure 2.28: Case C. Profiles of the power factor pf. Line A: pf variable; Line B: pf uniform. On the left along segment $\overline{ST}$; on the right along segment $\overline{MN}$.

properties in the range of operating temperatures of the reactor, are reported in Table 2.8 [12, 20, 21, 19]. The spatial distribution of power generation is well visible in Figures 2.27 and 2.28. The power factor is the ratio between the power generated per unit volume as a function of the position and the average power, namely

$$pf(\mathbf{x}) = \frac{q_g(\mathbf{x})}{\overline{q_g}} \,. \tag{2.13}$$

In Figure 2.28 one can see the power factor pf along the segment $\overline{ST}$ and along the segment $\overline{MN}$ on section a at $z = 2.7\ m$ ($M = (0,\, 0,\, 2.7)$, $N = (1,\, 1\, 2.7)$).

The variation of the power factor in the active part of the core has been implemented by means of the analytical function through the MEDMem interface. Different interfaces can be applied in different regions so that the setting can be limited to the core region. The imposed distribution is as follows

$$pf(\mathbf{x}) = (0.79 - 0.516\, r^3 + 0.363\, r^2 + 0.589\, r)\, \cos\left(\frac{\pi\,(z - 2.7)}{1.5}\right) \tag{2.14}$$

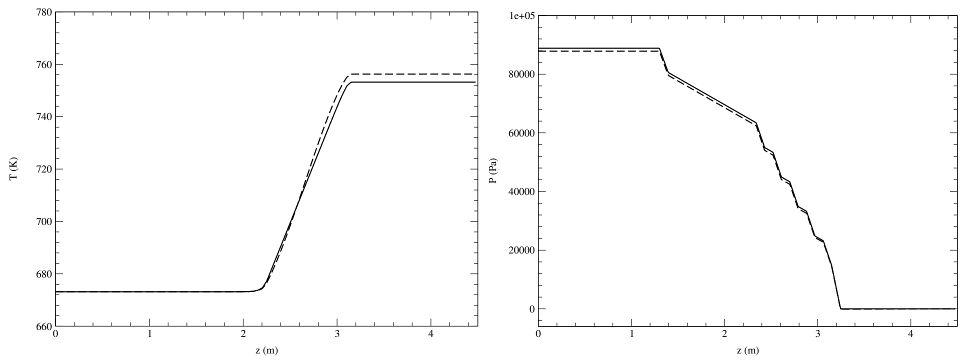


Figure 2.29: Case C. Comparison of temperature (left) and pressure (right) profiles along the line $\overline{ST}$. Dashed line: simulation with temperature dependent physical properties and $q_g = \text{const.}$; Solid line: simulation with constant physical properties and $q_g = q_g(\mathbf{x})$.

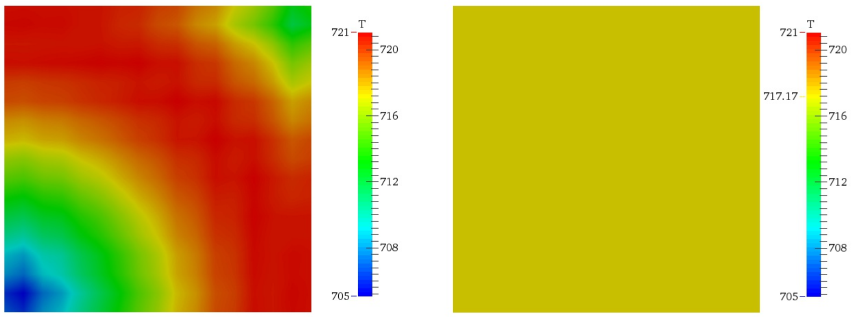


Figure 2.30: Case C. Comparison of temperature distributions on section a. On the left temperature dependent physical property case with $q_g = q_g(\mathbf{x})$. On the right temperature constant physical properties case with $q_g = \text{const.}$

