Agenzia Nazionale per le Nuove Tecnologie,
l'Energia e lo Sviluppo Economico Sostenibile

Ministero dello Sviluppo Economico

RICERCA DI SISTEMA ELETTRICO

Documento CERSE-UNIBO RL 1302/2010

FISSICU platform on CRESCO-ENEA grid for thermal-hydraulic nuclear engineering

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Report RdS/2010/138

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Settembre 2010

Report Ricerca di Sistema Elettrico
Accordo di Programma Ministero dello Sviluppo Economico – ENEA
Area: Produzione e fonti energetiche
Tema: Nuovo Nucleare da Fissione

Responsabile Tema: Stefano Monti, ENEA

CIRTEN

CONSORZIO INTERUNIVERSITARIO

PER LA RICERCA TECNOLOGICA NUCLEARE

ALMA MATER STUDIORUM - UNIVERSITÀ DI BOLOGNA

DIPARTIMENTO DI INGEGNERIA ENERGETICA, NUCLEARE E DEL CONTROLLO AMBIENTALE - LABORATORIO DI MONTECUCCOLINO

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Bologna, Settembre 2010

Lavoro svolto in esecuzione della linea progettuale LP5 punto B2 - AdP ENEA MSE del 21/06/07
Tema 5.2.5.8 – “Nuovo Nucleare da Fissione”.

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September 1 2010

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Abstract. The FISSICU (FISsione/SICUrezza) platform for CFD thermal-hydraulics is set on the CRESCO-ENEA GRID cluster located in Portici. The platform contains codes for microscale, intermediate and system scale simulations for components of nuclear plants and facilities. For direct three-dimensional numerical simulations the platform contains codes such as TRIO_U and SATURNE. At intermediate scale the platform implements codes such as NEPTUNE and for system level CATHARE will be available soon. The platform contains the SALOME application for code coupling and a large number of mesh generators and visualization tools. All the codes run starting from mesh input files with common formats. GMESH and SALOME MESH are open-source reference mesh generators that can be found in the platform together with conversion tools. The output is written in common format and can be visualized through the PARAVIEW application. A brief guide through the platform codes and tools with reference mesh and output formats is presented.

Contents

Introduction

CRESCO-ENEA GRID FISSICU PLATFORM								
		local		GRID				
	INSTALL	GUI	MPI	GUI	MPI	DNS	CFD	system
SALOME	yes	yes	yes	yes	no			
SATURNE	yes	yes	yes	no	no	x	x	
TRIO_U	yes	yes	yes	yes	no	x	x	
NEPTUNE	yes	yes	yes	no	no		x	
CATHARE	no	no	no	no	no			x
PARAVIEW	yes	yes	yes	yes	yes			

Table 1: Implementation status on CRESCO-ENEA GRID FISSICU platform

This document reports the status of the FISSICU (FISsione/SICUrezza) software platform for the study of the thermal-hydraulic behavior of nuclear reactors. The idea reflects the new European policy to develop a common European tools which has lead to fund the NURISP platform project. ENEA is a user group member of the project and under a direct agreement has obtained the use of several codes. The University of Bologna participates in the effort to use and install these computational tools and other in-house developed codes on the CRESCO-ENEA GRID cluster located in Portici (near Naples). The FISSICU platform has been constructed not only to collect a series of codes that has been extensively used in this field but also to harmonize them with reference input and output formats. The aim of the platform is to solve complex problems using file exchange between different codes and large multiprocessor architecture. In this way one hopes to investigate multi-physics and multi-scale problems arising in the study of nuclear reactor components. Reference mesh and output formats are considered and conversion tools are developed. The data visualization is performed with a unique application.

In Chapter 1 we give an overview of the organization of the platform. The purpose of solving multi-physics and multilevel problems is discussed together with the CRESCO-ENEA GRID. The reference mesh and output formats are introduced and the visualization open-source application PARAVIEW is described.

In Chapter 2 the SALOME platform is introduced along with its implementation on CRESCO-ENEA GRID. A brief explanation of the main modules KERNEL, GUI and MESH is given. The SALOME mesh generator and the file transfer service are discussed. The mesh generator is open-source but the main mesh format is the MED format which is not very popular so that conversion tools are necessary. A tutorial of the MESH module is presented.

Chapter 3 is a brief introduction to the SATURNE code. SATURNE code is an open-source code implemented on CRESCO-ENEA GRID for use in three-dimensional direct numerical simulations. The graphical user interface is introduced together with dataset and mesh generation. An example is illustrated step by step.

Chapter 4 is devoted to the presentation of TRIO_U and its implementation over the CRESCO-ENEA GRID. The generation of mesh and data format files is discussed together with a brief tutorial for the 2D cylindrical obstacle test. The code TRIO_U has capabilities at microscale and intermediate scale.

Finally in Chapter 5 NEPTUNE is described with its implementation over the CRESCO-ENEA GRID. NEPTUNE is a code that can be used in two-phase flow simulations at the intermediate scale.

Chapter 1

FISSICU platform organization

1.1 Multiphysics and Multilevel platform

1.1.1 Multiphysics analysis

The aim of the platform is to analyze complex nuclear systems that require the coupling of different equations for different components. At present nuclear reactor thermal-hydraulics consists of different physical models (heat transfer, two-phase flow, chemical poisoning) that cannot be analyzed all at the same time. Improvements are necessary both for the physical models (heat transfer coefficient at the interface between liquid and vapor, instabilities of the interface, diffusion coefficients) and mostly for the numerical schemes (accuracy, CPU time). In the absence of direct numerical simulations the improvement of CFD codes that rely on correlations must be based on experiments that offer sufficient resolution in space and time compared to the CFD computations. In many cases physical models lack of satisfactory experimental results and therefore numerical calculations cannot be accurate. In Figure 1.1 we show an example of the multi-physics approach where the physics of a nuclear core is coupled with the thermal-hydraulics of the steam generator and the pressurizer. In the upper plenum we can use a model that solves the Navier-Stokes equations while for the external loop we adopt a correlation approach. The two approaches require the use of different codes and the coupling at the interface between the two domains.

Even when experimental correlations are available for a single equation the complexity of the problems does not allow a whole-system simulation and even a greater computational power would be necessary to take into account the couplings. However, each physical model requires a number of parameters that are determined by the other state variables and the coupling between the equations is necessary to achieve an accurate and satisfactory result. For all these reasons it is important to develop tools that can manage different codes specific for a single application and perform easily a weak coupling. At the platform level there are three different types of coupling: weak, internal weak and strong coupling. In the first case the weak coupling is performed with the exchange of input and output files. In this case the file format must be compatible between

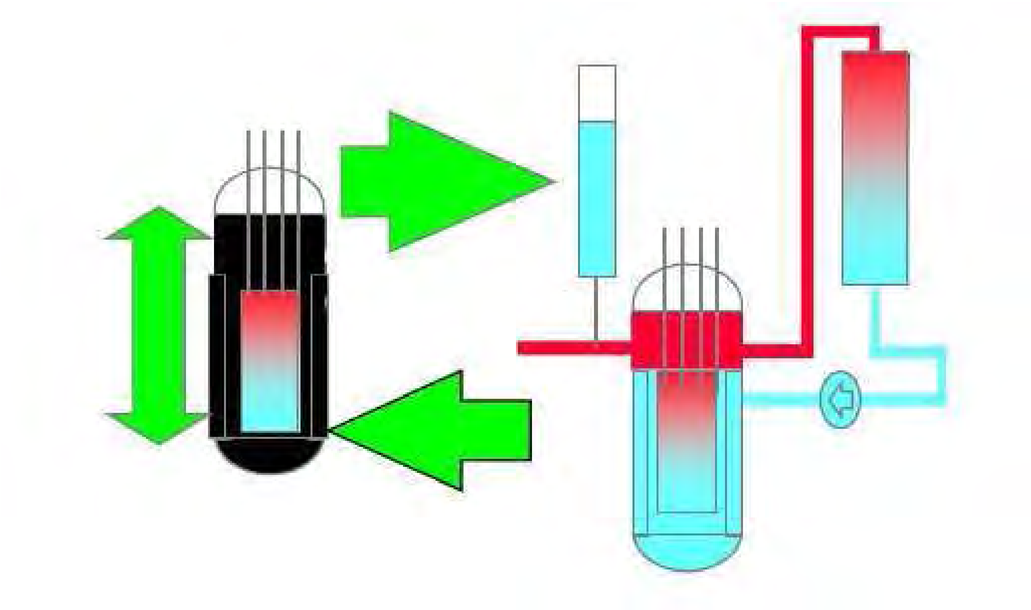


Figure 1.1: An example of multi-physics approach for nuclear reactor (NURISP) where different equation models can be coupled to analyze a complex system.

the applications or external conversion tools are required. In the internal weak coupling all the equations are solved in a segregated way using memory to exchange data between codes. A popular format for this purpose is the MED format. The strong coupling requires a larger computational power but can solve all the equations at the same time giving a more accurate result.

The platform should perform these tasks automatically together with runtime scheduling of the programs. Another important feature of the platform is the ability to manipulate and create input and output files with compatible formats. The SALOME software platform has been selected for these purposes and implemented on the ENEA-GRID cluster along with a selection of codes devoted to nuclear reactor thermal-hydraulics and safety analysis. Some key features of the SALOME platform are the following:

- interoperability between CAD modeling (input files) and computational software;
- integration of new components into heterogeneous systems;
- multi-physics weak coupling between computation software;
- a generic user friendly and efficient user interface;
- access to all functionalities via the integrated Python console.

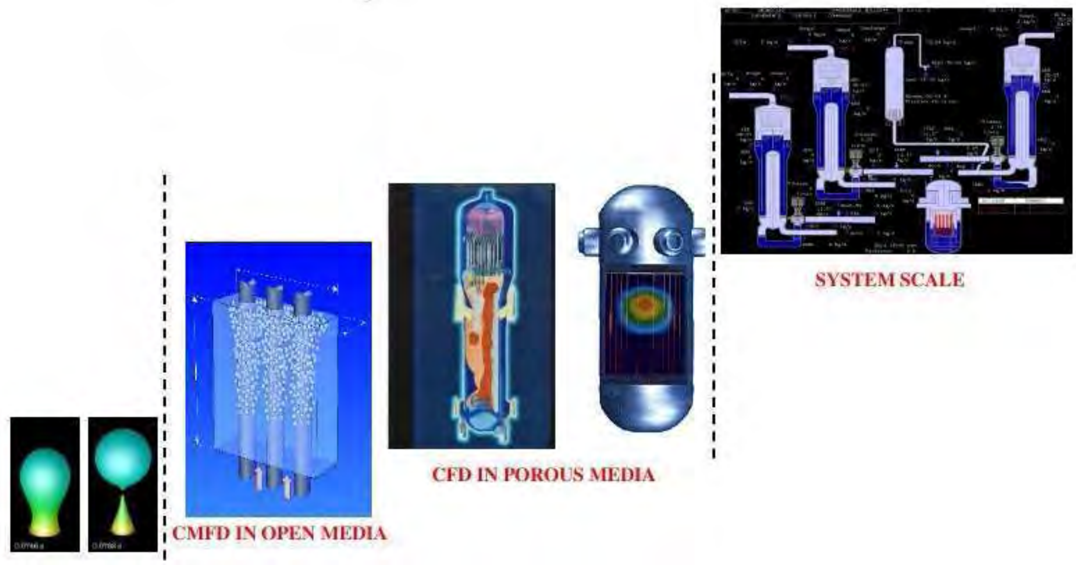


Figure 1.2: An example of multilevel approach for a nuclear reactor (NURISP).

1.1.2 Multilevel analysis

Another aspect of the complexity of nuclear reactor simulations is the different geometrical scales. As shown in Figure 1.2 we need to investigate problems with characteristic dimensions ranging from millimeters (bubbles) to several meters (nuclear plant loop). It is not possible to solve such a complex problem in a single simulation. Therefore we model different scales with different equations that take into account the relevant physics for the selected geometry. We can roughly subdivide the phenomena into three main groups.

- Micro-scale, where direct numerical simulations (DNS) are required. Usually the Navier-Stokes system and energy equation are directly implemented without approximations. The results obtained are very accurate but can only take into account small parts of the system and a limited number of processes.

- Meso-scale, where the Navier-Stokes equations can no longer be used directly. The introduction of correlations and modelings is required in order to analyze systems where thousands of microscale phenomena occur.

- Macro-scale, where the system is analyzed in its overall complexity. In this case heavy approximations must be assumed in order to simulate the whole system in a reasonable amount of time.

The phenomena in the DNS group can be simulated with commercial and open-source codes. For example ANSYS-FLUENT, CFX and Comsol multiphysics are viable commercial codes, while OPENFOAM and SATURNE are examples of open source software. A

DNS code focused on nuclear applications is TRIO_U, released only under closed agreement with CEA, that allows to perform simulations in three-dimensional domains. The high resolution and reliability of these codes lead to high accuracy and reproducibility of the results.

The meso-scale codes rely on correlations and averaged equations. Typical examples are turbulence models and two-phase thermal exchange. Turbulence models are widely available even for DNS codes while other correlations are specific of the applications. A nuclear engineering code of this type is NEPTUNE which is released only under closed agreement with EDF.

The system codes are very specific to the application field. In order to simulate all the system they need heavy simplifications such as the use of a mono-dimensional fluid equation. In the nuclear field we recall CATHARE (released by CEA) and the series of RELAP codes.

The CRESCO-ENEA FISSICU platform implements the following software:

- DNS: TRIO_U, SATURNE, FLUENT (already available from CRESCO), OPENFOAM (already available from CRESCO)
- Meso-scale: NEPTUNE, ELSY-CFD
- system level: CATHARE (coming soon)

along with SALOME which performs the input/output managing and code coupling.

1.2 CRESCO-ENEA GRID

1.2.1 CRESCO infrastructure

CRESCO (Centro Computazionale di RicErca sui Sistemi Complessi, Computational Research Center for Complex Systems) is an ENEA Project, co-funded by the Italian Ministry of Education, University and Research (MIUR). The CRESCO project is located in the Portici ENEA Center near Naples and consists of a High Performance Computing infrastructure mainly devoted to the study of Complex Systems [1]. The CRESCO project is built around the HPC platform through the creation of a number of scientific thematic laboratories:
a) the Computing Science Laboratory, hosting activities on hardware and software design, GRID technology, which will also integrate the HPC platform management;
b) the Computational Systems Biology Laboratory, hosting the activities in the Life Science domain;
c) the Complex Networks Systems Laboratory, hosting activities on complex technological infrastructures.

1.2.2 CRESCO access

There are four ways to access ENEA-GRID:
a) SSH client, with a terminal interface which can directly access to one of the front-end

Cluster name	Node Name	ACCESS SSH from enea domains	ACCESS SSH from world	OS
Bologna	graphlab03.bologna.enea.it	yes	no	IRIX
	pace.bologna.enea.it	yes	yes	AIX
Brindisi	campus03.brindisi.enea.it	yes	no	LINUX
	ercules.brindisi.enea.it	yes	yes	AIX
	graphbri.brindisi.enea.it	yes	no	IRIX
Casaccia	feronix0.casaccia.enea.it	yes	no	LINUX
	laran.casaccia.enea.it	yes	yes	LINUX
	prometeo.casaccia.enea.it	yes	yes	LINUX
	turan.casaccia.enea.it	yes	yes	LINUX
Frascati	bw305-1.frascati.enea.it	yes	no	LINUX
	eurofel00.frascati.enea.it	yes	no	LINUX
	lin4p.frascati.enea.it	yes	yes	LINUX
	onyx2ced.frascati.enea.it	yes	no	IRIX
	sp5-1.frascati.enea.it	yes	no	AIX
Portici	campus3.portici.enea.it	yes	no	LINUX
	graphpor.portici.enea.it	yes	no	IRIX
Portici CRESCO	cresco1-f1.portici.enea.it	yes	yes	LINUX
	cresco1-f2.portici.enea.it	yes	no	LINUX
	cresco1-f3.portici.enea.it	yes	no	LINUX
	cresco2-f1.portici.enea.it	yes	no	LINUX
	cresco2-f2.portici.enea.it	yes	no	LINUX
	cresco2-f3.portici.enea.it	yes	no	LINUX
	cresco1-fg1.portici.enea.it	yes	no	LINUX
	cresco1-fg2.portici.enea.it	yes	no	LINUX
	cresco1-fg3.portici.enea.it	yes	no	LINUX
	cresco1-fg4.portici.enea.it	yes	no	LINUX
	cresco-fpga6.portici.enea.it	yes	no	LINUX
Trisaia	campus03.trisaia.enea.it	yes	no	LINUX
	cluapple.trisaia.enea.it	not yet	not yet	MacOSX
	graphtri.trisaia.enea.it	yes	no	IRIX
	triafs.trisaia.enea.it	yes	yes	Solaris

Table 1.1: CRESCO front-end machines.

machines;
b) Citrix client, that can be installed on windows machines to access ENEA servers, including a terminal window to ENEA-GRID (INFOGRID);
c) FARO (Fast Access to Remote Objects) ENEA-GRID, that is a Java web interface available for all operating systems;
d) NX client.

The access is limited to authorized users that are provided with ENEA-GRID username and password to be used on every machine of the grid. Table 1.1 shows a list of available nodes. There are a number of front-end nodes to access the platform from the external world. The main ones are:
a) `sp5-1.frascati.enea.it`
b) `lin4p.frascati.enea.it`
c) `cresco1-f1.portici.enea.it`

In this report we consider the access to a front-end node with a ssh client from a linux terminal

```
$ ssh -X username@cresco1-f1.portici.enea.it
```

If one uses the web interface FARO (http://www.cresco.enea.it/nx.html), from any operating system, an `xterm` can be launched with a dedicated button. Further details on the login procedure can be found on the CRESCO website (http://www.cresco.enea.it/helpdesk.php).

1.2.3 CRESCO-ENEA FISSICU Platform

The FISSICU project is located in the directory

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

Inside the main directory `fissicu` (which stands as an abbreviation for nuclear fission safety), we find the three sub-directories

- `data`, where the simulation results should be stored;
- `html`, where the web pages are located (http://www.afs.enea.it/project/fissicu/);
- `soft`, where all the codes are installed.

At present, the following codes are available:

- SALOME (see Chapter 2, executable: `salome`);
- SATURNE (see Chapter 3, executable: `saturne`);
- NEPTUNE (see Chapter 5, executable: `neptune`);

- TRIO_U (see Chapter 4, executable: `triou`);
- FEM-UNIBO (the finite element Navier-Stokes solver developed at DIENCA - University of Bologna).

For each code, a script (`executable_env`) is also available which simply sets the proper environment variables to execute the code. This procedure can be used to run the code directly without any graphical interface on a single node where the user is logged. This is also the first step for production runs which use the batch queue to run the code in parallel.

Any executable is a script in the directory `/afs/enea.it/project/fissicu/soft/bin`. This directory should be added to the user environment variable `PATH`. With the `bash` shell, the command line is

```
$ export PATH=/afs/enea.it/project/fissicu/soft/bin:$PATH
```

This command line can also be added to the configuration file `.bashrc`.

1.2.4 Submission to CRESCO queues

CRESCO supports the LSF (Load Sharing Facility) job scheduler, which is a suite of several components to manage a large cluster of computers with different architectures and operating systems. The basic commands are

```
$ lshosts
```

It displays configuration information about the available hosts, as in the following output example

```
HOST_NAME type     model   cpuf ncpus maxmem maxswp server  RESOURCES
hostD     SUNSOL  SunSparc 6.0    1    64M    112M    Yes (solaris cserver)
hostB     ALPHA   DEC3000 10.0    1    94M    168M    Yes (alpha cserver)
hostM     RS6K    IBM350   7.0    1    64M    124M    Yes (cserver aix)
hostC     SGI6    R10K    14.0   16 1024M    1896M    Yes (irix cserver)
hostA     HPPA    HP715    6.0    1    98M    200M    Yes (hpux fserver)
```

```
$ lsload
```

It displays the current load information

```
HOST_NAME   status  r15s  r1m r15m  ut    pg   ls  it   tmp  swp  mem
hostD           ok   0.1  0.0  0.1   2%   0.0   5   3   81M  82M  45M
hostC           ok   0.7  1.2  0.5  50%   1.1  11   0  322M 337M 252M
hostM           ok   0.8  2.2  1.4  60%  15.4   0 136   62M  57M  45M
hostA         busy  *5.2  3.6  2.6  99% *34.4   4   0   70M  34M  18M
hostB        lockU   1.0  1.0  1.5  99%   0.8   5  33   12M  24M  23M
```

```
$ bhosts
```

It displays information about the hosts such as their status, the number of running jobs, etc.

```
HOST_NAME      STATUS    JL/U  MAX   NJOBS  RUN  SSUSP USUSP  RSV
hostA            ok       -     2      1     1     0     0     0
hostB            ok       -     3      2     1     0     0     1
hostC            ok       -     32    10     9     0     1     0
hostD            ok       -     32    10     9     0     1     0
hostM          unavail    -     3      3     1     1     1     0
```

```
$ bqueues
```

It lists the available LSF batch queues and their scheduling and control status

```
QUEUE_NAME PRIO NICE    STATUS     MAX  JL/U JL/P NJOBS  PEND  RUN  SUSP
owners       49   10  Open:Active    -    -    -     1     0     1     0
priority     43   10  Open:Active   10    -    -     8     5     3     0
night        40   10 Open:Inactive   -    -    -    44    44     0     0
short        35   20  Open:Active   20    -    2     4     0     4     0
license      33   10  Open:Active   40    -    -     1     1     0     0
normal       30   20  Open:Active    -    2    -     0     0     0     0
idle         20   20  Open:Active    -    2    1     2     0     0     2
```

```
$ bsub < job.lsf
```

It submits a job to a queue. The script `job.lsf` contains job submission options as well as command lines to be executed. A typical script is

```
#!/bin/bash
#BSUB -J JOBNAME
#BSUB -q quename
#BSUB -n nproc
#BSUB -oo stdout_file
#BSUB -eo errout_file
#BSUB -i input_file
triou_env
Trio_U datafile.data
```

where the options to `BSUB` specify respectively the name of the job, the name of the queue, the number of processors, the file names for the standard and error output, the input file. The last two lines set the environment variables for the code TrioU and launch the executable with a parameter file, without the graphical interface that clearly cannot be used when submitting a job with a batch queue.

```
$ bjobs
```

It reports the status of LSF batch jobs of the user.

```
JOBID USER  STAT  QUEUE     FROM_HOST EXEC_HOST JOB_NAME  SUBMIT_TIME
3926  user1 RUN   priority  hostF     hostC     verilog   Oct 22 13:51
605   user1 SSUSP idle      hostQ     hostC     Test4     Oct 17 18:07
1480  user1 PEND  priority  hostD               generator Oct 19 18:13
7678  user1 PEND  priority  hostD               verilog   Oct 28 13:08
7679  user1 PEND  priority  hostA               coreHunter Oct 28 13:12
7680  user1 PEND  priority  hostB               myjob     Oct 28 13:17
```

```
$ bkill  JOBID
```

It kills the job with number `JOBID`. This number can be retrieved with the command `bjobs`.