where ($r = \sqrt{x^2 + y^2}$). This distribution is similar to the actual distribution of the power reactor ELSY/ALFRED [8, 9, 10, 11, 12, 18]. In Figure 2.29 the comparison between the profiles of pressure and temperature along the segment $\overline{ST}$ for the two cases considered is shown. From Figure 2.30 and 2.31 it is quite evident the effect on the fields T and w of the space power generation distribution and of the temperature dependence of the refrigerant thermophysical properties. Finally, Figure 2.32 shows the stationary solution for three-dimensional fields of pressure, velocity and temperature in the case of non-uniform heat source in space with temperature dependent fluid properties. In this case we have forced the heat source to have an analytic form but with the same MEDMem interface we could transfer the solution from a neutronic code implemented over the SALOME platform.

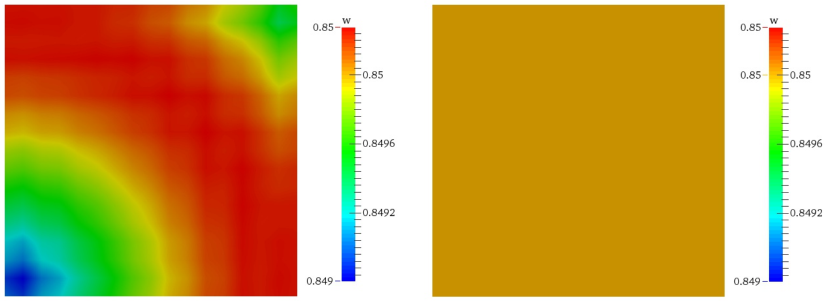


Figure 2.31: Case C. Comparison between the distributions of filtration velocity w on the section a. On the left temperature dependent physical property case with $q_g = q_g(\mathbf{x})$. On the right temperature constant physical properties case with $q_g = \text{const}$.