1.3 FISSICU platform input/output formats

Each software supports a large number of input and output formats that are not always fully compatible. The aim of the platform is to uniform all the codes to use the same format for input, in particular for the mesh, and for output files. Regarding the input format we select the MED and the XDMF formats. They rely on the HDF5 library that is responsible for the data storage in vector and matrix form. The MED and XDMF are driver files that access to the information stored by the HDF5 files. Regarding the output viewer we choose PARAVIEW because it is open source and can manage a large number of output formats.

1.3.1 Input mesh format

HDF5 format

Hierarchical Data Format, commonly abbreviated HDF5, is the name of a set of file formats and libraries designed to store and organize large amounts of numerical data [9].

The HDF format is available under a BSD license for general use and is supported by many commercial and non-commercial software platforms, including Java, Matlab, IDL, and Python. The freely available HDF distribution consists of the library, command-line utilities, test source, Java interface, and the Java-based HDF Viewer (HDFView). Further details are available at http://www.hdfgroup.org. This format supports a variety of datatypes, and is designed to give flexibility and efficiency to the input/output operations in the case of large data. HDF5 is portable from one operating system to another and allows forward compatibility. In fact old versions of HDF5 are compatible with newer versions.

The great advantage of the HDF format is that it is self-describing, allowing an application to interpret the structure and contents of a file without any outside information. There are structures designed to hold vector and matrix data. One HDF file can hold a mixture of related structures which can be accessed as a group or as individual objects.

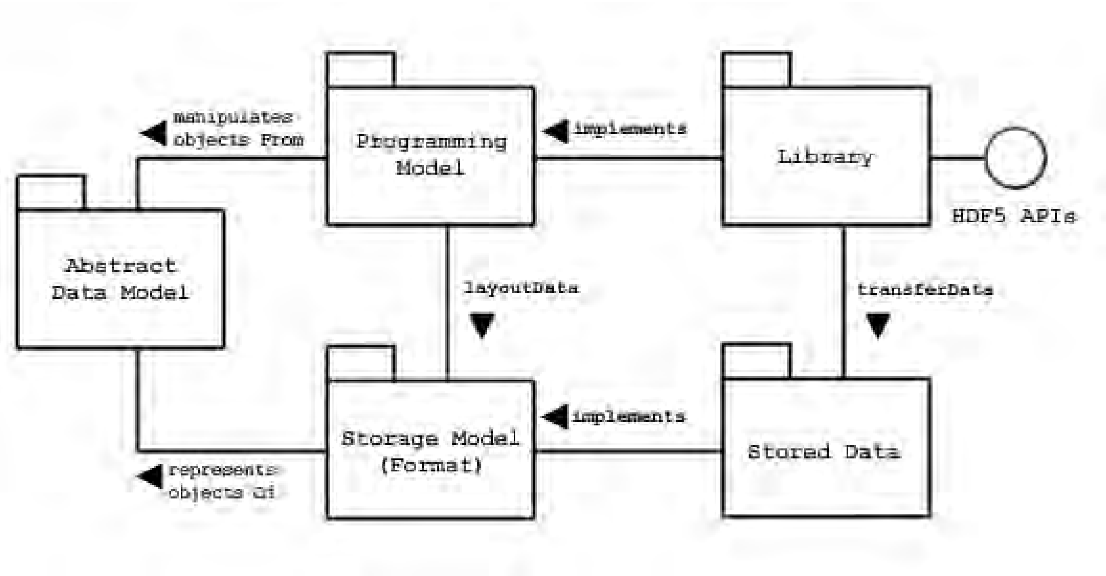


Figure 1.3: HDF5 storage model.

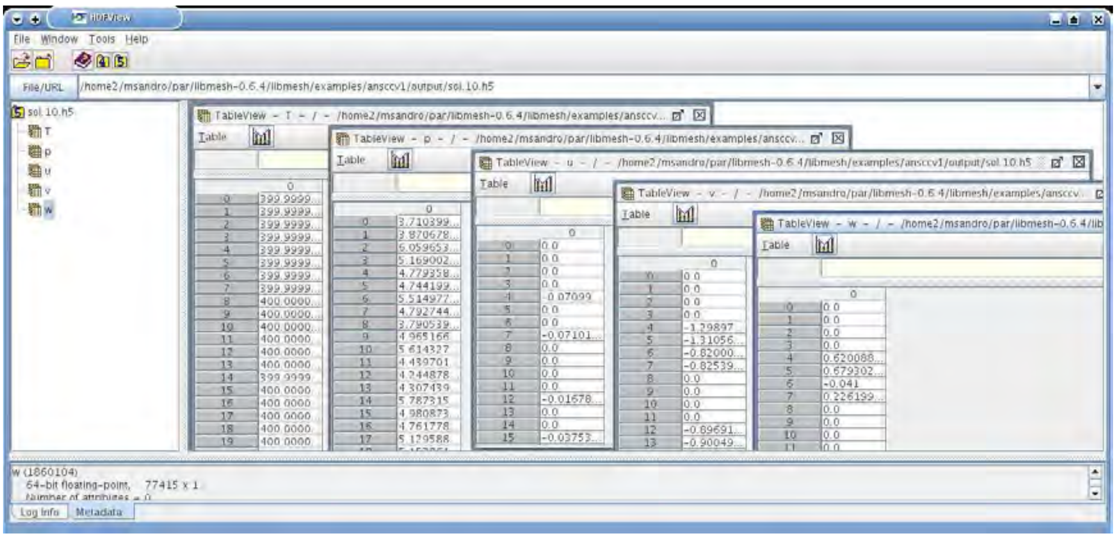


Figure 1.4: HDFVIEW opens HDF5 files.

The HDF5 has a very general model which is designed to conceptually cover many specific data models. Many different kinds of data can be mapped to HDF5 objects, and therefore stored and retrieved using HDF5. The key structures are:

- File, a contiguous string of bytes in a computer store (memory, disk, etc.).
- Group, a collection of objects.

- Dataset, a multidimensional array of Data Elements, with Attributes and other metadata.
- Datatype, a description of a specific class of data element, including its storage layout as a pattern of bits.
- Dataspace, a description of the dimensions of a multidimensional array.
- Attribute, a named data value associated with a group, dataset, or named datatype
- Property list, a collection of parameters controlling options in the library.

The HDF5 project provides also a visualization tool, HDFVIEW, to access raw HDF5 data. This program can be run from terminal with

```
$ hdfview
```

and a screenshot is given in Figure 1.4. The panel on the left shows the list of available datasets while on the right we can see the content of each of them.

XDMF format

XDMF (eXtensible Data Model and Format) is a library providing a standard way to access data produced by HPC codes. The information is subdivided into Light data, that are embedded directly in the XDMF file, and Heavy data that are stored in an external file. Light data are stored using XML, Heavy data are typically stored using HDF5. A Python interface exists for manipulating both Light and Heavy data. ParaView, VisIt and EnSight visualization tools are able to read XDMF [8].

A brief example of a typical XDMF driver file is

```
<?xml version="1.0" ?>
<!DOCTYPE Xdmf SYSTEM "../config/Xdmf.dtd" [<!ENTITY HeavyData ""> ]>
<Xdmf>
  <Domain>
   <Grid Name="Mesh">
     <Time Value ="0.1" />
      <Topology Type="Hexahedron" Dimensions="71400">
        <DataStructure DataType="Int" Dimensions="71400 8" Format="HDF">
meshxmf.h5:/MSHOCONN
        </DataStructure>
       </Topology>
      <Geometry Type="X_Y_Z">
        <DataStructure DataType="Float" Precision="8" Dimensions="77415 1"
         Format="HDF">
../data_in/mesh.h5:/COORD/X1
        </DataStructure>
        <DataStructure DataType="Float" Precision="8" Dimensions="77415 1"
```

```
          Format="HDF">
../data_in/mesh.h5:/COORD/X2
         </DataStructure>
         <DataStructure DataType="Float" Precision="8" Dimensions="77415 1"
          Format="HDF">
../data_in/mesh.h5:/COORD/X3
         </DataStructure>
       </Geometry>
       <Attribute Name="T" AttributeType="Scalar" Center="Node">
         <DataItem  DataType="Float" Precision="8" Dimensions="77415  1"
          Format="HDF">
sol.10.h5:T
         </DataItem>
       </Attribute>
     </Grid>
   </Domain>
</Xdmf>
```

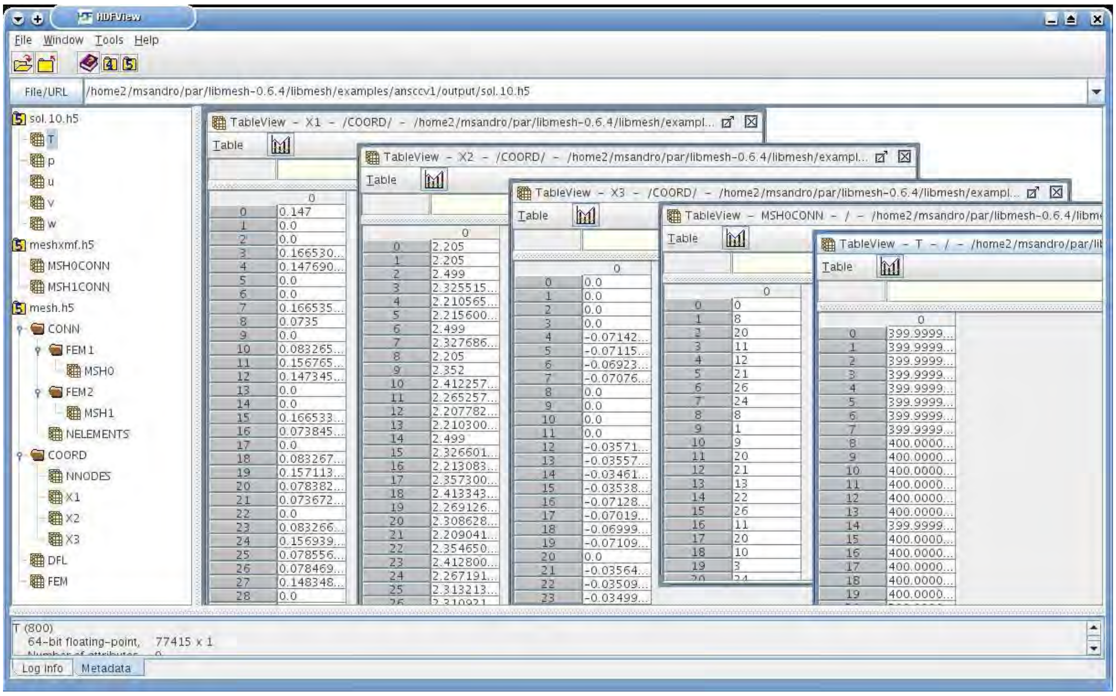


Figure 1.5: XDMF format stores heavy data in HDF5 files.

In this example all data are stored in external files (`meshxmf.h5`, `mesh.h5` and `sol.10.h5`), as shown in Figure 1.5. The data structures used in this example are `Domain`, `Grid`, `Topology`, `Geometry` and `Attribute`.

The organization of XDMF begins with the `Xdmf` element. Any element can have a `Name` or a `Reference` attribute. A `Domain` can have one or more `Grid` elements. Each `Grid` must contain a `Topology`, a `Geometry`, and zero or more `Attribute` elements. `Topology` specifies the connectivity of the grid while `Geometry` specifies the location of the grid nodes. `Attribute` elements are used to specify values such as scalars and vectors that are located at the node, edge, face, cell center, or grid center. A brief description of the keywords follows. **DataItem.** All the data for connectivity, geometry and attributes are stored in `DataItem` elements. A `DataItem` provides the actual values (for Light data) or the physical storage position (for Heavy data). There are six different types of `DataItem` :
- `Uniform`, that is a single array of values (default).
- `Collection`, that is a one dimensional array of DataItems.
- `Tree`, that is a hierarchical structure of DataItems.
- `HyperSlab`, that contains two data items. The first one selects which data must be selected from the second DataItem;
- `Coordinates`, that contains two DataItems. The first contains the topology of the second DataItem.
- `Function`, that is used to calculate an expression that combines different DataItems.

Grid. The data model portion of XDMF begins with the `Grid` element. A `Grid` is a container for information related to 2D and 3D points, structured or unstructured connectivity, and assigned values. The `Grid` element has a `GridType` attribute that can assume the values:
- `Uniform` (a homogeneous single grid (i.e. a pile of triangles));
- `Collection` (an array of Uniform grids all with the same Attributes);
- `Tree` (a hierarchical group);
- `SubSet` (a portion of another Grid).

Geometry. The `Geometry` element describes the XYZ coordinates of the mesh. Possible organizations are:
- `XYZ` (interlaced locations, an X,Y, and Z for each point);
- `XY` (Z is set to 0.0);
- `X_Y_Z` (X,Y, and Z are separate arrays);
- `VXVYVZ` (Three arrays, one for each axis);
- `ORIGIN_DXDYDZ` (Six values : Ox,Oy,Oz + Dx,Dy,Dz).

The default `Geometry` configurations is `XYZ`.

Topology. The `Topology` element describes the general organization of the data. This is the part of the computational grid that is invariant under rotation, translation, and scaling. For structured grids, the connectivity is implicit. For unstructured grids, if the connectivity differs from the standard, an `Order` may be specified. Currently, the following `Topology` cell types are defined: `Polyvertex` (a group of unconnected points), `Polyline` (a group of line segments), `Polygon`, `Triangle`, `Quadrilateral`, `Tetrahedron`, `Pyramid`, `Wedge`, `Hexahedron`, `Edge_3` (Quadratic line with 3 nodes), `Tri_6`, `Quad_8`, `Tet_10`, `Pyramid_13`, `Wedge_15`, `Hex_20`.

Attribute. The `Attribute` element defines values associated with the mesh. Currently the supported types of values are : `Scalar`, `Vector`, `Tensor`, `Tensor6`, `Matrix`. These values can be centered on : `Node`, `Edge`, `Face`, `Cell`, `Grid`. A summary of all XDMF structures and keywords is given in Table 1.2.

MED format

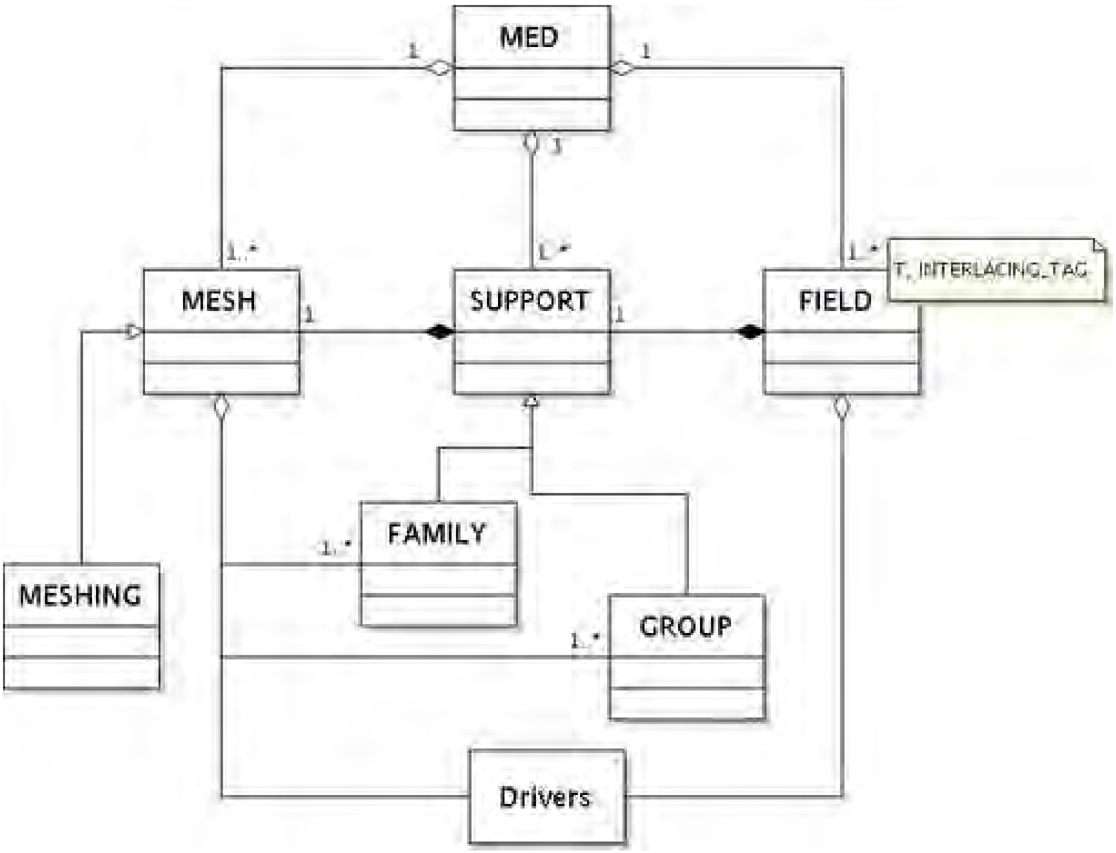


Figure 1.6: MED storage format.

The MED (Modèle d'Echange de Données) data exchange model is the format used in the SALOME platform for communicating data between different components. It manipulates objects that describe the meshes underlying scientific computations and the value fields lying on these meshes. This data exchange can be achieved either through files using the MED-file formalism or directly through memory with the MED Memory (MEDMEM) library. The MED libraries are organized in multiple layers:
- The MED file layer : C and Fortran API to implement mesh and field persistency.
- The MED Memory level: C++ API to create and manipulate mesh and field objects in memory.
- Python API generated using SWIG which wraps the complete C++ API of the MED

Attribute (XdmfAttribute)	
Name AttributeType Center	(no default) Scalar, Vector, Tensor, Tensor6, Matrix, GlobalID Node, Cell, Grid, Face, Edge
DataItem (XdmfDataItem)	
Name ItemType Dimensions NumberType Precision Format	(no default) Uniform, Collection, tree, HyperSlab, coordinates | Function (no default) in KJI Order Float, Int, UInt, Char, UChar 1, 4, 8 XML, HDF
Domain (XdmfDomain)	
Name	(no default)
Geometry (XdmfGeometry)	
GeometryType	XYZ, XY, X_Y_Z, VxVyVz, Origin_DxDyDz
Grid (XdmfGrid)	
Name GridType CollectionType Section	(no default) Uniform, Collection, Tree, Subset Spatial, Temporal (if GridType="Collection") DataItem, All (if GridType="Subset")
Topology (XdmfTopology)	
Name TopologyType NodesPerElement NumberOfElement OR Dimensions Order BaseOffset	(no default) Polyvertex, Polyline, Polygon, Triangle, Quadrilateral,Tetrahedron, Pyramid,Wedge, Edge_3, Triangle_6, Quadrilateral_8, Tetrahedron_10, Wedge_15, Hexahedron_20, Hexahedron, Pyramid_13, Mixed, 2DSMesh, 2DRectMesh, 2DCoRectMesh, 3DSMesh, 3DRectMesh (no default) (no default) (no default) each cell type has its own default 0, #
Time	
TimeType Value	Single, HyperSlab, List, Range (no default, Only valid for TimeType="Single")

Table 1.2: XML Element (Xdmf ClassName) and Default XML Attributes

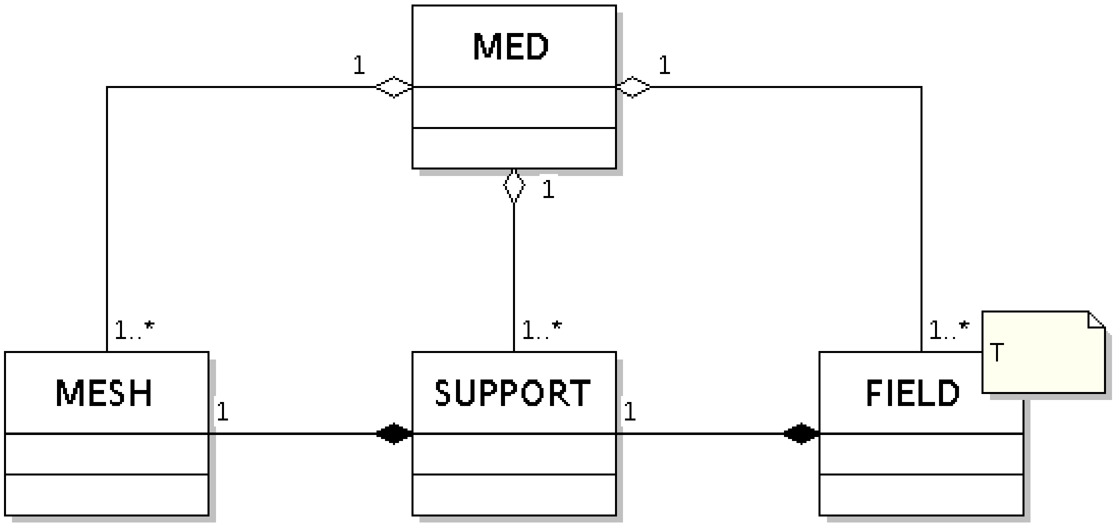


Figure 1.7: MEDMEM memory storage format.

Memory.
- CORBA API to simplify distributed computation inside SALOME (Server Side).
- MED Client classes to simplify and optimize interaction of distant objects within the local solver.

Two codes running on different machines can thus exchange meshes and fields. These meshes and fields can easily be read/written in a MED file format, enabling access to the whole SALOME suite of tools (CAD, meshing, visualization, other components) [4].

With MED Memory any component can access a mesh or field object generated by another application. Though the MEDMEM library can recompute a descending connectivity from a nodal connectivity, MEDMEM drivers can only read MED files containing the nodal connectivities of the entities. In MEDMEM, constituent entities are stored as MED_FACE or MED_EDGE, whereas in MED File they should be stored as MED_MAILLE.

The field notion in MED File and MEDMEM is quite different. In MEDMEM a field is of course defined by its name, but also by its iteration number and its order number. In MED File a field is only flagged by its name. For instance, a temperature at times $t = 0.0\,s$, $t = 1.0\,s$, $t = 2.0\,s$ will be considered as a single field in MED File terminology, while it will be considered as three distinct fields in the MED Memory sense.

MEDMEM supports data exchange in following formats:
- GIBI, for reading and writing the mesh and the fields in ASCII format.
- VTK, for writing the mesh and the fields in ASCII and binary formats.
- EnSight, for reading and writing the mesh and the fields in ASCII and binary formats.
- PORFLOW, for reading the mesh in ASCII format.

Classes. At a basic usage level, the MEDMEM library consists of few classes which are

located in the MEDMEM C++ namespace:
- MED the global container;
- MESH the class containing 2D or 3D mesh objects;
- SUPPORT the class containing mainly a list of mesh elements;
- FIELD the class template containing a list of values lying on a particular support.

The MEDMEM classes are sufficient for most of the component integrations in the SALOME platform. The use of the MED Memory libraries may make the code coupling easier in the SALOME framework. With these classes, it is possible to:
- read/write meshes and fields from MED-files;
- create fields containing scalar or vectorial values on a list of elements of the mesh;
- communicate these fields between different components;
- read/write such fields.

Advanced classes. A more advanced usage of the MED Memory is possible through other classes. Figure 1.6 gives a complete view of the MED Memory API. It includes:
- GROUP, a class inherited from the SUPPORT class used to create supports linked to mesh groups. It stores a restricted list of elements used to set boundary conditions and initial values.
- FAMILY which is used to manipulate a certain kind of support which does not intersect each other.
- MESHING which builds meshes from scratch, it can be used to transform meshes from a specific format to the MED format or to integrate a mesher within the SALOME platform.
- GRID which enables the user to manipulate specific functions for structured grids.

Note that in Figure 1.6 as well as in Figure 1.7 the MED container controls all the objects it contains: its destructor destroys all the objects inside. On the other hand, the MESH, SUPPORT and FIELD objects are independent. Destroying a SUPPORT (resp. a FIELD) will have no effect on the MESH (resp. SUPPORT) which refers to it. But the user has to maintain the link: a MESH aggregates a SUPPORT which aggregates a FIELD. If the user has to delete MED Memory objects, the FIELD has to be deleted first, then the SUPPORT and finally the MESH.

MEDMEM Lists. A few enums (C enumerations) are defined in the MEDMEM namespace :

- an enum which describes the way node coordinates or field values are stored:
  - `MED_FULL_INTERLACE` for arrays such that $x_1, y_1, z_1, \ldots, x_n, y_n, z_n$;
  - `MED_NO_INTERLACE` for arrays such that $x_1, \ldots, x_n, y_1, \ldots, y_n, z_1, \ldots, z_n$;
  - `MED_UNDEFINED_INTERLACE`, the undefined interlacing mode,

- an enum which describes the type of connectivity:
  - `MED_NODAL` for nodal connectivity;

- MED_DESCENDING for descending connectivity.
The user has to be aware of the fact that the MED Memory considers only meshes defined by their nodal connectivity. Nevertheless, the user may, after loading a file in memory, ask to the mesh object to calculate the descending connectivity.

- an enum which contains the different mesh entities, medEntityMesh, the entries of which being: MED_CELL, MED_FACE, MED_EDGE, MED_NODE, MED_ALL_ENTITIES. the mesh entity MED_FACE is only for 3D and the In 3D (resp. 2D), only mesh entities MED_NODE, MED_CELL and MED_FACE (resp. MED_EDGE) are considered. In 1D, only mesh entities MED_NODE and MED_CELL are taken into account.

- The medGeometryElement enum which defines geometric types. The available types are linear and quadratic elements: MED_NONE, MED_POINT1, MED_SEG2, MED_SEG3, MED_TRIA3, MED_QUAD4, MED_TRIA6, MED_QUAD8, MED_TETRA4, MED_PYRA5, MED_PENTA6, MED_HEXA8,MED_TETRA10, MED_PYRA13, MED_PENTA15, MED_HEXA20, MED_POLYGON, MED_POLYHEDRA, MED_ALL_ELEMENTS.

1.3.2 Platform visualization

PARAVIEW on CRESCO-ENEA GRID

Inside the platform there are many applications for visualization. In order to uniform the output and the visualization we use only the PARAVIEW software. The reasons for this choice are:

- it is open-source, scalable and multi-platform;
- it supports distributed computation models to process large data sets;
- it has an open, flexible and intuitive user interface;
- it has an extensible, modular architecture based on open standards.

For all these reasons the output files must be saved in a PARAVIEW readable format. From the practical point of view this is not a limitation since PARAVIEW reads a large number of formats. The following is an incomplete list of currently available readers:
- ParaView Data (.pvd)
- VTK (.vtp, .vtu, .vti, .vts, .vtr, .vtm, .vtmb,.vtmg, .vthd, .vthb, .pvtu, .pvti, .pvts, .pvtr, .vtk)
- Exodus
- XDMF and hdf5 (.xmf, .xdmf)
- LS-DYNA
- EnSight (.case, .sos)
- netCDF (.ncdf, .nc)
- PLOT3D
- Stereo Lithography (.stl)

- Meta Image (.mhd, .mha)
- SESAME Tables
- Fluent Case Files (.cas)
- OpenFOAM Files (.foam)
- PNG, TIFF, Raw Image Files
- Comma Separated Values (.csv)
- Tecplot ASCII (.tec, .tp)

In ENEA-CRESCO cluster, PARAVIEW can run in two different ways:
a) from console;
b) as a remote application through FARO.

From console the command is :

```
$ paraview-3.8.0
```

to run the latest version of PARAVIEW (3.8.0). The other versions are available by changing the version number in the command after the − sign. We remark that PARAVIEW can be launched only from machines with graphical capability (with a letter `g` in the name). For example PARAVIEW can run from `cresco1-fg1.portici.enea.it`.

As a remote application one must login from the FARO web page (see Section 1.2.2) and then select the PARAVIEW button. If the program runs in this mode the rendering is pre-processed on the remote machine, which guarantees a higher speed.

The PARAVIEW application

PARAVIEW is an open-source, multi-platform application designed to visualize data sets of large size. It is built on an extensible architecture and runs on distributed and shared memory parallel as well as single processor systems. PARAVIEW uses the Visualization Toolkit (VTK) as the data processing and rendering engine and has a user interface written using the Qt cross-platform application framework. The Visualization Toolkit (VTK) provides the basic visualization and rendering algorithms. VTK incorporates several other libraries to provide basic functionalities such as rendering, parallel processing, file I/O and parallel rendering [7].

A brief explanation of the PARAVIEW GUI is given in Figure 1.8. The GUI has many panels that control the visualization. The two main panels are the View Area and the Pipeline Browser panel. The data are loaded in the View Area which displays visual representations of the data in 3D View, XY Plot View, Bar Chart View or Spreadsheet View. The visualization on the View Area is managed by the Pipeline Browser panel. The `Open` and `Save data` buttons perform the loading and saving operations for all the supported file formats. The Object Inspector panel contains controls and information about the reader, source, or filter selected in the Pipeline Browser. The most important menu is the Filters menu that is used to manipulate the data. For example one can draw the isolines of any dataset using the Contour filter. The Sources menu is used to create

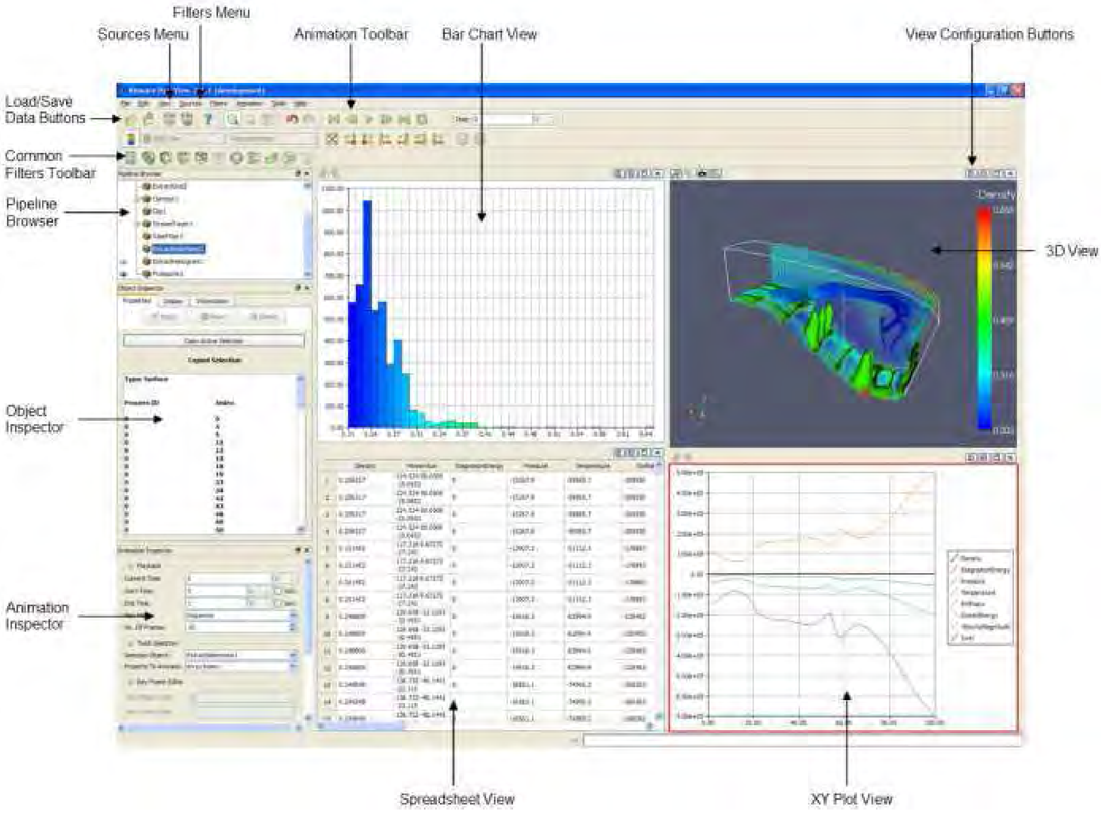


Figure 1.8: Basic interface for PARAVIEW

new geometrical objects while the Animation toolbar navigates through the different time steps of the simulation [6].

Documentation

More information is available on the ParaView web site:
http://www.paraview.org
A wiki is also available at
http://www.paraview.org/Wiki/ParaView
and a tutorial
http://public.kitware.com/Wiki/The_ParaView_Tutorial
A list of all sources and filters can be found at
http://www.paraview.org/New/help.html

Chapter 2

SALOME

2.1 Introduction

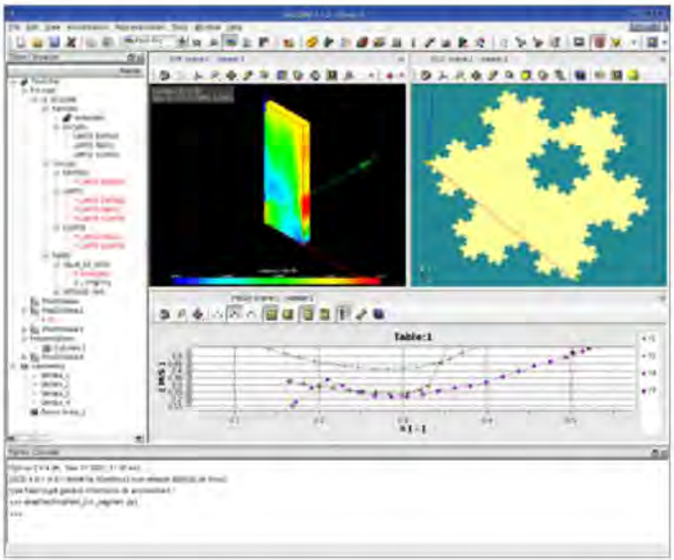


Figure 2.1: SALOME graphical user interface

2.1.1 Code development

Developer(s)	Open CASCADE, NURISP, EDF
Stable release	`5.1.4 / June 2010`
Operating system	`Unix/Linux`
License	`GNU Lesser General Public License`
Website	`www.salome-platform.org`

2.1.2 Location on CRESCO-ENEA GRID

CRESCO-ENEA GRID:

executable:	`salome`
install directory:	`/afs/enea.it/project/fissicu/soft/SALOME`

2.1.3 SALOME overview

SALOME is a free and open-source software that provides a generic platform for numerical simulations. The SALOME application is based on an open and modular architecture that is released under the GNU Lesser General Public License. The source code and executables in binary form may be downloaded from its official website at http://www.salome-platform.org. There are several version available, such as Debian, Mandriva and a universal package with all dependencies inside. All versions have a 32 and 64 bit version. The source code is also available to any programmer who wishes to develop and make it available for other operative system. On the CRESCO-ENEA GRID the Mandriva version (for 64 bits) is installed.

SALOME, which is also developed under the project NURISP, is a base software for integration of custom modules and developing of the custom CAD applications. The main modules are:
a) KERNEL: distributed components management, study management, general services;
b) GUI: graphical user interface
c) GEOM: CAD models creation, editing, import/export
d) MESH: standard meshing algorithm with support for any external mesher (plugin-system)
e) MED: MED data files management
f) POST: dedicated post-processor to analyze the results of solver computations (scalar, vectorial)
g) YACS: computational schema manager for multi-solver coupling and supervision module.

In the FISSICU project SALOME is mainly used as mesh generator but it has many other features: interoperability between CAD modeling and computational software, integration of new components into heterogeneous systems, multi-physics weak coupling between computational software. The platform may integrate different additional codes on which perform code coupling. At the moment the integration among codes is far to be completed but some basic functionality can be used. In the platform the ideas of weak, internal weak and strong coupling are implemented. The weak coupling is performed with the exchange of output and input files. In the internal weak coupling all the equations are solved in a segregated way using memory to exchange data between codes. A popular format for this purpose is the MED library and its MEDMEM API classes. Among the various available SALOME modules, there are some samples that can be used by the developers to learn how to create and integrate custom modules in the SALOME platform. SATURNE has a module that links to the SALOME platform, but only a beta version is available. The integration module is in development at EDF. NEPTUNE and CATHARE codes are also developing an integration module for the SALOME platform [4, 5].

2.2 SALOME on CRESCO-ENEA GRID

The SALOME platform is located on CRESCO-ENEA GRID in the directory

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

The salome platform can be run in two ways:
a) from console
b) from FARO website

From console one must first set the access to the bin directory

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

by executing the script

```
$ source pathbin.sh
```

Remark. The script `pathbin.sh` must be in the home directory. One must copy the template script `pathbin.sh` from the directory

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

and then execute the script to add the bin directory to the `PATH`. If the `pathbin.sh` script is not available one must enter the `bin` directory to run the program.

Once the bin directory is on your own `PATH` all the programs of the platform can be launched. The command needed to start the SALOME application is

```
$ salome
```

Remark. The script `salome` consists of two commands: the environment setting and the start command. The environment script sets the environment of shell. The start command is a simple command that launches the `runSalome` command.

From FARO web application it is possible to access the SALOME platform with remote accelerated graphics. Once FARO has been started (see Section 1.2.2) one must open an xterm. In the xterm console one must follow the same procedure as before. First, set the access to the bin directory

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

by executing the script

```
$ source pathbin.sh
```

SALOME starts with the command

```
$ salome
```

Remark. When exiting the SALOME application we are left in a python shell. To exit press CTRL+D.

2.3 SALOME platform modules

2.3.1 Introduction

SALOME platform has seven components:

- KERNEL, that provides component management, study management and general services
- GUI, that provides a graphical user interface
- GEO, that provides a geometry module to create, edit, import/export CAD models
- MESH, that provides a CAD model with standard meshing algorithms
- MED, that provides the data files management
- POST-PRO, that provides a post-processor dedicated viewer to analyze the results of solver computations
- YACS, that provides a computational schema involving multi-solver coupling

2.3.2 KERNEL

The KERNEL components is the key component of the SALOME platform. The KERNEL module provides communication among distributed components, servers and clients: dynamic loading of a distributed component, execution of a component and data exchange between components. CORBA interfaces are defined via IDL files and are available for users in Python. CORBA interfaces for some services are encapsulated in C++ classes providing a simple interface. Python SWIG interface is also generated from C++, to ensure a consistent behavior between C++ modules and Python modules or user scripts.

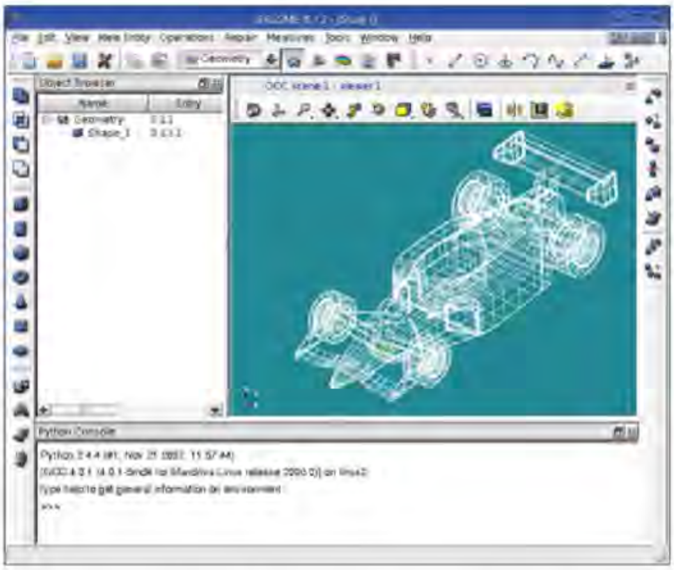


Figure 2.2: GUI for the GEOM module.

2.3.3 GUI

GUI (Graphical User Interface) provides a common shell for all components, which can be integrated into the SALOME platform. GUI component in SALOME platform provides a common desktop environment (SALOME desktop) for all components and component integration and management by uploading, switching and menus/toolbars handling of the different components. The GUI provides also standard viewers for data visualization as VTK 3D viewer, OCC 3D viewer, Plot 2D viewer and supervision viewer.

2.3.4 GEOM

This component provides functionalities for creation, visualization and modification of geometric CAD models. Also the GEOM module provides visualization of models in 3D viewers in shading and wireframe modes. SALOME imports and exports CAD models in formats as IGES 5.3, STEP AP203/214 schemas and BREP (Open CASCADE internal format). One can create basic geometrical objects and 3D primitives together with modeling operations such as extrusion, revolution and pipe creation. Inside the GEOM component we can get topological information and dimensions such as center of gravity, axis of inertia and minimal distance.

2.3.5 MED

The purpose of the MED module is to provide a standard for storing and recovering computer data associated to numerical meshes and fields, and to facilitate the exchange between codes and solvers. For details one can see Section 1.3.1.

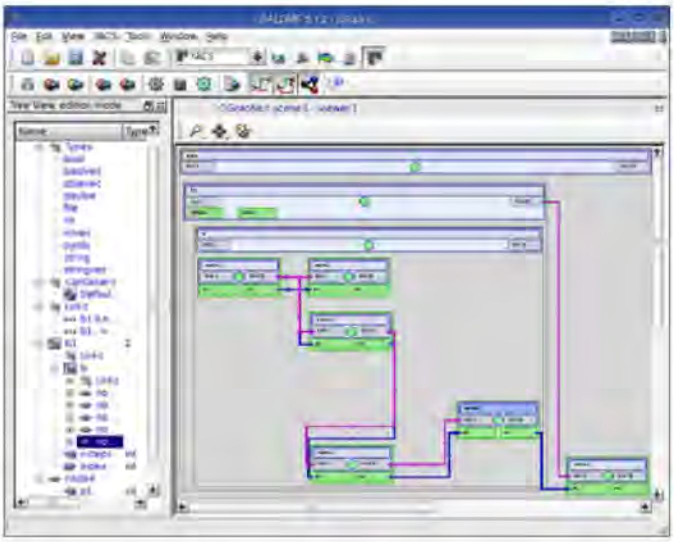


Figure 2.3: GUI for the YACS module

2.3.6 MESH

The goal of the MESH module is to create a mesh on the basis of the geometrical models created or imported into the GEOM module. A set of meshing algorithms and their corresponding conditions (hypotheses) to compute meshes are available to the user. For details see Section 2.5.3.

2.3.7 POST-PRO

The purpose of this module is to supply visualization tools to help the end-user analyze the results issued from a solver after a numerical computation. It proposes standard functionalities to display information through a wide range of functions. In the CRESCO-ENEA GRID we do not use this module since the PARAVIEW application will be used for post-processing.

2.3.8 YACS

YACS module allows to build, edit and execute calculation schemes. A calculation scheme defines a chain or a coupling of computer codes. Some common general operations are the activation of the YACS module, the import/export schema, the modification of a schema (create, edit, delete an object). All these operations can be performed graphically, as shown in a typical screen of this module in Figure 2.3.

2.4 SALOME file transfer service

This section introduces the SALOME file feature (`Salome_file`) which can be used to transfer files from one computer to another. This can be used from one program to retrieve the output file from another application and use it as input file.

2.4.1 File transfer service inside a program

`Salome_file` is a CORBA object which may manage different files. First a `Salome_file` must be created. It is a container with no files. Files may be added to the `Salome_file` using the `Salome_file_i` interface. A file is represented by a name and a path. There are two different types of files that can be added to the `Salome_file`:
- Local file: the file added exists or it will be created by the user with the path and the name used in its registration.
- Distributed file: the file added exists into a distributed localization.
In order to get a distributed file, the Salome_file has to be connected with an another `Salome_file` that has this file.

In the following we show a simple `Salome_file` with the objective to create two `Salome_files`: one with a local file and the other with a distributed file. Then, these `Salome_files` are connected to enable the copy of the real file between the two files.

```
#include "Salome_file_i.hxx"
int main (int argc, char * argv[]){
  Salome_file_i myfile;
  Salome_file_i filedist;
  myfile.setLocalFile("localdir");
  filedist.connectDistributedFile("distrdir", myfile);
  filedist.setDistributedSourceFile("distrdir", "localdir");
  filedist.recvFiles();
};
```

The include `Salome_file_i.hxx` is necessary to use the functions and the class. In the first two lines two `Salome_files` are created with the command `Salome_file_i`. The file names are `myfile` and `filedist`. The function `setLocalFile` sets the path `localdir` of the local `myfile` file. The function `setDistributedFile` sets the path `distrdir` of the distributed file with name `filedist`. The directories must exist. Now the files are defined by name and path. The `connect` command connects the distributed `filedist` file with the local `myfile` file. The transfer starts with the command `recvFiles`.

2.4.2 Python file transfer service

The file transfer can also be obtained by using python commands. If the remote hostname is `computername` and we would like to copy `myfile` from the remote to a local computer the following python program can be used

```
import salome
salome.salome_init()
import LifeCycleCORBA
remotefile="myfile"
aFileTransfer= \
       LifeCycleCORBA.SALOME_FileTransferCORBA('computername',remotefile)
localFile=aFileTransfer.getLocalFile()
```

2.4.3 Batch file transfer service

A third way to have a service access is through the SALOME batch service. The interested reader can consult the SALOME documentation.

2.5 SALOME Mesh creation

2.5.1 Import and export of mesh files in SALOME

At the moment the SALOME platform on CRESCO-ENEA GRID is not used to distribute files and the implementation of coupled codes is not fully operational. The most important use of the SALOME platform is the mesh generation. SALOME offers a good open source application able to generate meshes for other applications as SATURNE and many others. For this reason it is important to use the MED format or convert such a format in more popular formats. The mesh functionality of SALOME is performed by the MESH module. In the SMESH module there is a functionality allowing importation and exportation of meshes from MED, UNV (I-DEAS 10), DAT (Nastran) and STL format files. These formats are not very popular and local converters may be necessary.