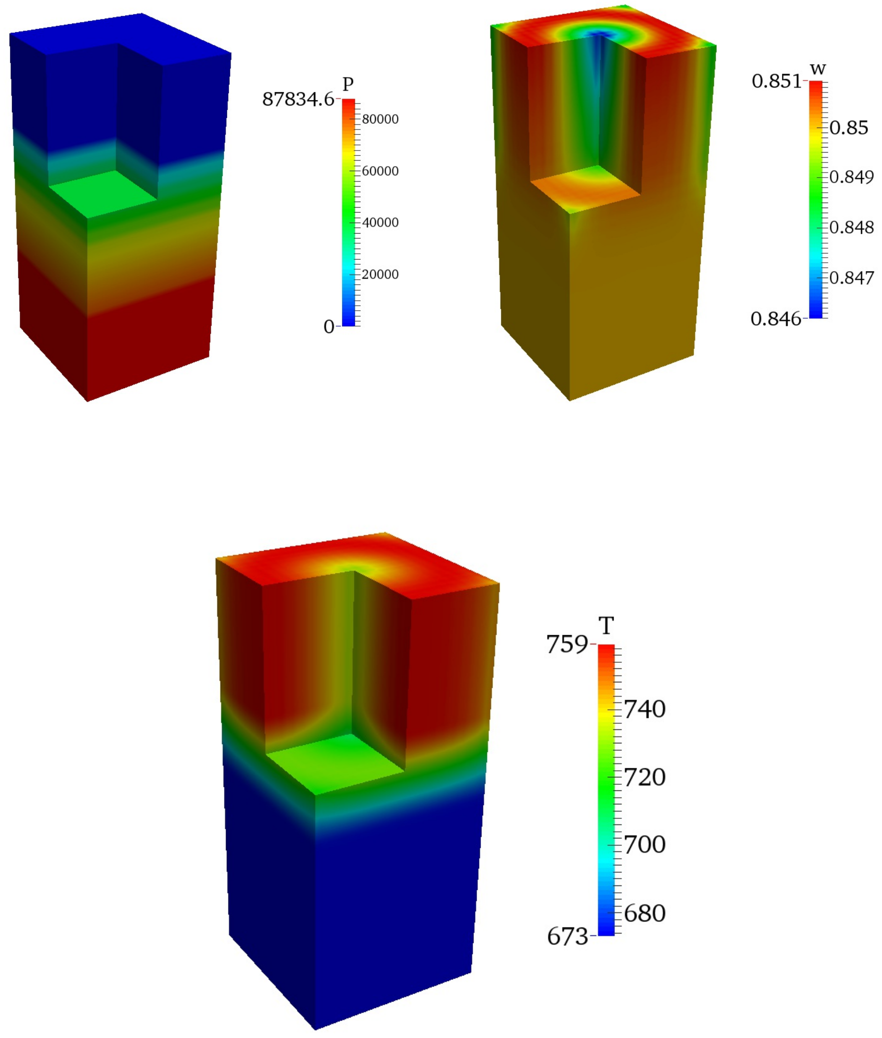


Figure 2.32: Case C. Pressure, velocity and temperature fields. Tests with inlet filtration velocity $w = 0.85\ m/s$, variable fluid properties and with all pressure drops.

2.3.4 Coupling 3D-FEMLCORE and 1D libMesh primary loop module

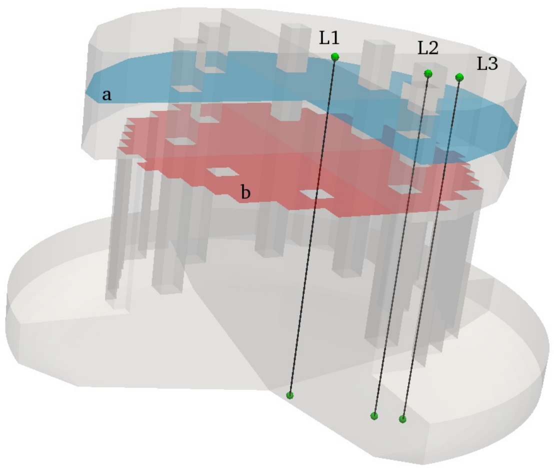


Figure 2.33: FEMLCORE module. Placement of figures and charts. Cross-sectional portion of a at $z = 3.9$ m; Cross section b at $z = 3.244$ m; line L1 at $x = y = 0.2$ m; line L2 at $x = y = 1$ m; line L3 at $x = 1.323$ m and $y = 1.176$ m.

In this test we couple the FEMLCORE code with a monodimensional code based on libmesh libraries. The monodimensional code solves the conservation equations where we add some sources to model a simple pump and vapor generator model [5]. The coupling gives the boundary conditions for the FEMLCORE. The *FEMUS* interfaces are three: the inlet and the two outlets of the reactor. On the inlet we transfer the velocity field from the monodimensional system to the inlet surface. At the outlet we pass the velocity field from the outlet surface to the monodimensional libMesh problem. The pressure field transfers in the opposite direction. We use the MEDMem tools to integrate the field over the surfaces and transfer the average value from one scale to the other. The temperature is always tranfer in the motion direction, i.e, from the libMesh module to the FEMLCORE inlet and from the FEMLCORE outlet to the monodimensional libMesh module.

In this test we analyze the working behavior of a stationary reactor with 1500 MW of power. The reactor, along the vertical coordinate, is divided into three parts: the *lower plenum* (from $z = 0$ to $z = 1.3\,m$) the *core* (from $z = 1.3$ to $z = 3.245\,m$) and the *upper plenum* (from 3.245 to $z = 4.485\,m$). At the top of the core, between $z = 2.25$ and $z = 3.5$ m, the source of thermal power is placed together with the corresponding fuel elements. As shown in Figure 2.34, with regard to the primary loop, both the steam generator (SG) and the pump (pump) are positioned in the "horizontal portion" of the ducts that links the inlet to outlet of the reactor. Let s be curvilinear coordinate of