Mesh import. In order to import a mesh inside the `SMESH` module from other formats these steps must be followed:
- From the File menu choose the Import item, from its sub-menu select the corresponding format (MED, UNV and DAT) of the file containing your mesh.
- In the standard Search File dialog box select the desired file. It is possible to select multiple files.
- Click the OK button.

Mesh export. Once the mesh is generated by the SALOME MESH module the procedure to export a mesh is the following
- Select the object you wish to export.
- From the File menu choose the Export item and from its sub-menu select one of the available formats (MED, UNV, DAT and STL).
- In the standard Search File select a location for the exported file and enter its name.
- Click the OK button.

2.5.2 Mesh tutorial from SALOME documentation

Help for mesh creation can be found at

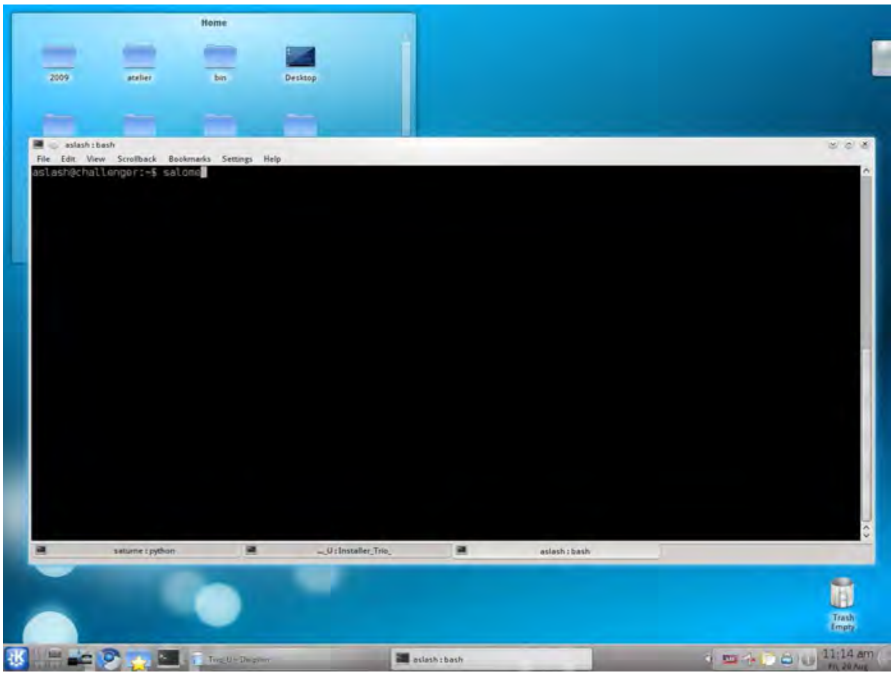
http://www.salome-platform.org/user-section/salome-tutorials

In this web page there are ten exercises from EDF:
EDF Exercise 1: Primitives, partition and meshing example. Geometric Primitives, tetrahedral and hexahedral 3D meshing, Partitions.
EDF Exercise 2: 2D Modeling and Meshing Example. Geometrical Primitives, triangular 2D mesh, Zone Refinement, mesh modification, sewing.
EDF Exercise 3: Complex Geometry meshed with hexahedra, quality controls. 3D Geometry, Partition, Hexahedral mesh, mesh display, quality controls.
EDF Exercise 4: Extrusion along Path and meshing example. The purpose is to produce a prismatic meshing on a curved geometry.
EDF Exercise 5: Geometry by blocks, shape healing. Creation of a geometric object by Blocks, Primitive, Boolean Operation, Shape healing.
EDF Exercise 6: Complex Geometry, hexahedral mesh. 3D Geometry, Partition, Hexahedral Mesh.
EDF Exercise 7: Creation of mesh without geometry. Manual creation of a mesh.
EDF Exercise 8: Pattern Mapping. Creation of a Pattern mapping.
EDF Exercise 9: Joint use of TUI and GUI. Learn to use GUI dialogs with TUI commands to generate a pipe with different sections.
EDF Exercise 10: Work with scripts only. This exercise is to learn working with Python scripts in SALOME. The scripts allow to parameterize studies and to limit the disk space for the storage.

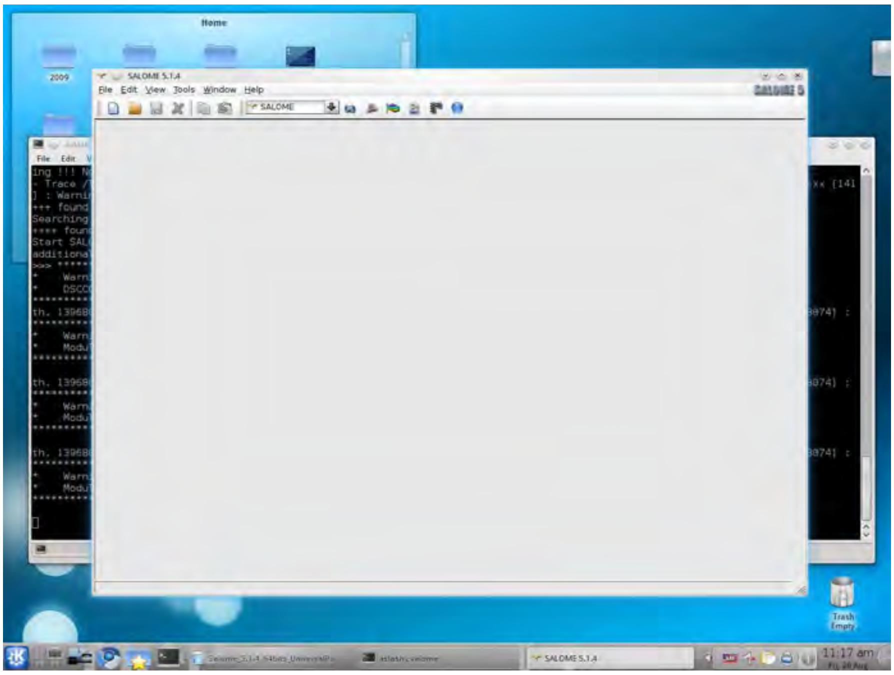
2.5.3 Tutorial: step by step mesh on CRESCO-ENEA GRID

In this section we introduce step by step a mesh generation on CRESCO-ENEA GRID from the MESH module of the SALOME application.

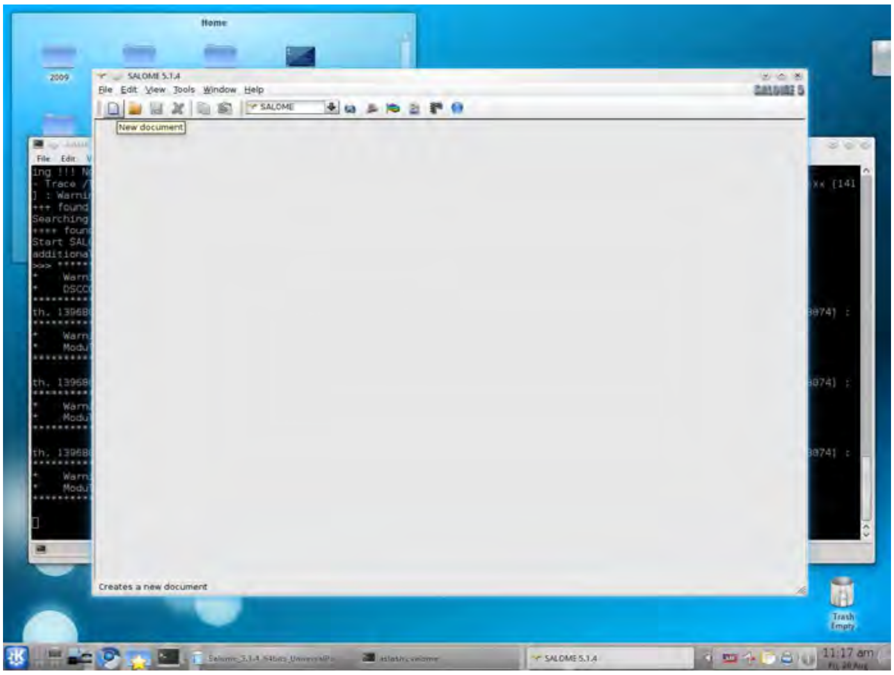
1. Launch `salome` from command line.



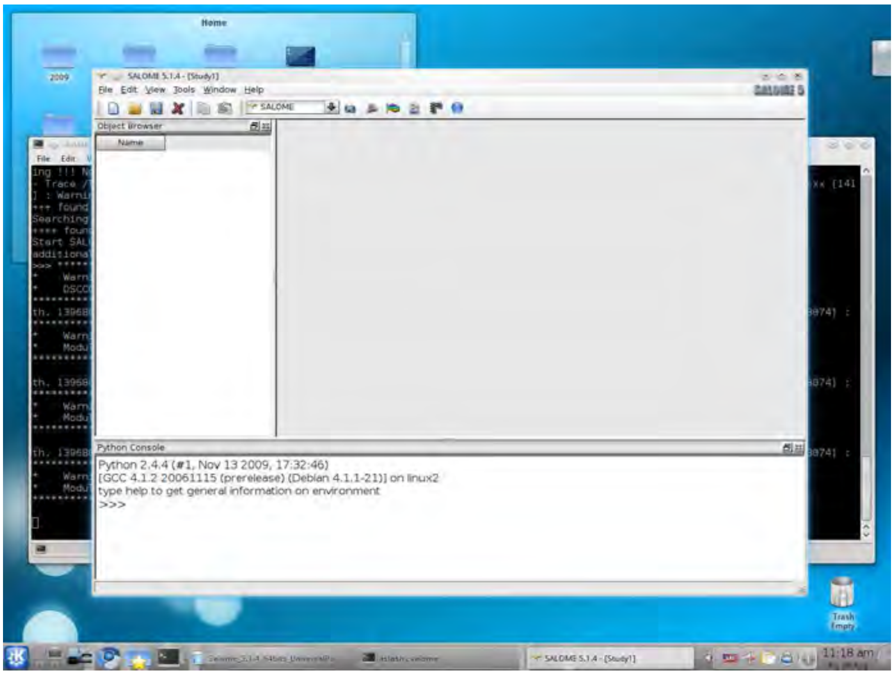
2. The SALOME main window will appear.



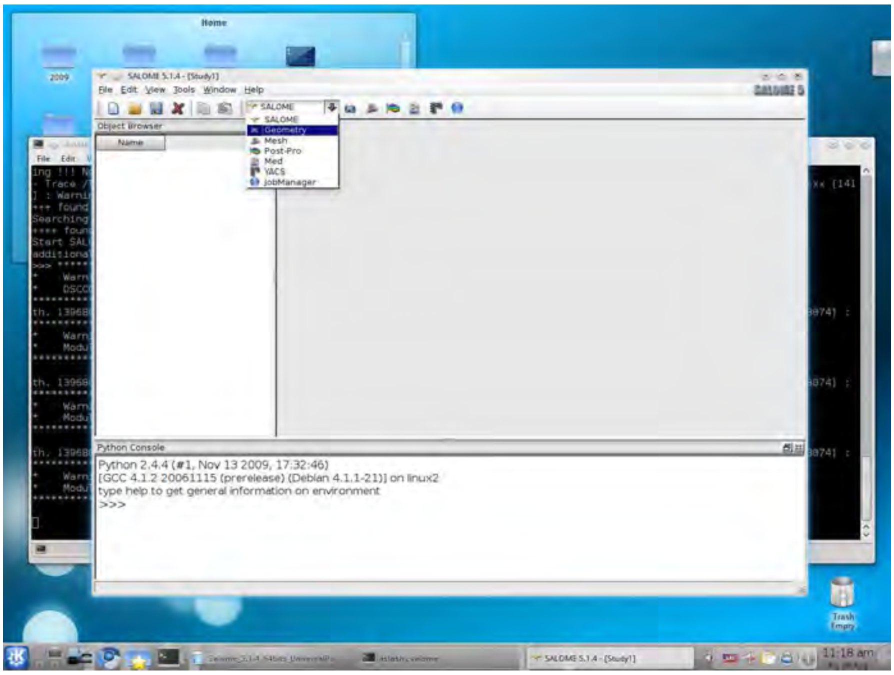
3. Click the $\boxed{\text{New document}}$ button.



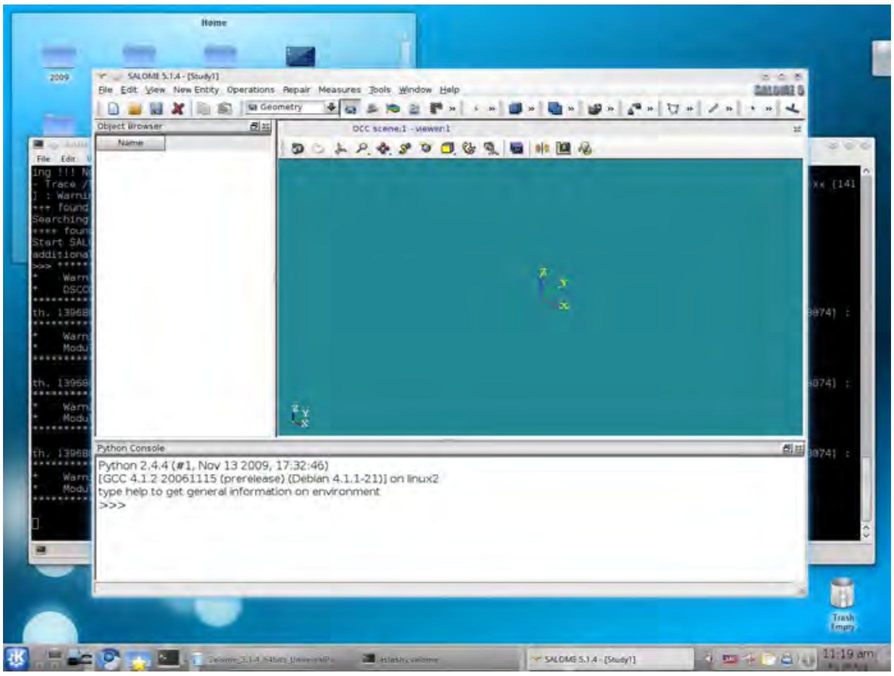
4. The list on the left will show all the elements added to the working study.



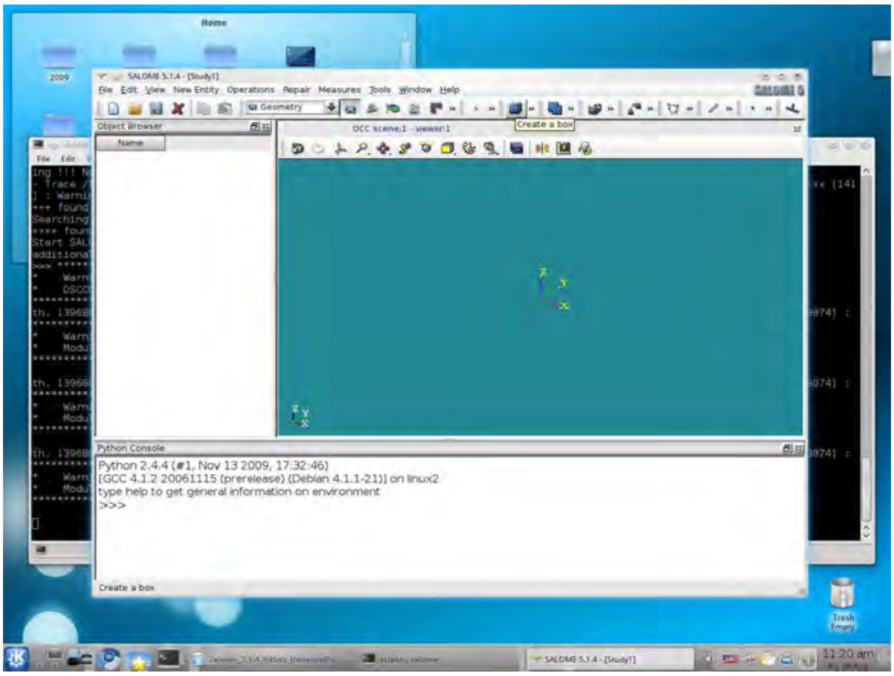
5. Select the Geometry module form the dropdown menu.



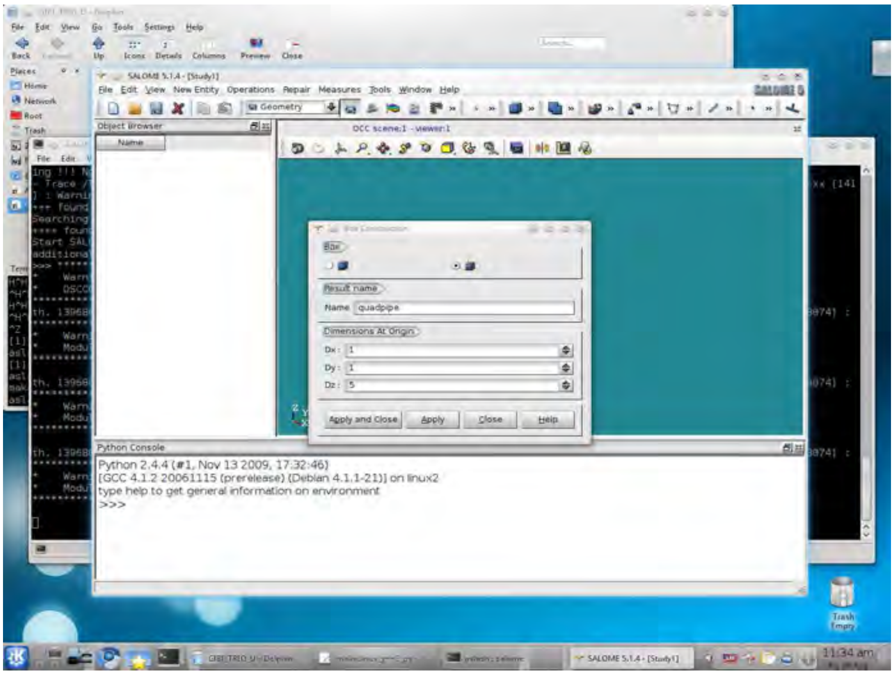
6. The main window will switch to an OpenCascade scene.



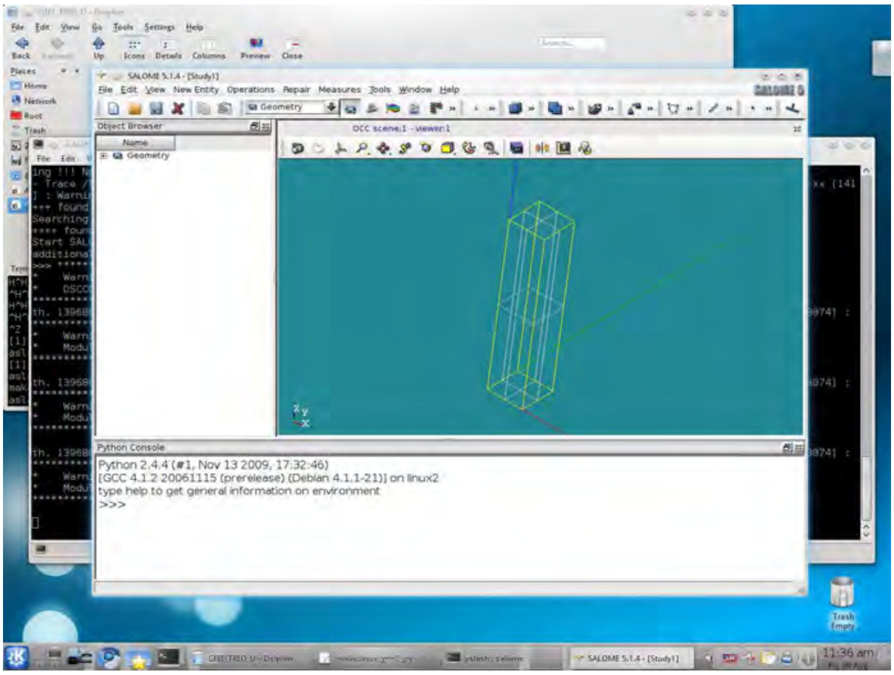
7. Click the Create a box button.



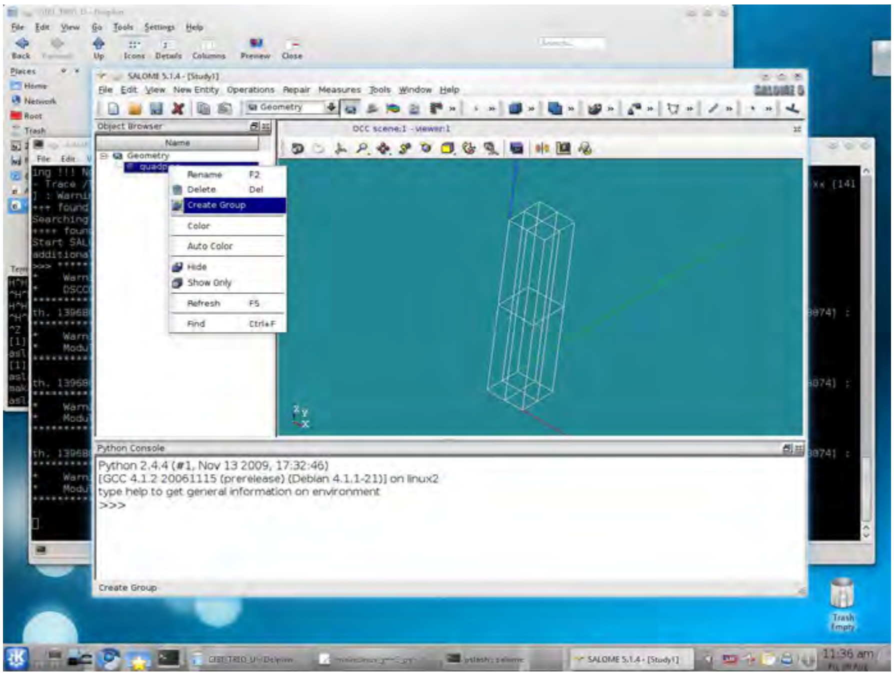
8. On the dialog, use `quadpipe` for the Name. The dimension of the box shall be 1, 1 and 5.