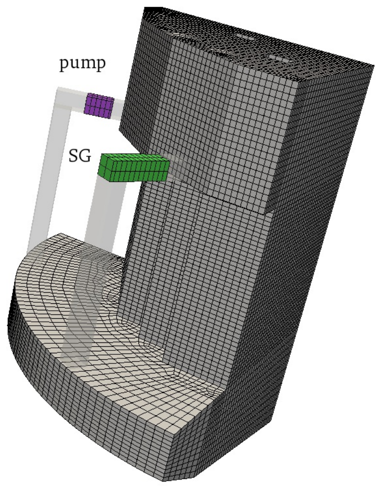


Figure 2.34: LibMesh module. Location of the pump and steam generator in the computational primary loop.

PARAMETER	VALUE
P_{nom}	1482.235 MW
q_l	0.023753 MW/m
m	$\approx$ 124000 Kg/s
T_{in}	673.15 K
T_{out}	$\approx$ 753 K
ΔT	$\approx$ 80 K
w^*_{core}	$\approx$ 1.5 m/s
A_{FA}	0.086436 m^2
$A_{Coolant}$	0.046744 m^2
r	0.5408

Table 2.9: Operating parameters at steady working condition.

the centerline that connects the upper to the lower plenum. We set the pumps in the segment with curvilinear coordinate s = 0.4-0.7 m, and the SG between s = 0.4 and $s = 1$ m.

The pump is placed exactly at the entrance of the steam generator. In Table 2.9 the main operating conditions of the system are summarized. In particular, the overall mass

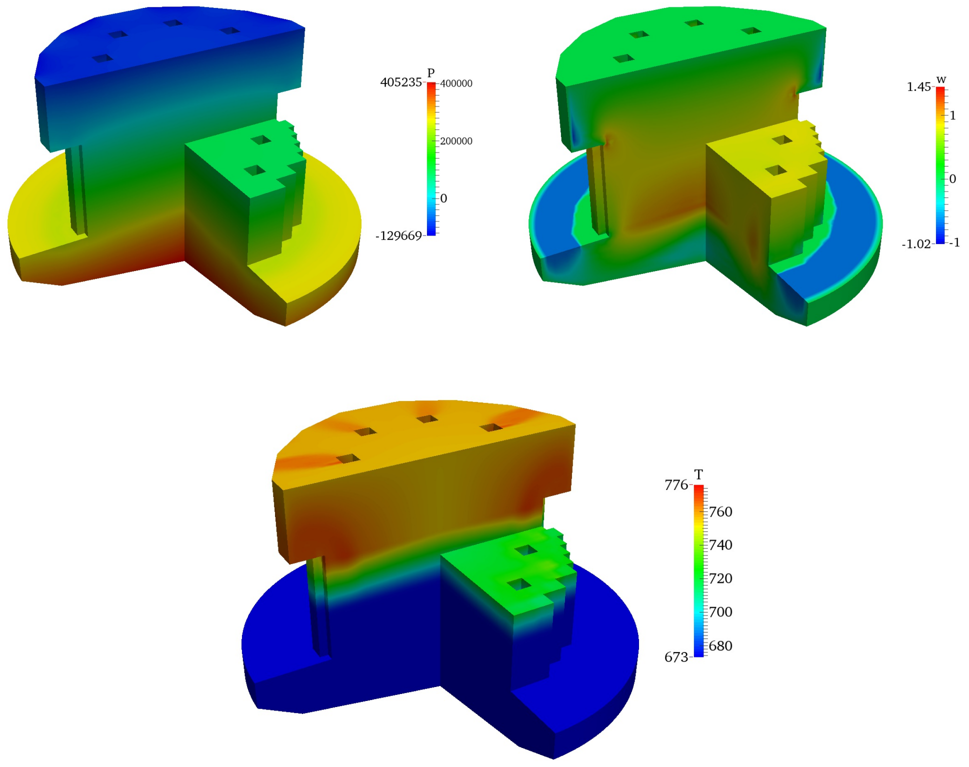


Figure 2.35: FEMLCORE module. Temperature, pressure and velocity field at working conditions.