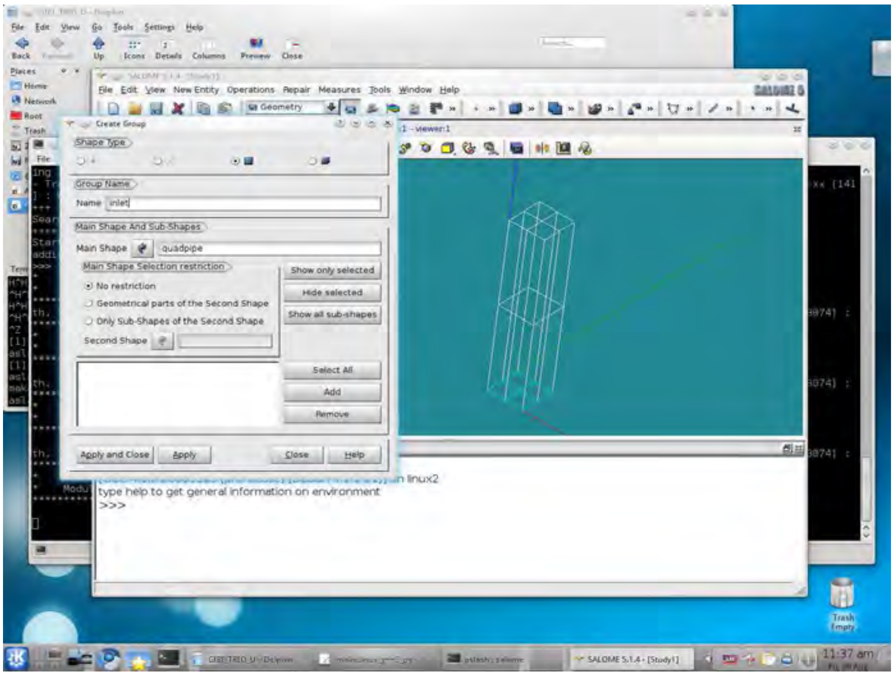
9. Zoom to the just created object.



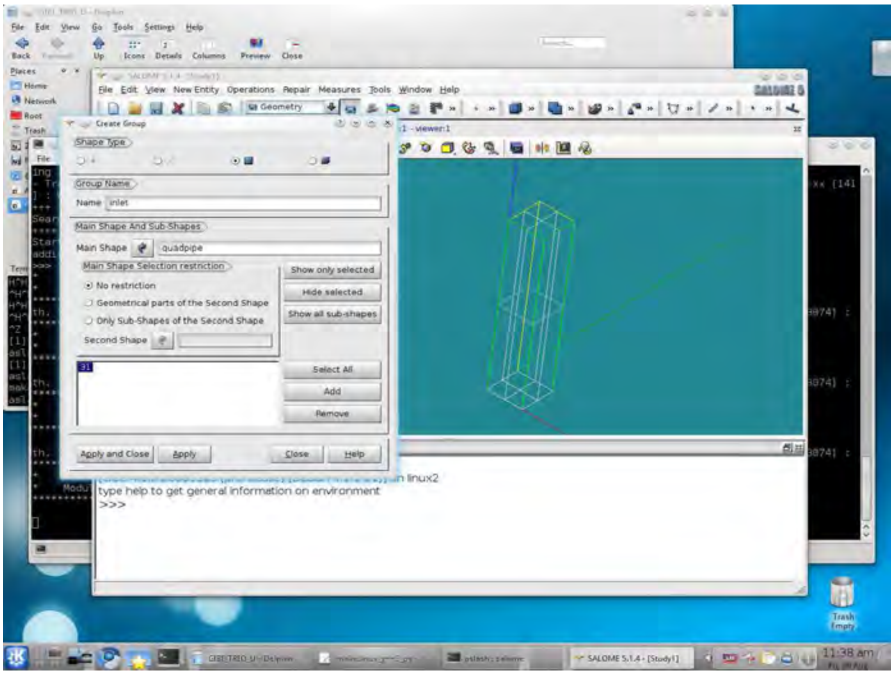
10. Right-click on the `quadpipe` object in the left column. Select the Create Group option.



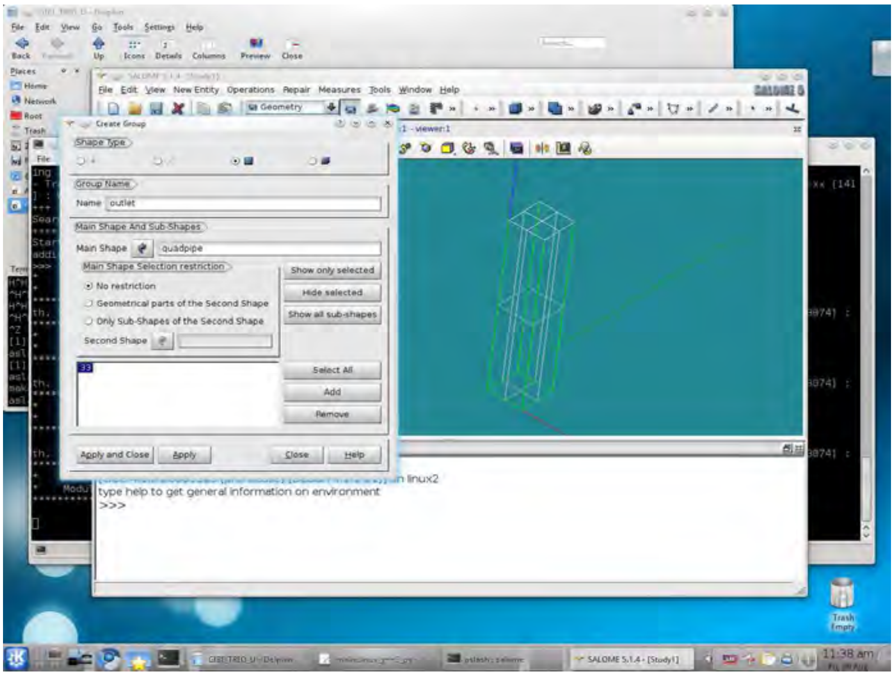
11. We create all the boundary regions of the box in order to put boundary conditions on them. We start from the `inlet` region, selecting it directly in the OCC scene.



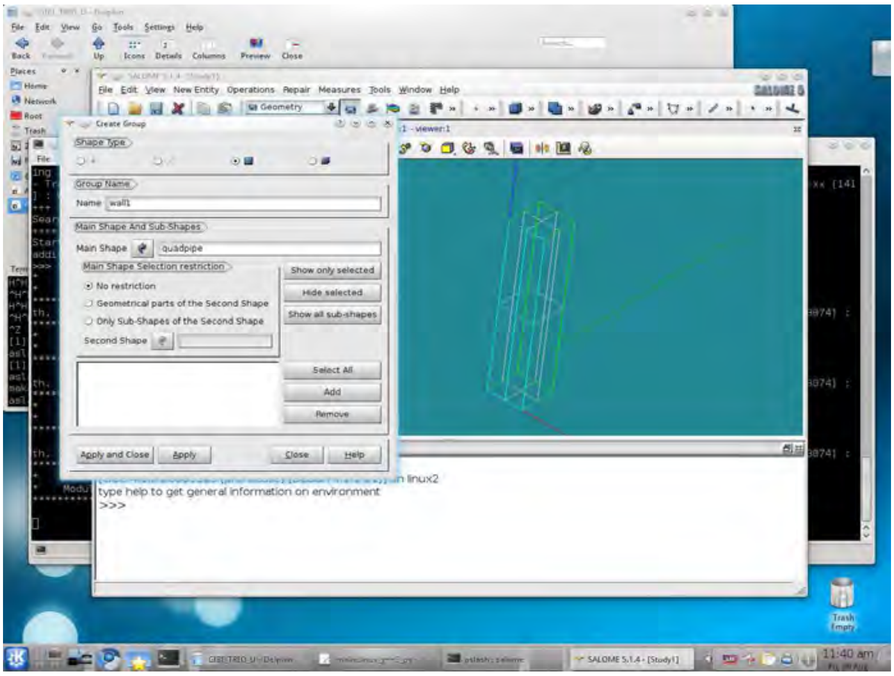
12. Clicking the Add button, the surface should appear in the list. The number of this region must be `31`. Click the Apply button.



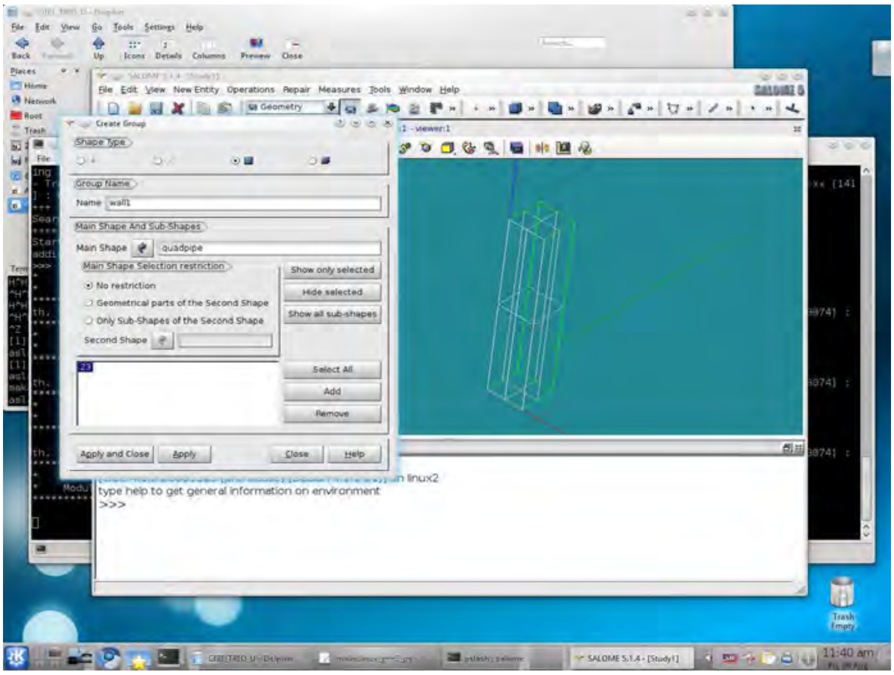
13. Similarly we create the `outlet` region (number 33).



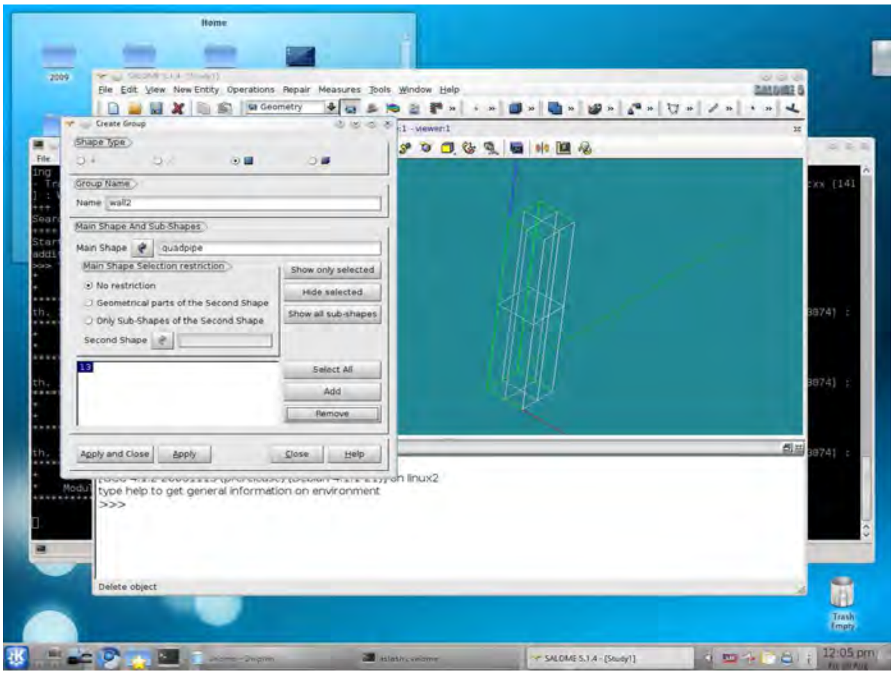
14. We split the lateral surface in 4 regions. We start from the front one and name it `wall1`.



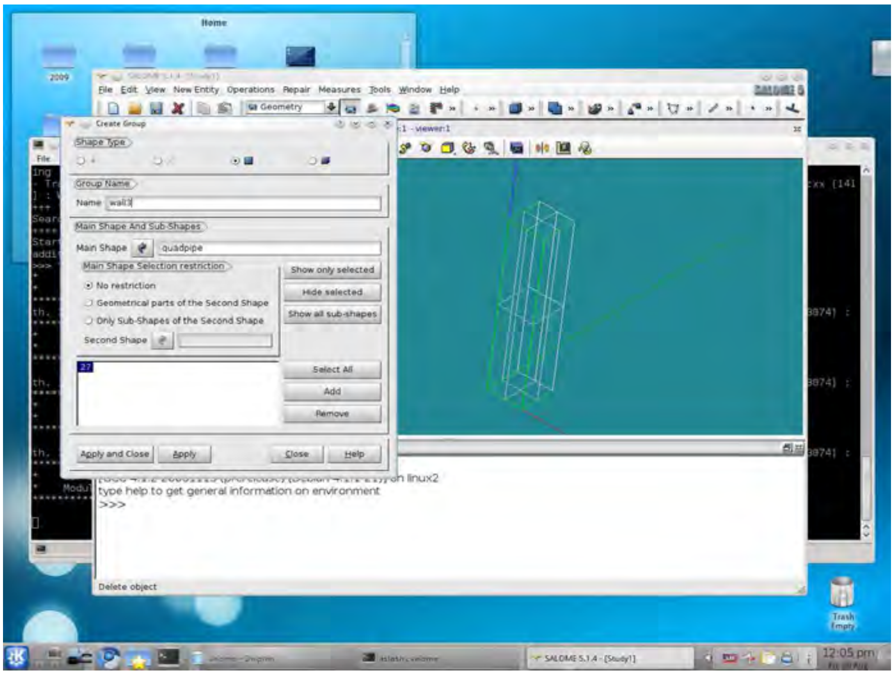
15. The number of this region is 23.



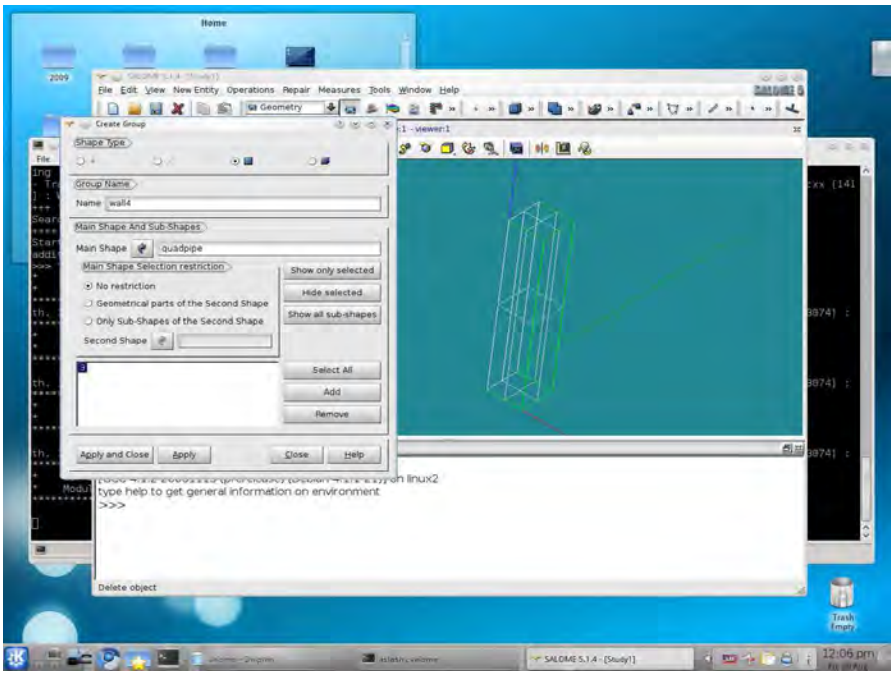
16. wall2 region is numbered 13.



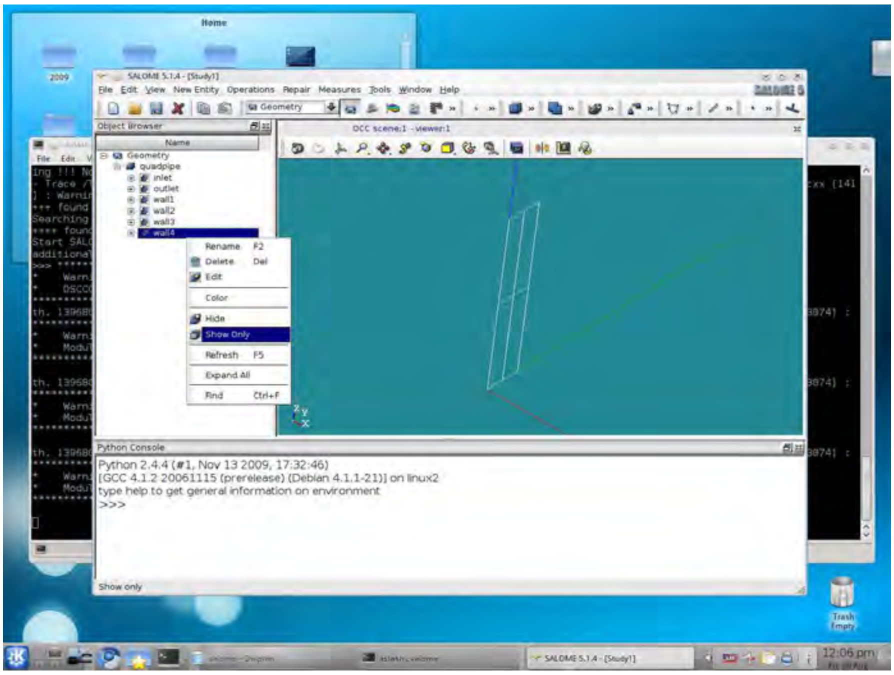
17. `wall3` region is numbered 27.



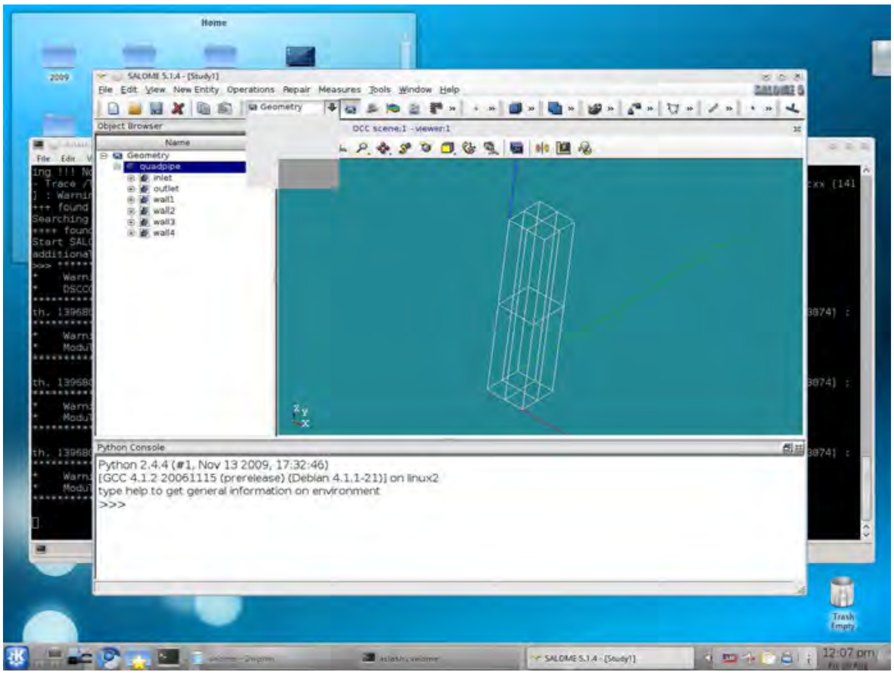
18. `wall2` region is numbered 3. We can now click the Apply and Close button, since this is the last region to create.



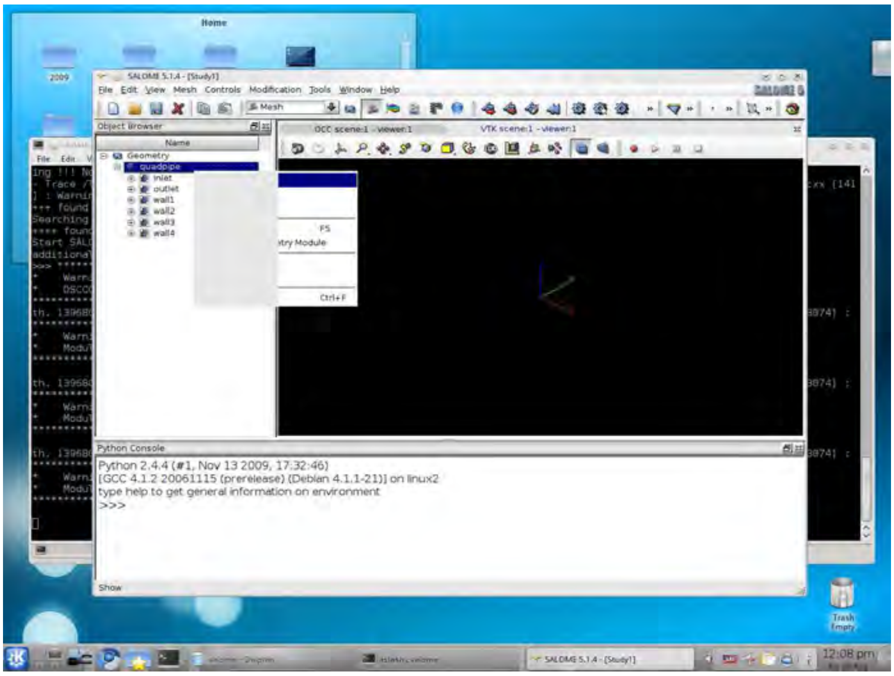
19. To check if all the regions have been created correctly, we can use the Show Only option in the right-click menu of each object.



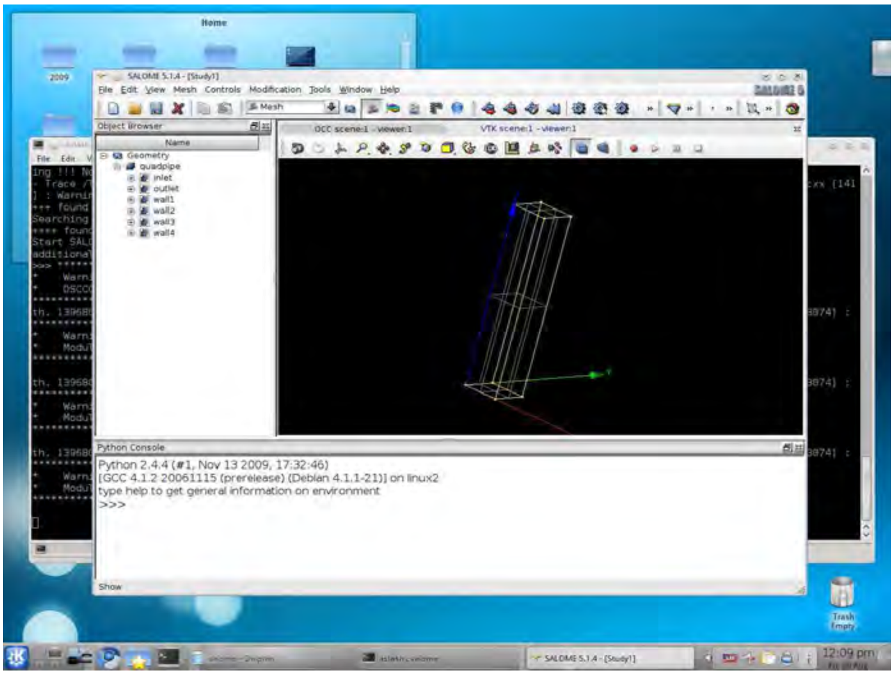
20. We select the Mesh module from the drop-down menu.