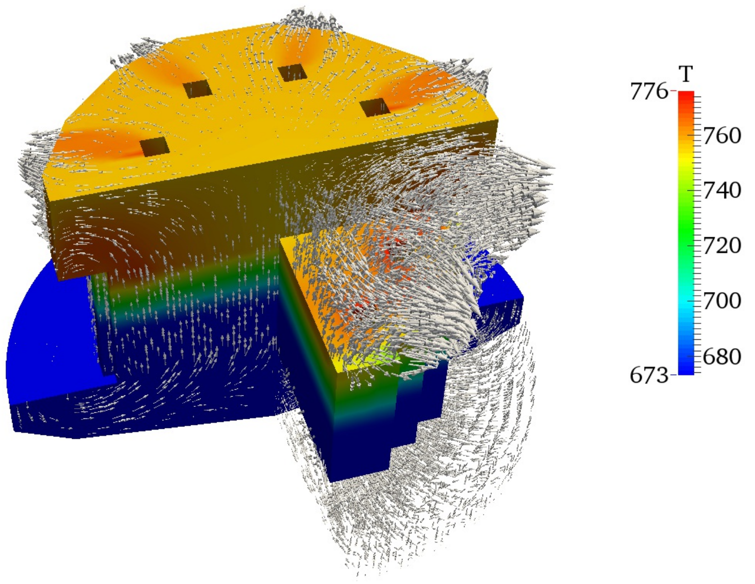
flow is approximately 124,000 kg/s, while the volumetric density of power (average) is

$$q_g = \frac{P_{nom}}{N_a\, A_{FA}\, H_a} = \frac{1482.235}{162 \times 0.294^2 \times 0.9} = 117.6156\, MW/m^3\,, \qquad (2.15)$$

and the linear power density (average)

$$q_l = \frac{P_{nom}}{N_a\, n_r\, H_a} = \frac{1482.235}{162 \times 428 \times 0.9} = 0.023753\, MW/m\,. \qquad (2.16)$$

For the thermal-hydraulic simulation of the core a FEMLCORE porous medium module is used in which geometrical details describing the fuel element sub-channels are neglected. The code solves the time dependent equation for the filtration velocity $\mathbf{v}$. The real velocity $\mathbf{v}^*$ owned by the coolant is given by the ratio between the filtration velocity and the occupancy factor r. The occupancy factor is defined by the ratio between the section actually available for the passage of the fluid and the total section of the *core* and it is assumed to be $r = A_C/A_{FA} = 0.5408$. It is clear that the coolant is subject to



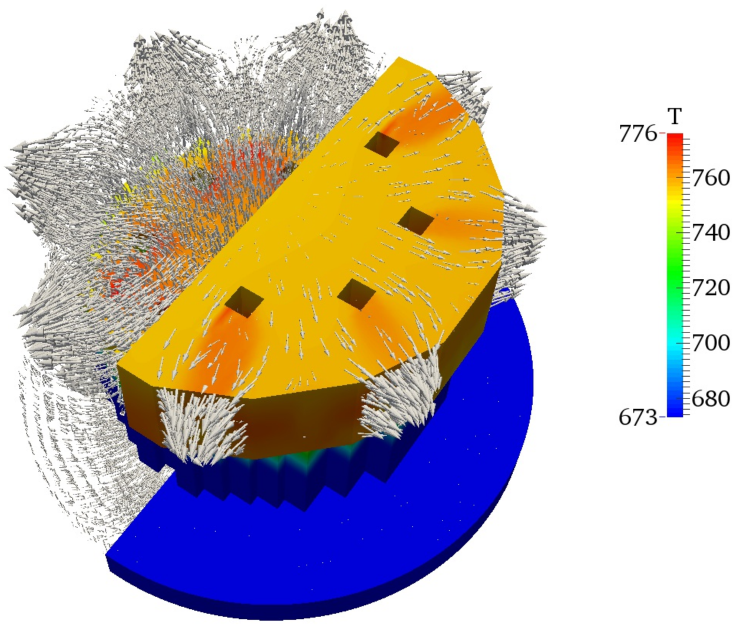


Figure 2.36: FEMLCORE module. Vectorial representation of the velocity and temperature field for the stationary solution at nominal power.

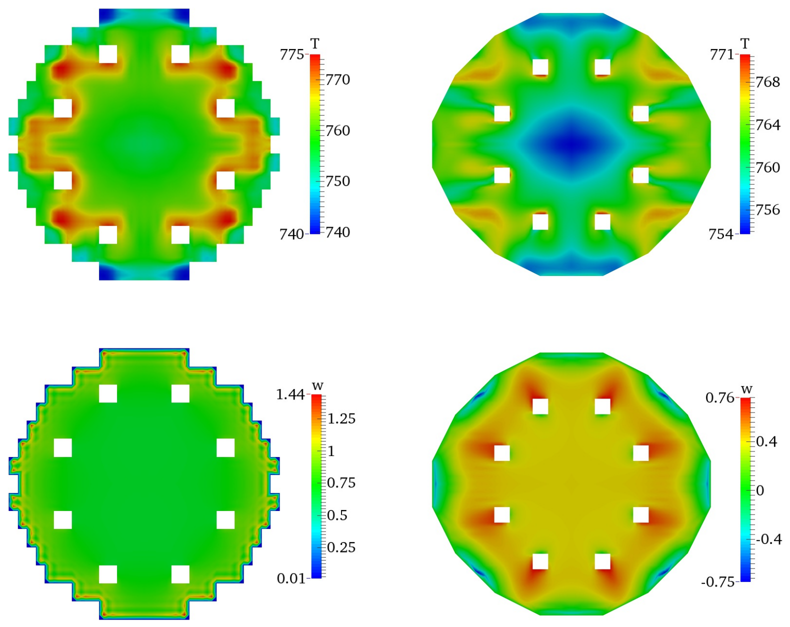


Figure 2.37: FEMLCORE module. Stationary solution of the temperature and velocity fields on sections a and b in the case of operation at nominal power.

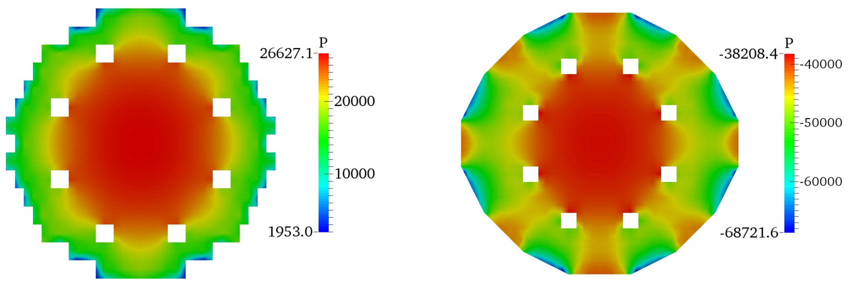


Figure 2.38: FEMLCORE module. Pressure stationary solution over the sections a and b in the case of operation at nominal power.

a sharp acceleration at the core inlet due to the narrowing of the section in the presence of structure mechanical material. Figure 2.35 shows the fields of temperature, vertical velocity w and pressure in steady state conditions.