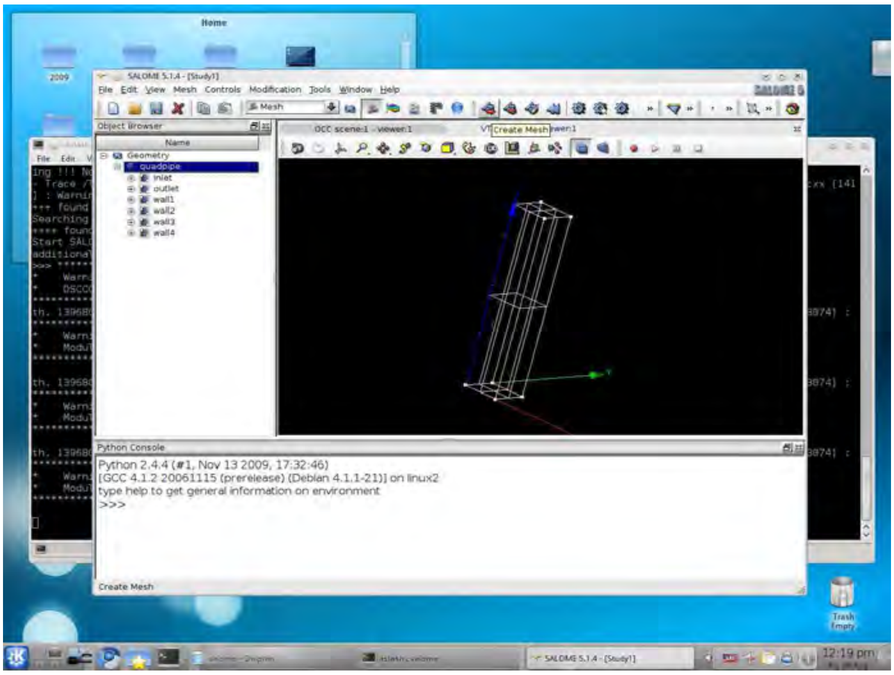
21. In order to show the `quadpipe` object, we select show in the right-click menu.



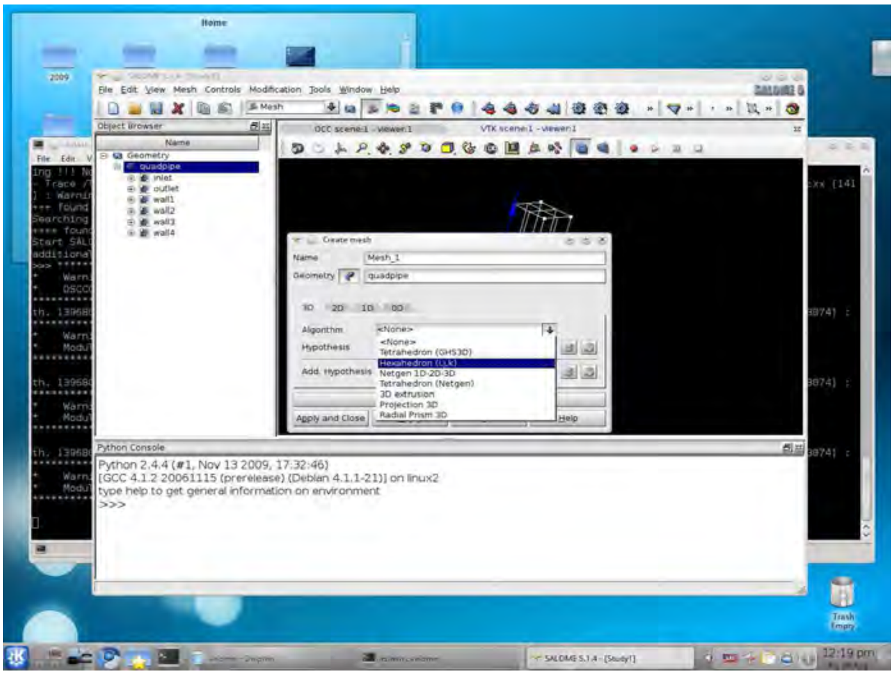
22. We zoom to the object in the VTK scene.



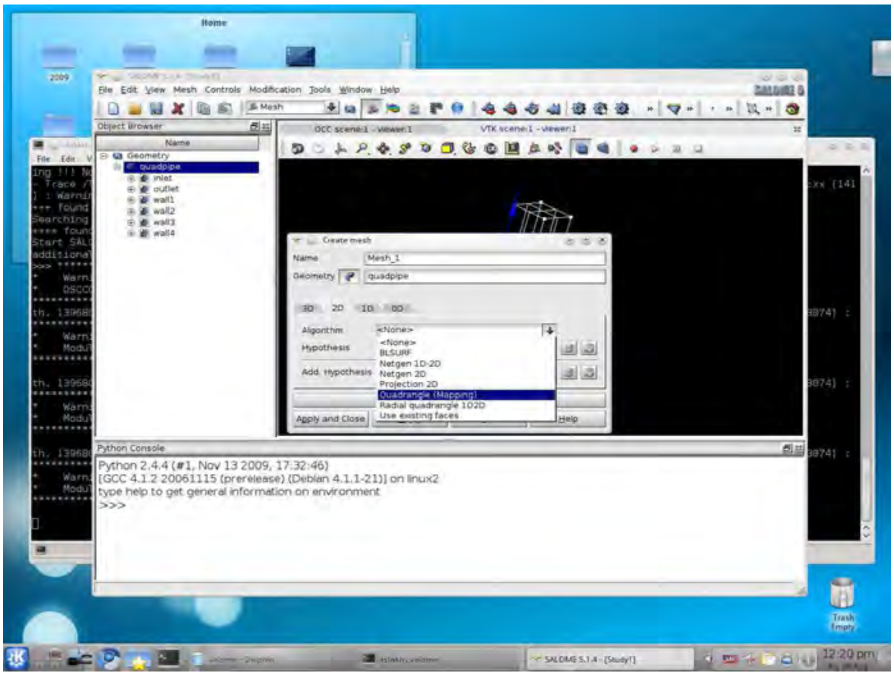
23. We click on the create mesh button.



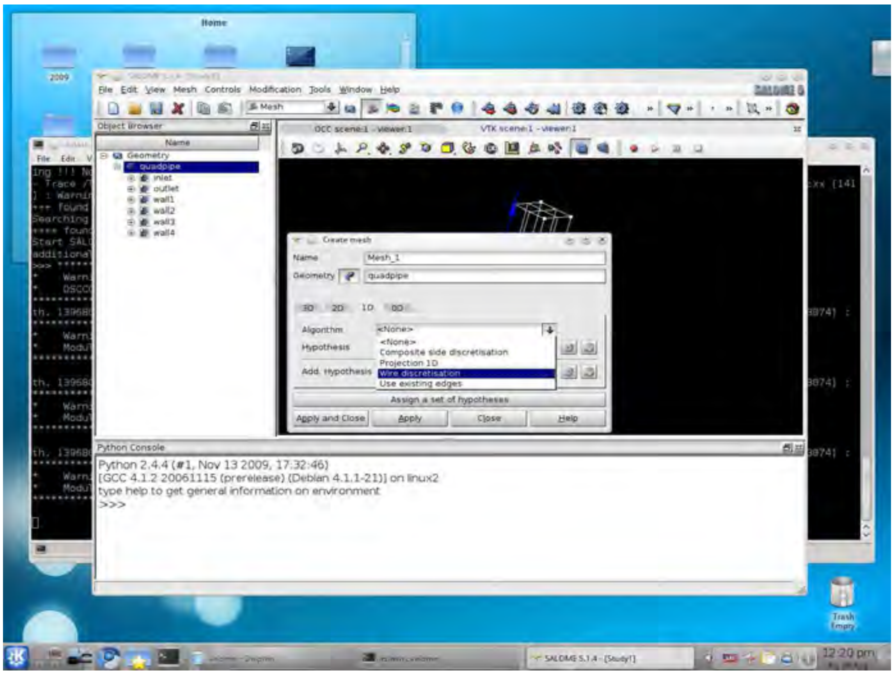
24. In the appearing dialog, we select Hexahedron (i,j,k) in the `Algorithm` drop-down menu for the `3D` tab.



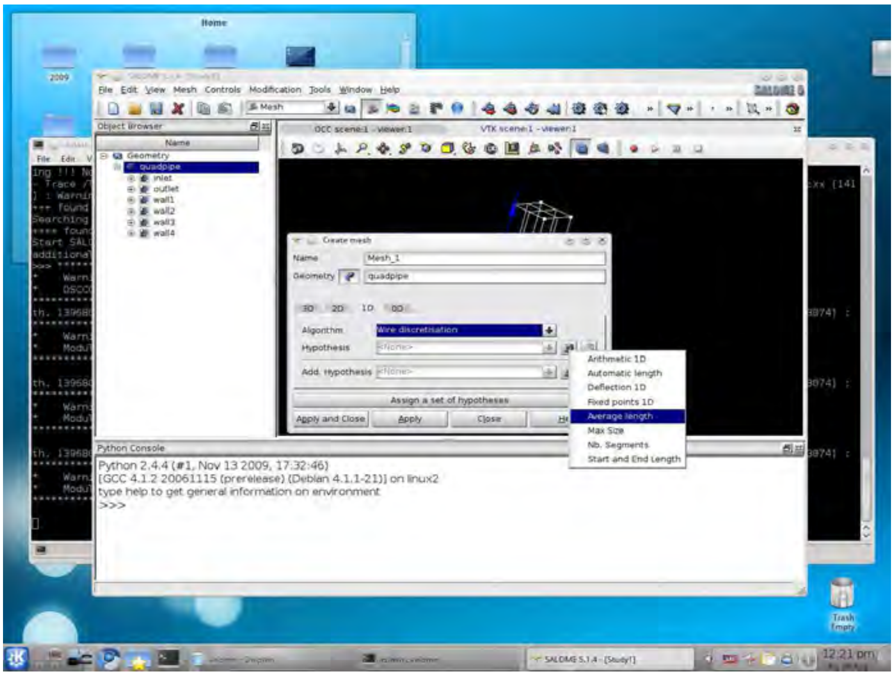
25. In the 2D tab, we select the Quadrangle (Mapping) algorithm.



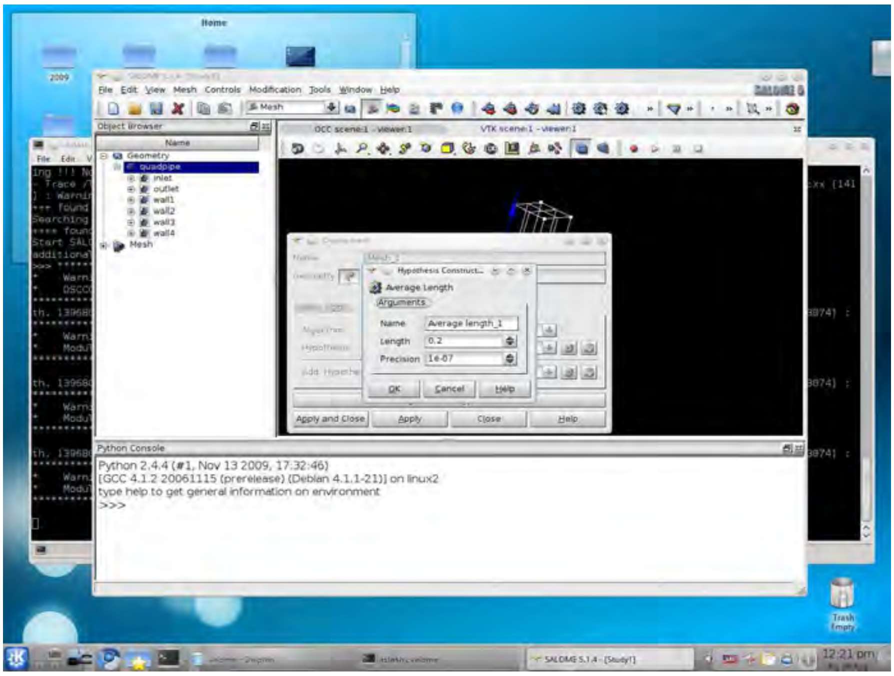
26. In the 1D tab, we select the Wire discretization algorithm.



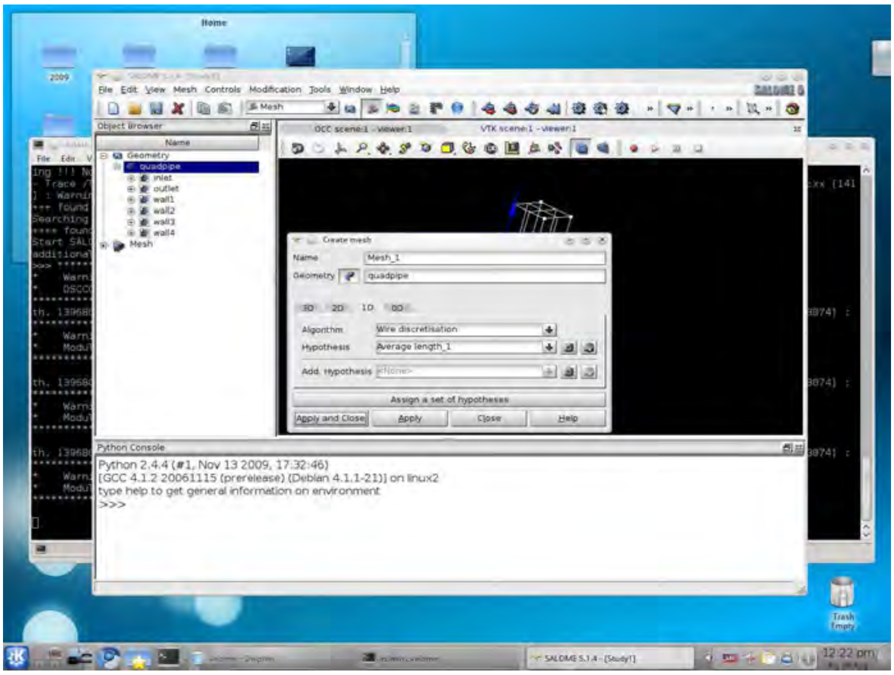
27. Clicking on the the gear icon, we can configure the selected algorithm. We choose Average length.



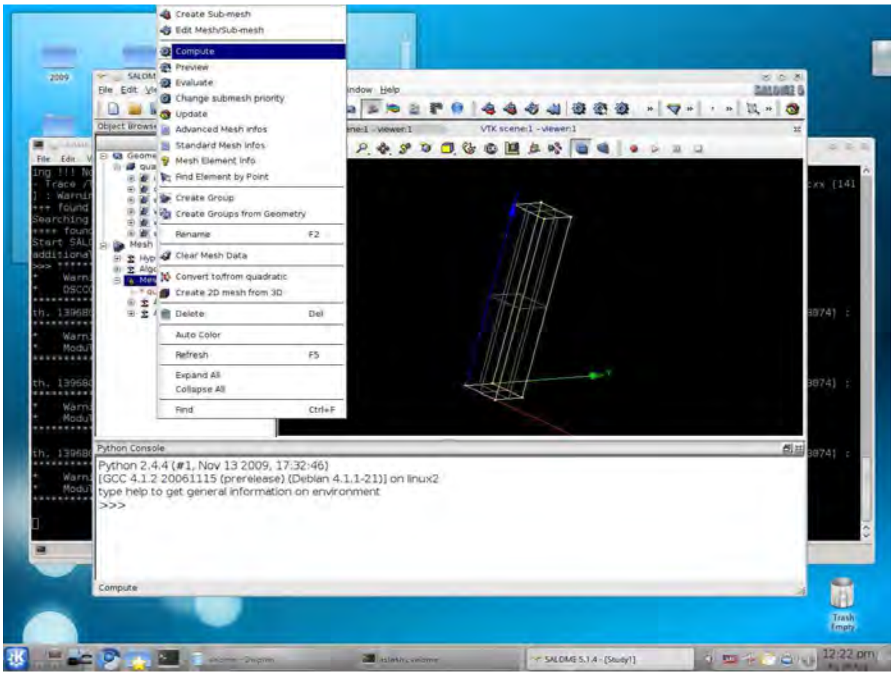
28. We set the `Length` to 0.1 and click OK.



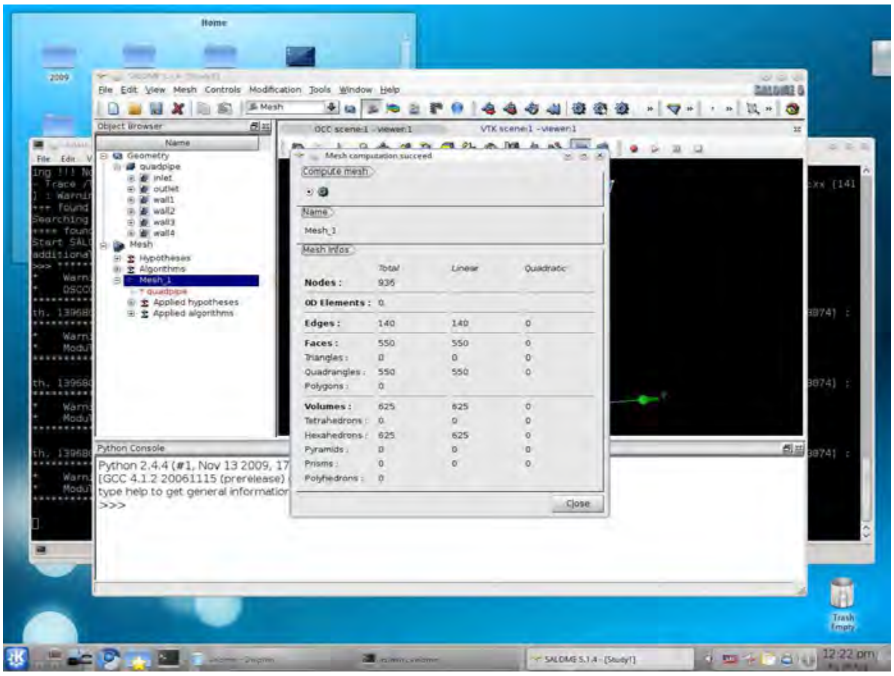
29. The mesh is now ready: we can click on Apply and Close.



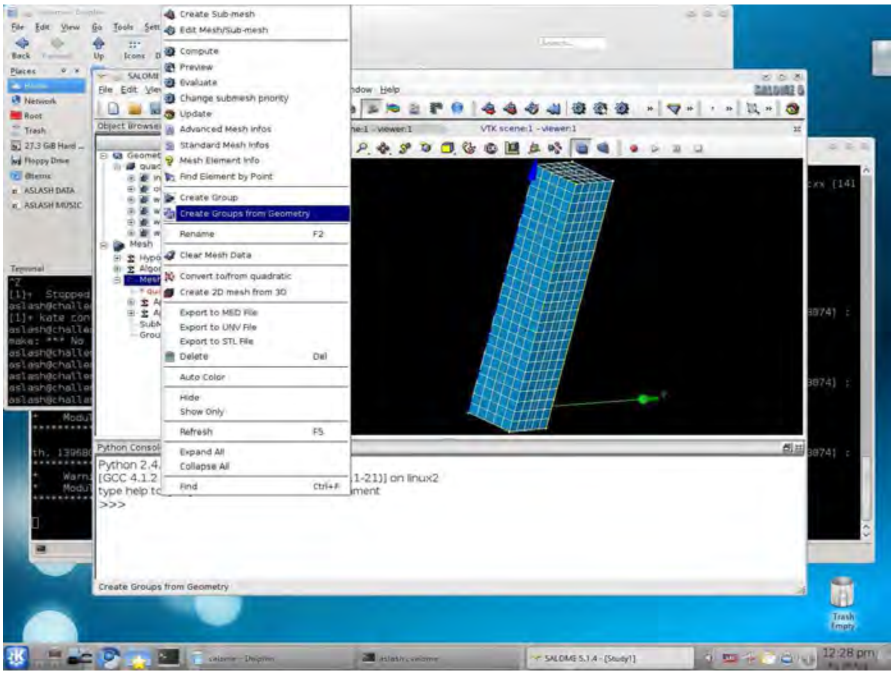
30. In order to calculate the mesh, we click the Compute button in the right-click menu of the mesh we have just created.



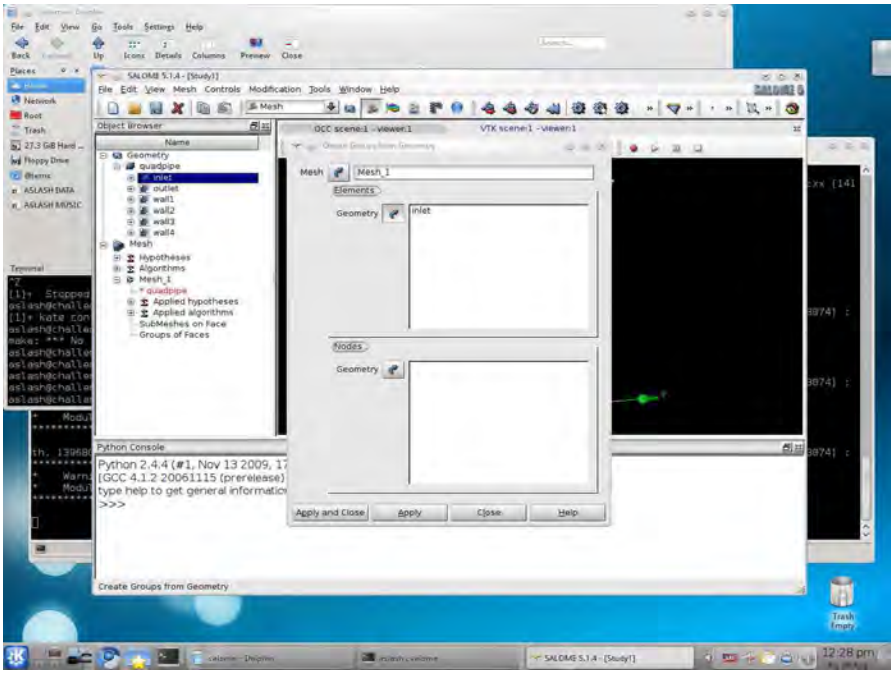
31. If everything has gone well, a summary window will appear with some details on the mesh. In particular, we have to check that there are 1D, 2D and 3D elements.