The fluid enters the low plenum along the normal direction to the input surface at $z = 1.3\ m$ ($\mathbf{v} = w\widehat{k}$) at a rate of about $1\ m/s$ (Figure 2.35 on the right and 2.36) with a

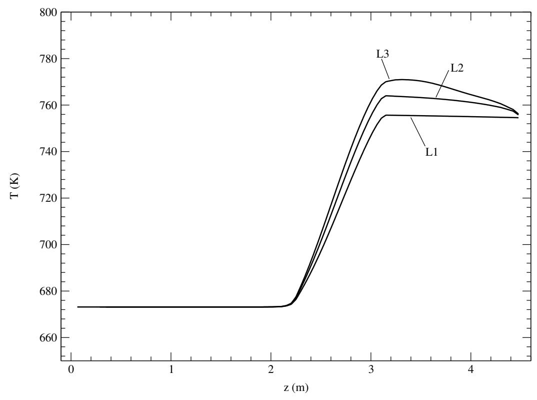


Figure 2.39: FEMLCORE module. Temperature of the coolant along the lines $L1$, $L2$ and $L3$. Steady state solution in case of nominal power.

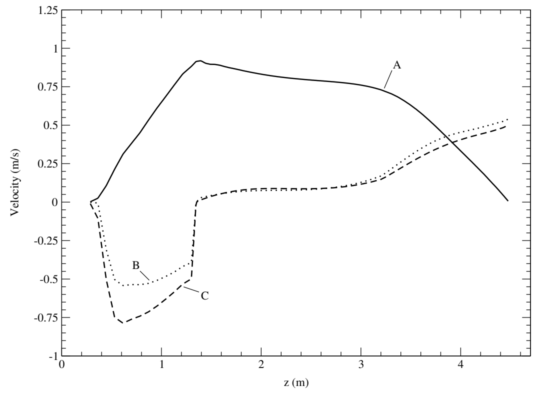


Figure 2.40: FEMLCORE module. Components of the velocity vector along the line L2. Steady state solution when operating at nominal power. A: component w; B: Component u; C: component v.

temperature of 672 K. The thermophysical properties of the refrigerant at the reactor entrance are $rho = 10562.99\ kg/m^3$, $mu = 0.002227\ Pa\,s$, $Kappa = 16.5857\ W/mK$ and $C_P = 147.3\ J/kgK$. The average temperature on the outlet surface of the core, as well as the input of upper plenum, is about 752 K with an increase in temperature of about 80 degrees. However since the generation of power is not uniform some peaks reach around 772 K as shown in Figures 2.35, 2.37 and 2.39. In Figure 2.36 the path of the fluid is shown within the reactor. As it is visible in the Figure, in the core the velocity components u and v vanish.

The maximum pressure, just over 4 bar, is reached at the base of the reactor. This value is mostly due to the hydrostatic load caused by the high density of lead and only minimally to the pressure losses. In Figure 2.37 and 2.38 the fields of temperature,

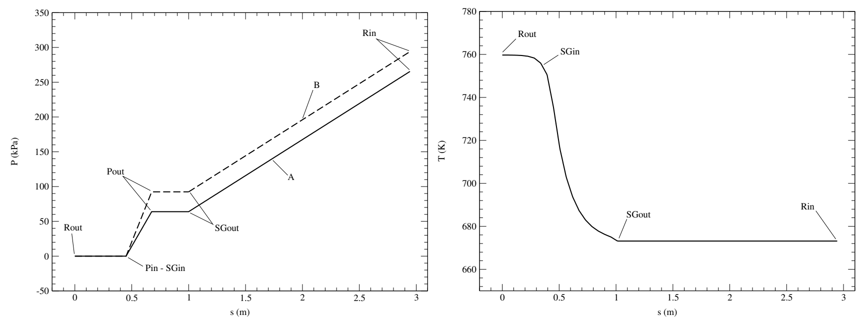


Figure 2.41: LibMesh module. Pressure (top) and temperature (bottom) solution in the primary loop in case of operation at nominal power. Rin, Rout: input and output reactor; SGin, SGout: input and output steam generator; Pin, Pout; input and output pump.

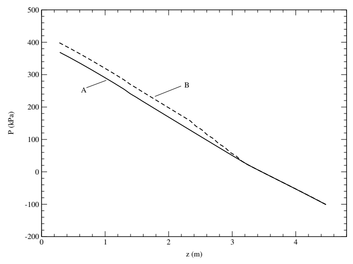


Figure 2.42: FEMLCORE module. Pressure drop along the line $L2$; steady state solution in nominal operating conditions. Line A: pressure drop considering the only losses distributed; Line B: pressure drop considering both the hydraulic losses and those accidental due to the spacer grids.

pressure and vertical velocity w are shown at the core exit b placed at an intermediate position within the upper plenum (see Figure 2.33 for details). In Figure 2.37 we can see the effect on the temperature field of the distribution of the power factor pf on different horizontal planes. In the same Figure one can see the flat profile of the velocity and the formation of recirculation fluid structure near the walls of the upper plenum. In Figure 2.39 the temperature field is shown along the three vertical lines $L1$, $L2$ and $L3$: the latter corresponds to the hot channel on which there is the highest values of power factor and therefore local temperature peaks may occur.

The evolution of the vertical profile of temperature is almost the same along all three segments. At the entrance of the active part of the core at $z = 2.25\ m$ the temperature begins to rise up to its maximum value at the output of the core at $z \approx 3.25\, m$. Within the plenum, due to the strong mixing regime, the temperature along the hot channel ($L3$) tends to decrease reaching, as the other profiles, a value of approximately 756 K. In Figure 2.40 the profile of the three components of velocity along the line $L2$ are shown. As already mentioned earlier, within the core the velocity components u and v (lines B and C) vanish, while the vertical component w reaches a mean value of about 0.8 m/s ($w^* \approx 1.48\,m/s$).

Two different simulations are carried out: the first considering only the hydraulic losses due to viscous friction; the second considering the pressure losses due to the presence of spacer grids too.

In Figure 2.42 the pressure drop along the line $L2$ is shown for both cases: distributed losses only (A), accidental and distributed losses (B). The presence of the spacer grids is clearly visible where the pressure profile is not linear between $z = 2.25$ and $z = 3.245$. From Figure 2.41, in which the steady state solution is shown for the temperature and pressure fields in the primary loop, it is easy to see the total value of all the pressure drops (distributed and concentrated), which equals the pressure contribution supplied by the pump (Figure 2.41 (a)). This total value is equal to about 95 kPa ($\approx 1\,bar$) while the contribution of only the distributed load losses is about 60 kPa.

The domain does not have axial symmetry. This implies that the ranges for the pressure P, velocity $\mathbf{v}$ and temperature T assume different values on the two outlets. For this reason, to study in detail the 3D effects on various physical phenomena, it would be necessary to consider two different primary loops and then solve two libMesh problems.

Conclusions

In this report we have described the integration of the FEMLCORE code in the SALOME platform. Because of the unavailability of a system code on SALOME platform for the first evaluation of FEMLCORE integration, we have decided to use the libMesh library to simulate a mono-dimensional loop to be integrated with FEMLCORE results. An interface for coupling libMesh-SALOME was originally developed by CEA and EDF over the open-source libMesh library. Starting from this work we have further developed the libMesh-SALOME interface and on this model we have build a FEMLCORE integration interface. This allows us to drive three-dimensional modules of FEMLCORE with boundary conditions from any system code present on SALOME platform.

Coupling examples with CFD and porous modules have been presented and evaluated. We have reported 3D-CFD/3D-CFD coupling for energy and Navier Stokes equations tests with codes based both on libMesh and FEMus libraries. Multiscale coupling has been also investigated in two FEMLCORE tests. First the data transfer interface has been used to transfer heat generation and pressure drop analytical distributions inside the FEMLCORE core module. Finally a 3D-porous/1D-porous coupling FEMLCORE-libMesh has been tested. In this integrated version the FEMLCORE code on the SALOME platform can be considered a stand-alone code with a CAD, a mesh generator and a visualization software. At the same time FEMLCORE code can be coupled with system codes that have a SALOME interface.

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