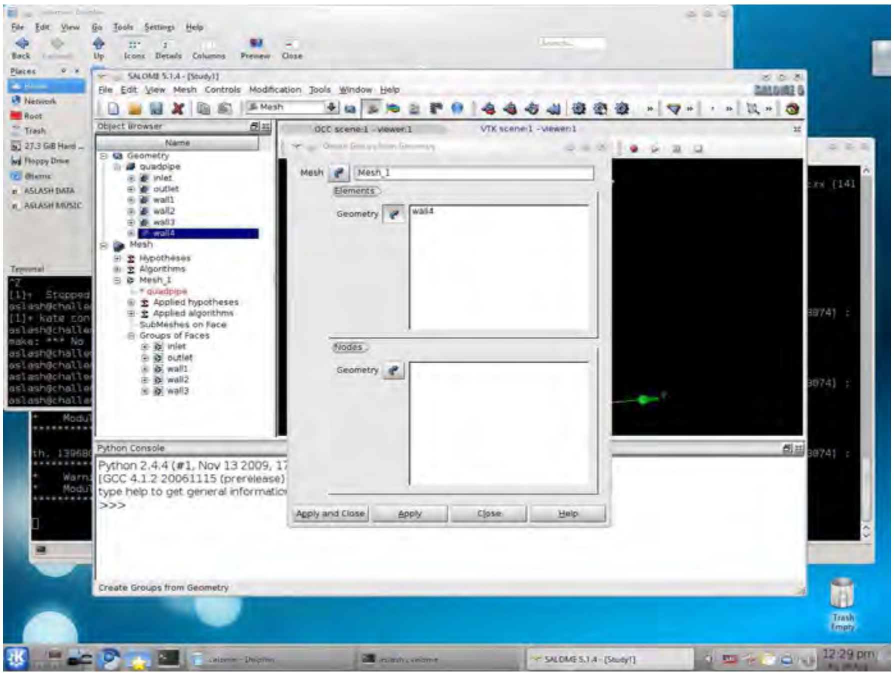
32. Now we create the sub-regions that correspond to the boundary surfaces. We select Create groups from geometry from the right-click menu of the mesh.



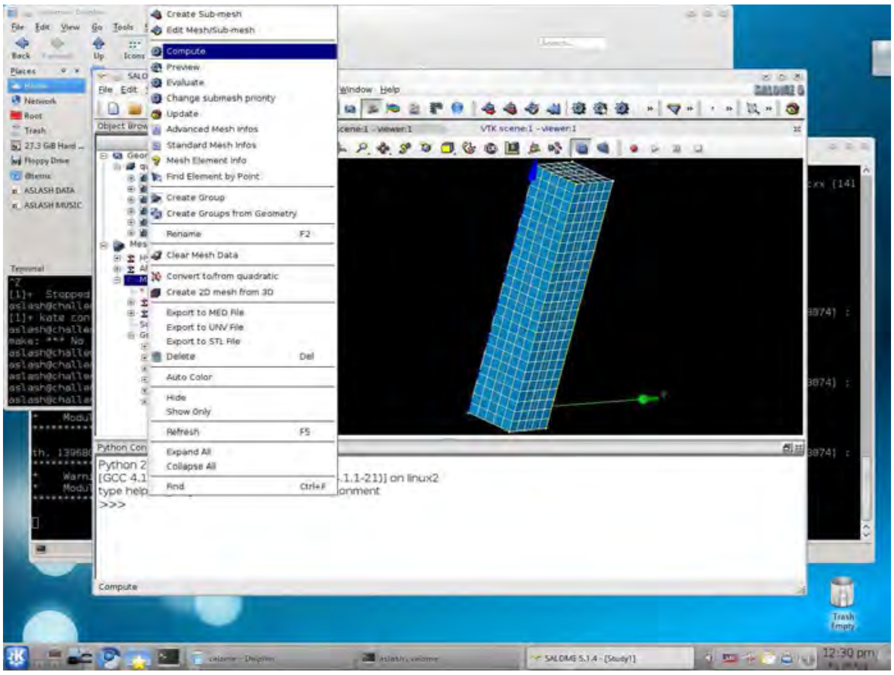
33. We select the inlet region in the left column and and click Apply.



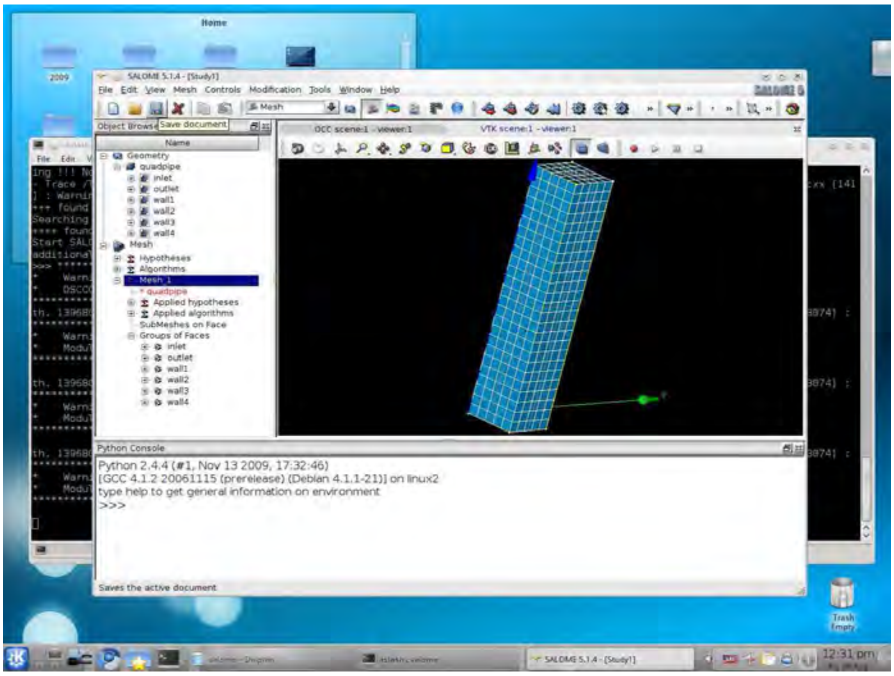
34. We create all the six regions in the same way, selecting the mesh and the geometry element and clicking Apply until we reach the last one (`wall4`).



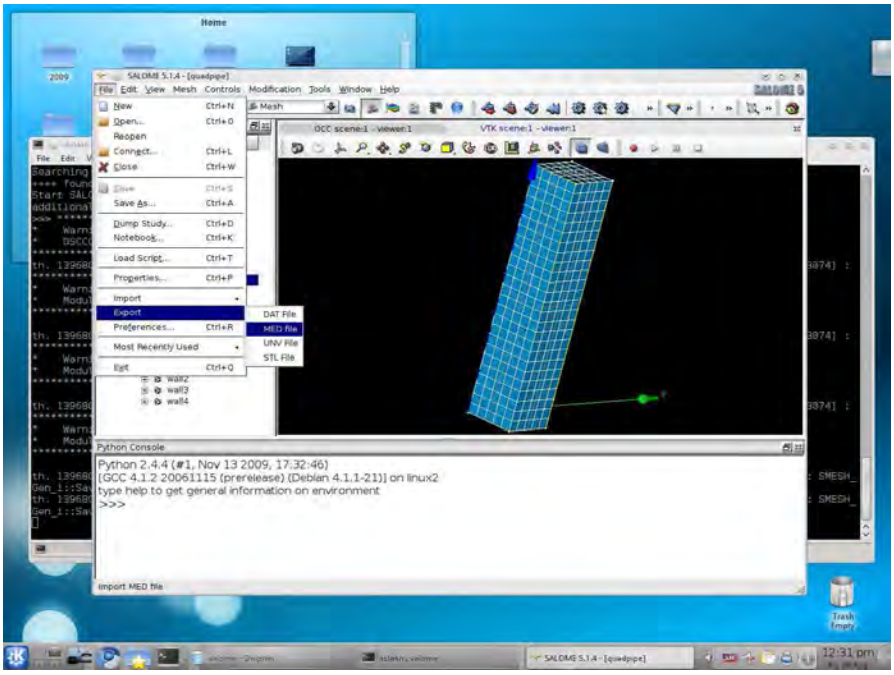
35. We recompute the mesh by clicking again Compute in order to update the mesh.



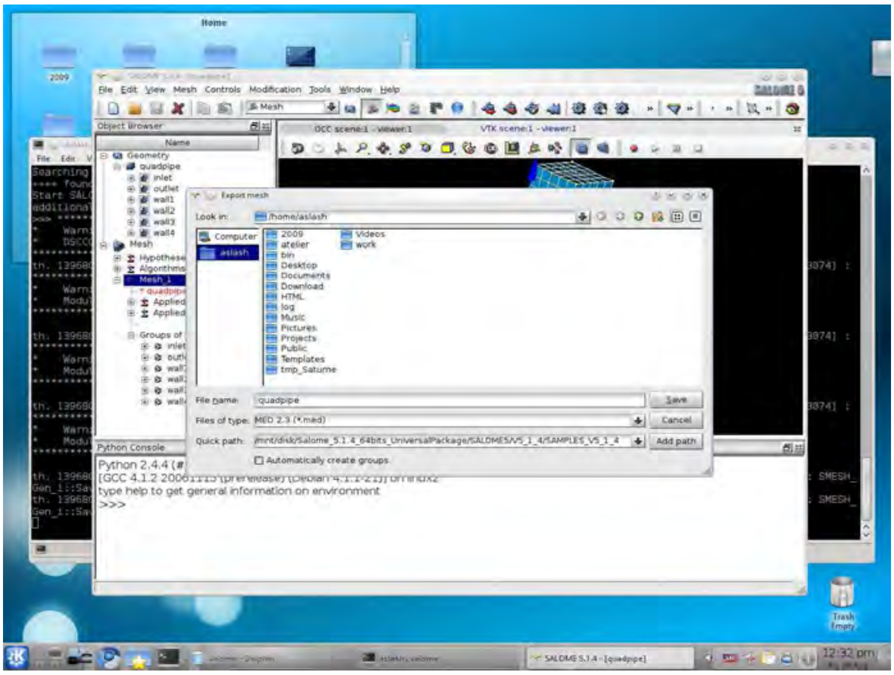
36. We can now save the SALOME study by clicking the Save button. we can name the file `quadpipe.hdf`.



37. In SATURNE we need the mesh file in MED format. We can generate it via the File -> Export -> MED menu. The mesh must be selected to perform this action.



38. We name the file `quadpipe.med`.



This is a very simple but significative example of mesh generation, since it covers all the required steps to generate a mesh with all the features needed touse it in SATURNE or NEPTUNE. For more complete examples one can follow the tutorial suggested in Sections 2.5.2. This mesh can be converted into a more popular format or used directly in many applications as, for examples, SATURNE or TRIO_U.

Chapter 3

SATURNE

3.1 Introduction

Figure 3.1: SATURNE graphical user interface.

3.1.1 Code development

Developer(s)	EDF
Stable release	2.0.0 RC2 / July 7, 2010;
Operating system	Linux and Cross-platform
License	GNU General Public License
Website	http://www.code-saturne.org

3.1.2 Location on CRESCO-ENEA GRID

CRESCO-ENEA GRID:	
executable:	`saturne`
install directory:	`/afs/enea.it/project/fissicu/soft/Saturne`

3.1.3 SATURNE overview

SATURNE is a general purpose CFD free software. Developed since 1997 at EDF R&D, SATURNE is now distributed under the GNU GPL license. It is based on a collocated Finite Volume approach that accepts meshes with any type of cell. The code works with tetrahedral, hexahedral, prismatic, pyramidal and polyhedral finite volumes and any type of grid structures such as unstructured, block structured, hybrid, conforming or with hanging node geometries.

Its basic capabilities enable the handling of either incompressible or compressible flows with or without heat transfer and turbulence. Many turbulence model are implemented such as mixing length, κ-ϵ models, κ-ω models, $v2f$, Reynolds stress models and Large Eddy Simulation (LES). Dedicated modules are available for additional physics such as radiative heat transfer, combustion (gas, coal and heavy fuel oil), magneto-hydro dynamics, compressible flows, two-phase flows (Euler-Lagrange approach with two-way coupling), extensions to specific applications (e.g. for atmospheric environment) [2, 3].

SATURNE can be coupled to the thermal software SYRTHES for conjugate heat transfer. It can also be used jointly with structural analysis software CODE_ASTER, in particular in the SALOME platform. SYRTHES and CODE_ASTER are developed by EDF and distributed under the GNU GPL license.

3.2 SATURNE dataset and mesh files

SATURNE requires a specific structure for the configuration and input files. Each simulation is denoted as *case*. One must therefore create a `case` directory and put all SATURNE simulations inside. For details on SATURNE file structure see Section 3.3.2.

SATURNE requires a dataset file (with extension `xml`) and a mesh file (with extension `med`) with the mesh geometry.

3.2.1 SATURNE mesh file

The mesh file must be in MED format. For MED format file one can see Section 1.3.1 and for mesh generation the SALOME section 2.5.

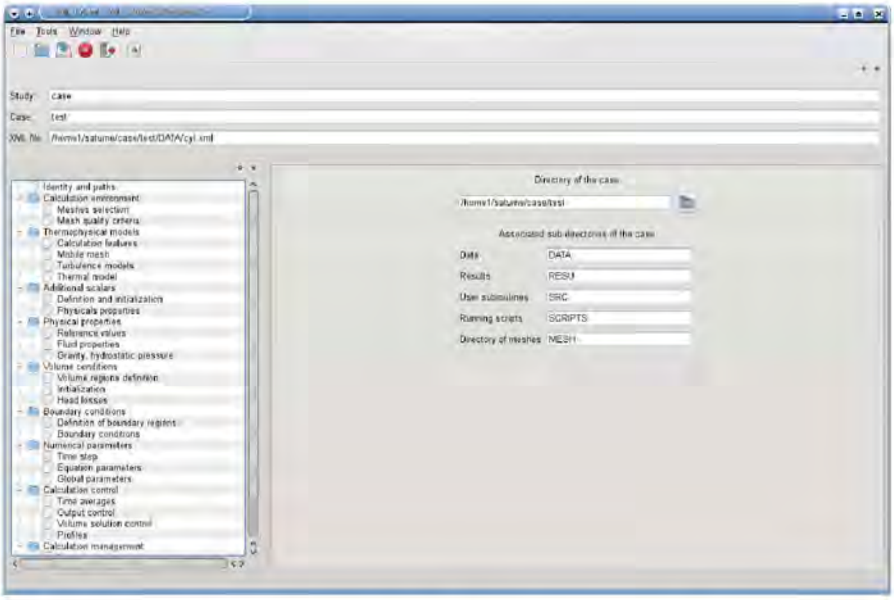


Figure 3.2: SATURNE graphical user interface.

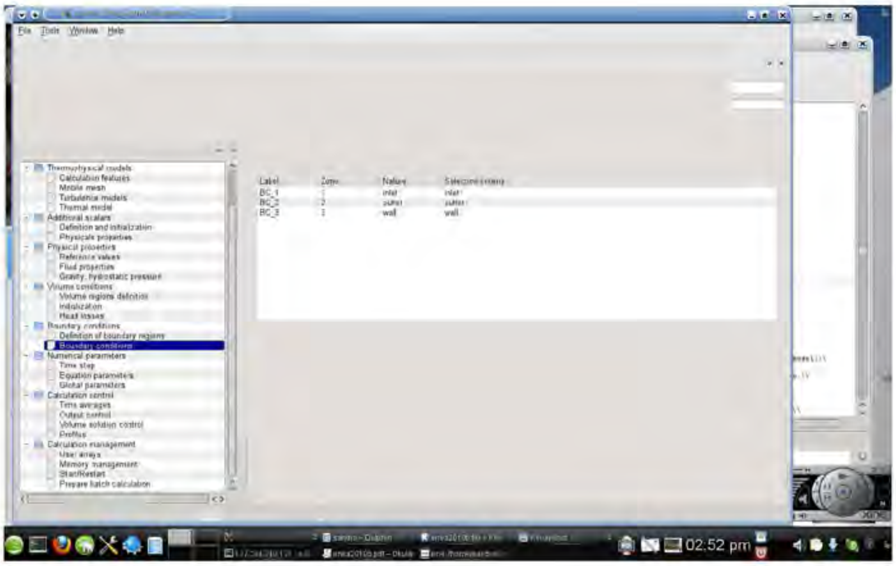


Figure 3.3: SATURNE GUI for boundary condition options.

3.2.2 SATURNE dataset file

The dataset file for the definition of the parameters is a XML file which is in the `case` directory (subdirectory DATA). There are two different ways to generate the dataset file:

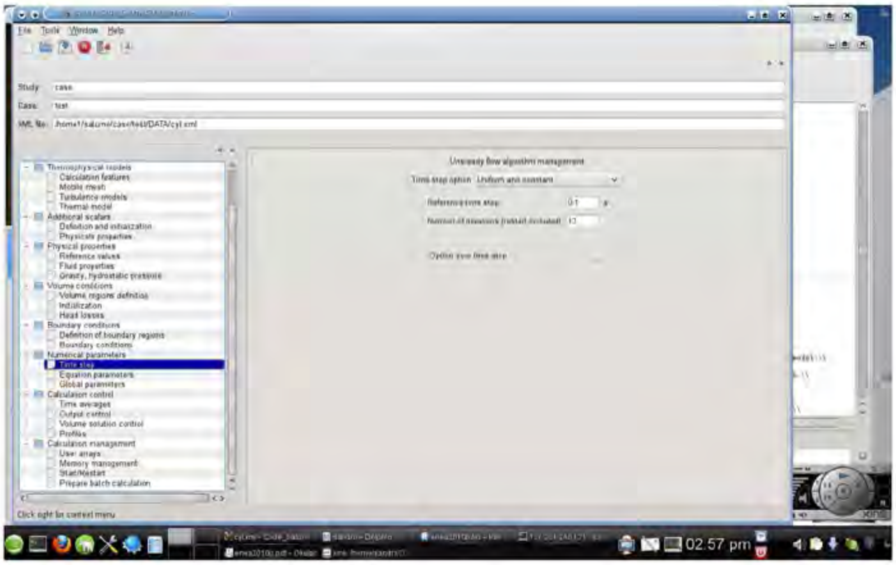


Figure 3.4: SATURNE GUI for numerical parameter option.

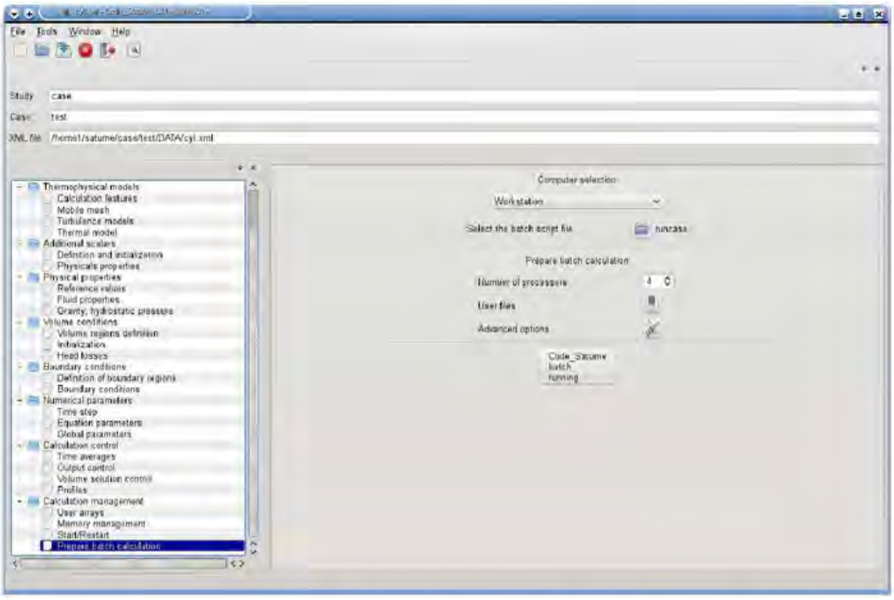


Figure 3.5: SATURNE GUI start/stop computation panel.

a) Using the SATURNE GUI
b) editing the dataset template XML file directly

The application control file consists of several sections. As shown in Figure 3.2 the

SATURNE GUI opens a window which is divided into three panels: top panel, option panel and view panel. The name of the study and the name of the dataset file with the corresponding path must be introduced in the top panel. The option panel consists of a tree menu with different sections. The sections are the following:

- `Identity and paths` where the path to the case is written;
- `Calculation environment` with mesh selection;
- `Thermophysical models` with turbulence and thermal model options;
- `Additional scalars` with the definition and initialization of physical properties;
- `Physical properties` with reference values, fluid properties, gravity and hydrostatic pressure options;
- `Volume conditions` with volume region definition and initialization;
- `Boundary conditions` with the definition of boundary regions and conditions;
- `Numerical parameters` with time step, equation parameters and global parameters;
- `Calculation control` with time average option, output control, volume solution control and output profiles;
- `Calculation management` with user arrays, memory management and start/restart options.

The mesh should be opened and checked through the section `Calculation environment`. In this section there are also some mesh quality tools. The mesh must be saved in MED format and constructed in such a way that the boundary zones are marked as special regions. These regions will appear in the `Boundary conditions` section where the boundary conditions must be defined. The SALOME GUI defines the boundary conditions as shown in Figure 3.3. The parameters as the time step length and the number of the time steps can be set in `Numerical parameters`. A screenshot of the `Numerical parameters` is shown in Figure 3.4. The computation can be started from the start/stop computation panel in the `Calculation management` section. This panel appears in Figure 3.5 where the number of processors can be set. For more details one can see the example in Section 3.4 or the documentation of the SATURNE code. The SATURNE GUI generates a dataset file like the following:

```
<?xml version="1.0" encoding="utf-8"?>
<Code_Saturne_GUI case="cyl" study="case" version="2.0">
<solution_domain>
           ...........
<meshes_list>
<mesh format="med" name="cyl1.med" num="1"/>
```

```
</meshes_list>
    .......
</solution_domain>
<thermophysical_models>
<velocity_pressure>
<variable label="Pressure" name="pressure">
<reference_pressure>101325</reference_pressure>
</variable>
      ..............
</thermophysical_models>
<numerical_parameters>
<multigrid status="on"/>
<gradient_transposed status="on"/>
<velocity_pressure_coupling status="off"/>
<pressure_relaxation>1</pressure_relaxation>
<wall_pressure_extrapolation>0</wall_pressure_extrapolation>
<gradient_reconstruction choice="0"/>
</numerical_parameters>
<physical_properties>
<fluid_properties>
<property choice="constant" label="Density" name="density">
<initial_value>1</initial_value>
<listing_printing status="off"/>
<postprocessing_recording status="off"/>
</property>
             .............
</fluid_properties>
            ..........
</physical_properties>
<boundary_conditions>
<variable/>
<boundary label="BC_1" name="1" nature="inlet">inlet</boundary>
            ...........
</boundary_conditions>
<analysis_control>
<output>
<postprocessing_mesh_options choice="0"/>
           .............
</output>
<time_parameters>
<time_step_ref>0.01</time_step_ref>
<iterations>100</iterations>
<time_passing>0</time_passing>
```

```
<zero_time_step status="off"/>
</time_parameters>
<time_averages/>
<profiles/>
</analysis_control>
<calcul_management>
           ..............
</calcul_management>
<lagrangian model="off"/>
</Code_Saturne_GUI>
```

This file can also be modified without the GUI by editing a template dataset XML file. The file is subdivided into various sections such as `Calculation environment`, `Thermophysical models`, `Additional scalars`, `Boundary conditions`, `Numerical parameters` and `Calculation management`. Inside each section we can see the corresponding options.

3.3 SATURNE on CRESCO-ENEA GRID

3.3.1 Graphical interface

The SATURNE code is located on CRESCO-ENEA GRID in the directory

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

Once the `PATH` is set for the directory

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

by executing the script

`$ source pathbin.sh`

as it is explained in Section 1.2.3, the SATURNE GUI starts with the command

`$ saturne`

Remark. Not all libraries are yet available at the moment for the CRESCO architecture. We suggest to run SATURNE GUI on a personal workstation.

The GUI is used to set up the simulation creating a `data.xml` file. The solution of the case must be run in command line mode or in batch mode as explained in the next section.

3.3.2 Data structure

SATURNE requires a specific structure for the configuration and input files. Each simulation is denoted as *case*. We can therefore create a `cases` directory and put all SATURNE simulation files inside.

Inside this directory, each case will have its own directory (for example `case1`, `case2`) and there must be a `MESH` directory, where all the meshes are stored.

```
cases
+-- case1
+-- case2
...
+-- MESH
```

Inside each case directory, we have to create the four sub-directories

- `DATA`, where the xml configuration file is stored;
- `RESU`, that is used for the outputs;
- `SCRIPTS`, that hosts the execution scripts;
- `SRC`, in which we can put some additional source file.

During the execution, SATURNE will generate some temporary files that are by default stored in the `tmp_Saturne` directory in the user home directory. This directory must be periodically cleaned by hand, as there is no automatic procedure.

3.3.3 Command line execution

In order to execute the application in a shell we must first set up the environment using the script

```
saturne_env
```

that is located in the directory

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

Remark. The `saturne_env` script consists of the following lines

```
#! /bin/bash
export cspath= \
 /afs/enea.it/project/fissicu/soft/Saturne/2.0rc1/cs-2.0-beta2/bin
export CSMPI=$cspath/../../openmpi-1.4.1/bin
export PATH=$cspath:$PATH
```

In order to run a case one must first create a directory and put the following files in it:

- `data.xml` that is the configuration file of the case
- `mesh.med` that is the mesh file (in MED format)

There are two ways to run the code:
a) from console
b) using the `runcase` script

From console there are two steps to follow:
1) preprocess the mesh with the command

```
$ cs_preprocess --mesh mesh.med --case data.xml
```

This command generates the file

```
preprocessor_output
```

where all the informations of the mesh are stored.
2) run the application with
- serial mode

```
$ cs_solver --log 0 --param data.xml
```

- parallel model

```
$ $CSMPI/mpirun -np NPROC cs_solver --log 0 --param data.xml --mpi
```

where `$CSMPI` is defined in the `saturne_env` script. `NPROC` defines the number of processors used.

To use the `runcase` file, one starts from a template available inside the directory

```
/afs/enea.it/project/fissicu/soft/Saturne/data
```

There are two templates, one to be launched from the GUI interface (`runcase`) and another for console execution (`runcase_sh`). The runcase for the GUI takes into account the data structure explained in Section 3.3.2 while the `runcase_sh` needs only the data and the mesh file in the current directory just like we have seen above for console running.

3.3.4 Batch running

This is the template file for queue submission using LSF on CRESCO-ENEA GRID:

```
#!/bin/bash
#BSUB -J JOBNAME
#BSUB -n NPROC
#BSUB -oo stdout_file
#BSUB -eo errout_file
saturne_env
cs_solver --log 0 --param data.xml
```

where the options `-J` sets the job name, `-n` the number of processors, `-oo` the file for the standard output and `-eo` the error output. The last two lines set the environment variables for the code SATURNE and launch the executable with a parameter file, without the graphical interface that clearly cannot be used when submitting a job with a batch queue. This template is located at

```
/afs/enea.it/project/fissicu/soft/Saturne/data/saturne.lsf
```

Once the script is ready the command

Property	Value
Density [kg/m^3]	10340
Viscosity [Pa · s]	0.00184
Specific heat [J/KgK]	145.75
Thermal conductivity [W/mK]	11.732
Inlet Temperature [K]	673.15
Inlet Velocity [m/s]	0.01

Table 3.1: Physical properties and operating conditions for the SATURNE tutorial.

```
$ bsub < saturne.lsf
```

starts the batch execution.

When one uses the `runcase` script the LSF options are already placed at the beginning of the script. There is a space between the `#` and `BSUB` to be erased. In this case the batch run is started with the command

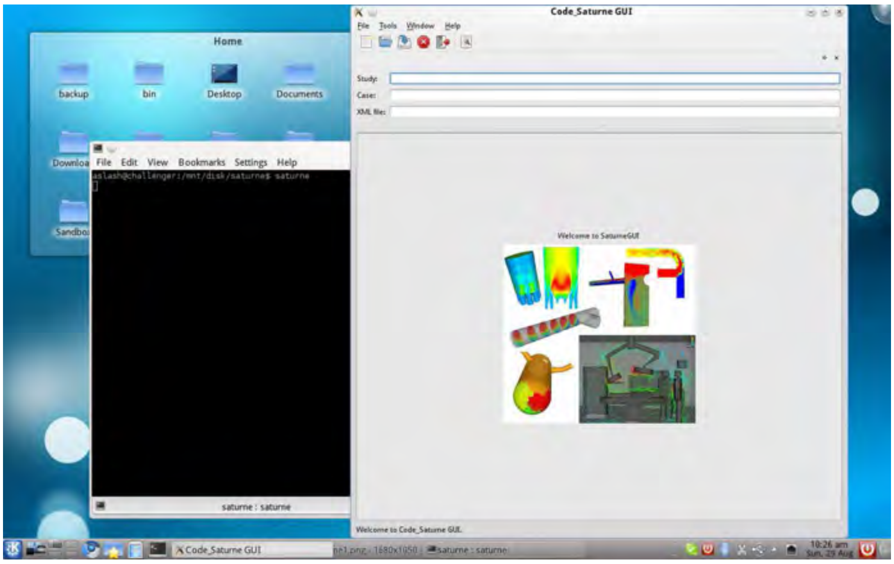
```
$ bsub < runcase
```

Further informations on batch commands are available in Section 1.2.4.

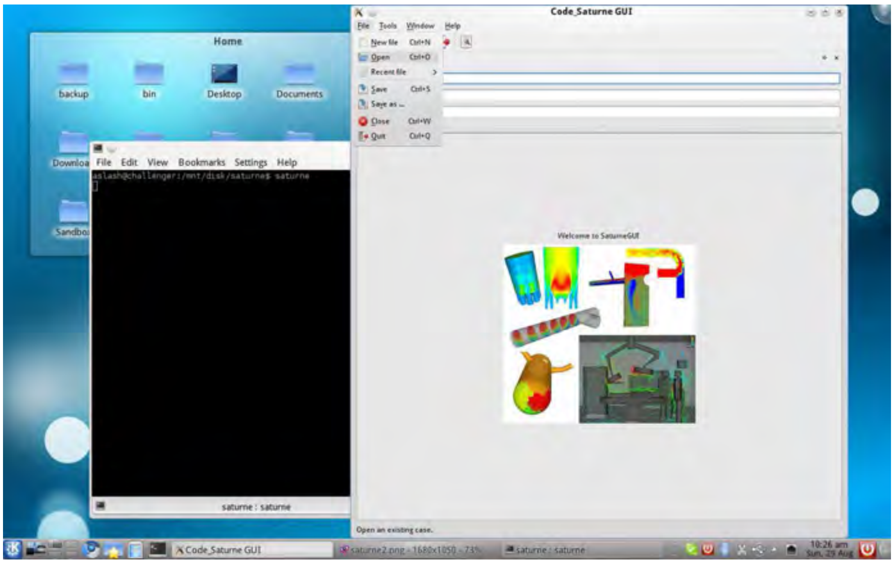
3.4 SATURNE tutorial: a simple heated channel test

In this tutorial we will study a square pipe with one heated surface. The fluid is lead, with the physical properties and operating conditions of Tab. 3.1. The mesh has been created with SALOME in Sec. 2.5. In order to configure the simulation, we will start from a simple template that we have already put in the `DATA` directory, along with the generic `runcase` script in the `SCRIPTS` directory.

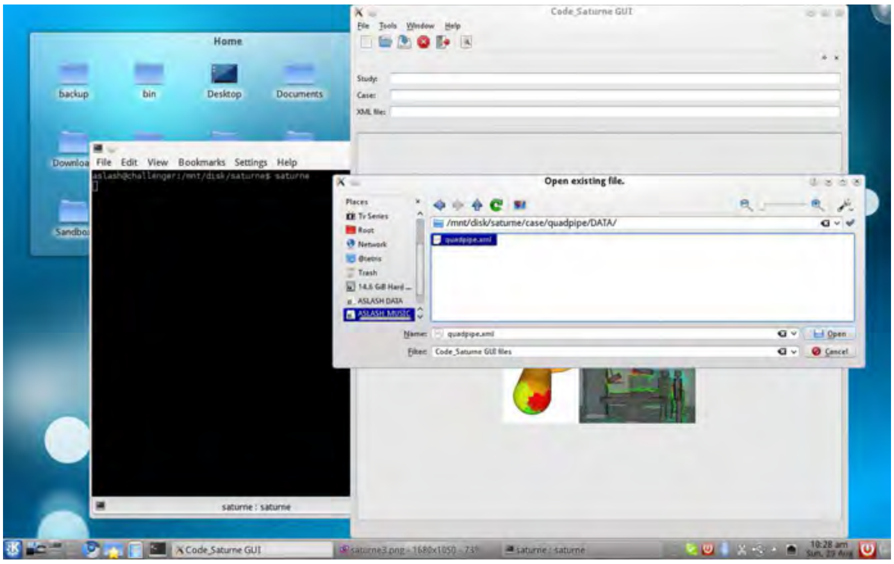
1. Run `saturne` from command line



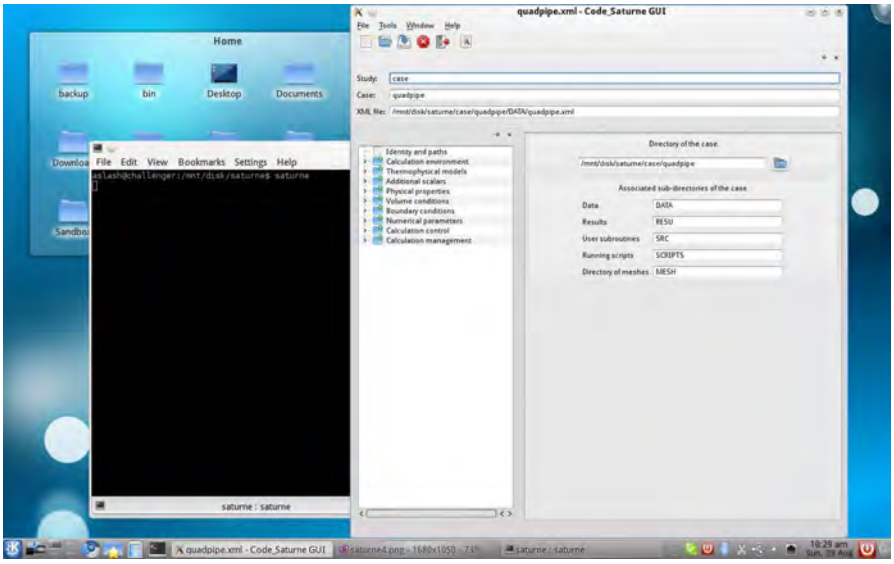
2. Click the Open button, or go to the File menu and click Open



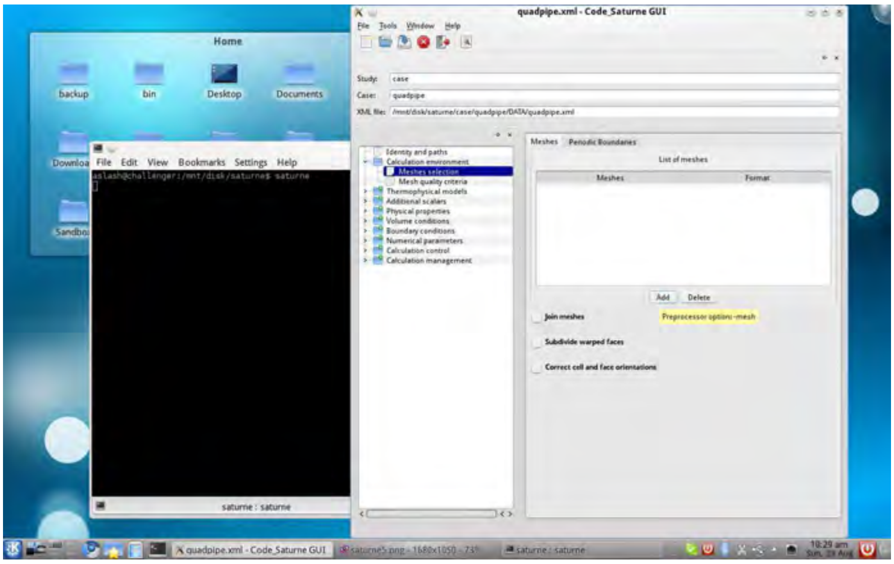
3. Browse to the case directory, and then inside the `DATA` sub-directory. In this example, the case is named `quadpipe`. Select the xml file (here `quadpipe.xml`) and click Open.



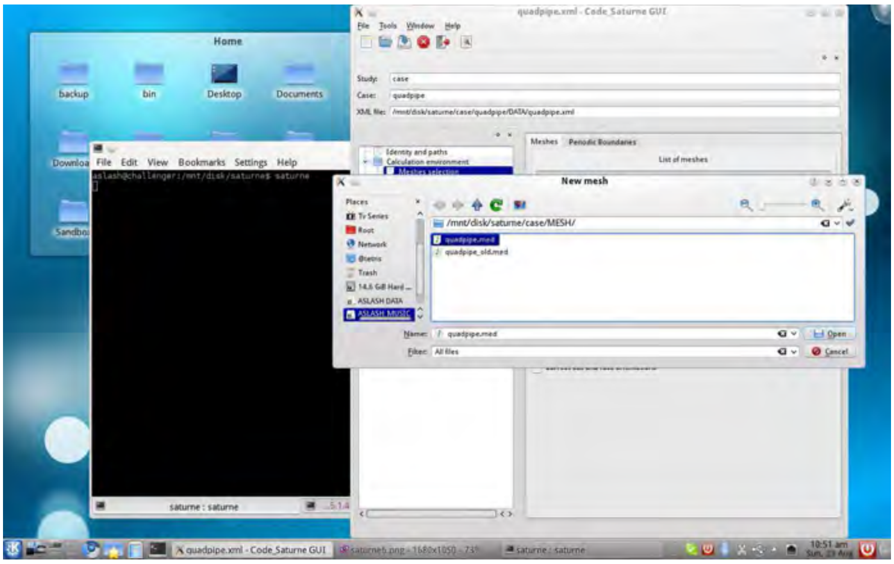
4. We can check that the directory structure has been created correctly. If some directory is missing, it will be displayed in red. We can adjust the directory structure and start again.



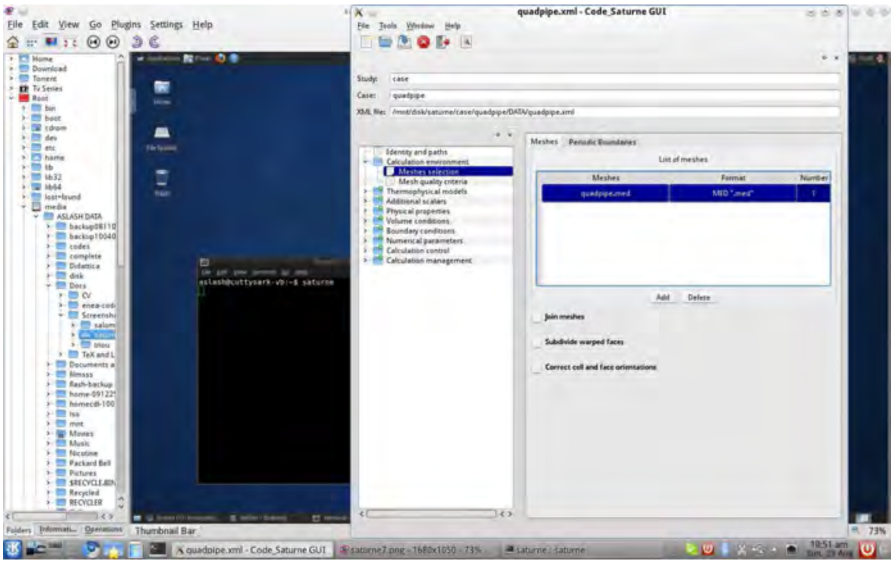
5. The configuration is subdivided in multiple directories. The first one is the Calculation environment, that includes the Meshes selection and Mesh quality criteria tabs. We select the first one. In here, we will find the list of meshes selected for the simulation. We can add a new mesh with the Add button.



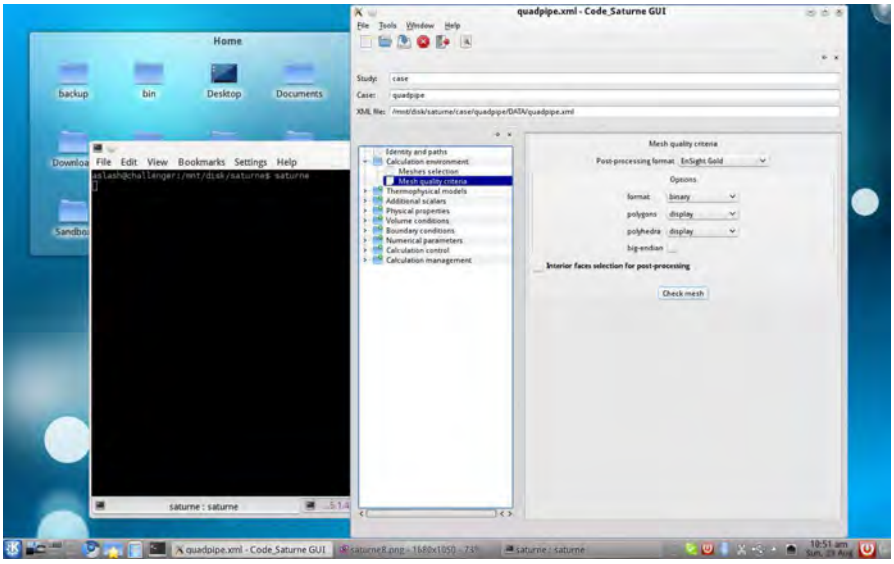
6. We select the quadpipe.med mesh created in Sec. 2.5.



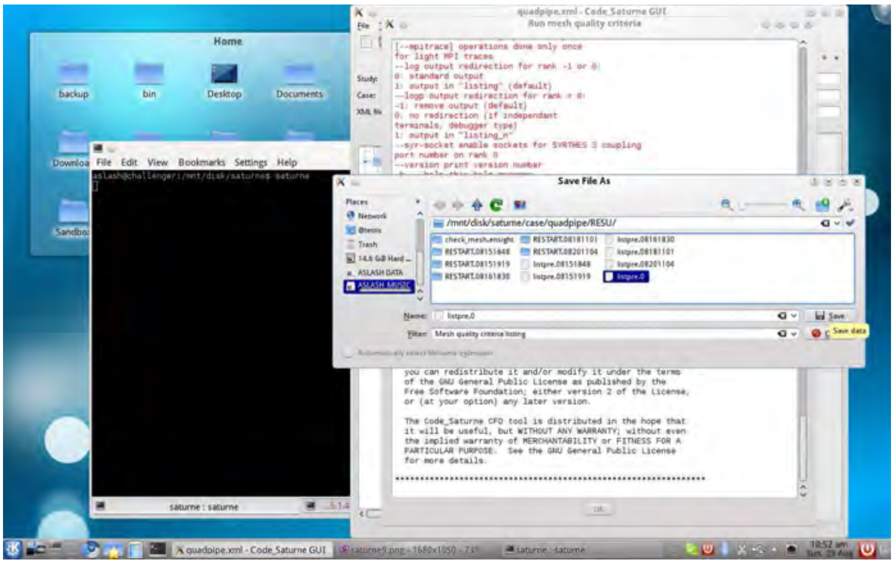
7. The mesh must appear in the list with the right format.



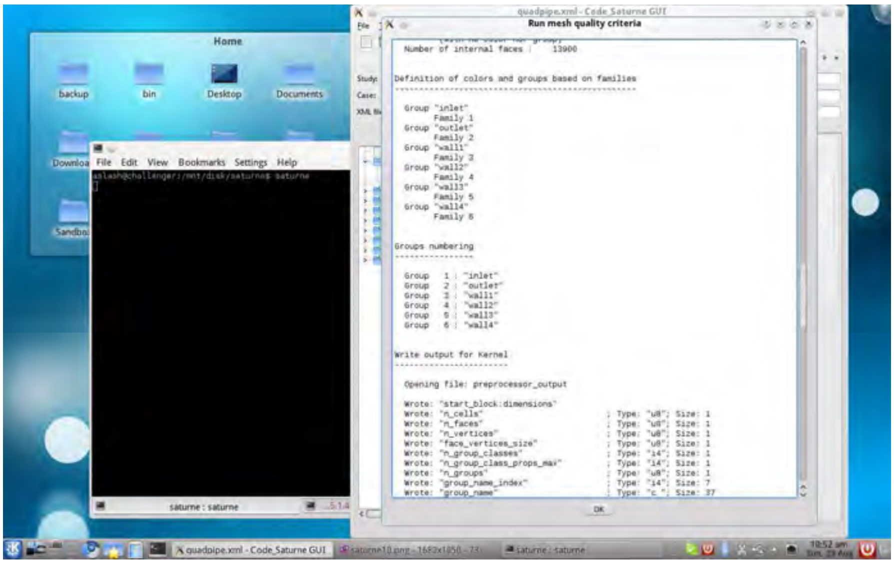
8. In the Mesh quality criteria we can check if the mesh has been recognized correctly with the Check Mesh button.



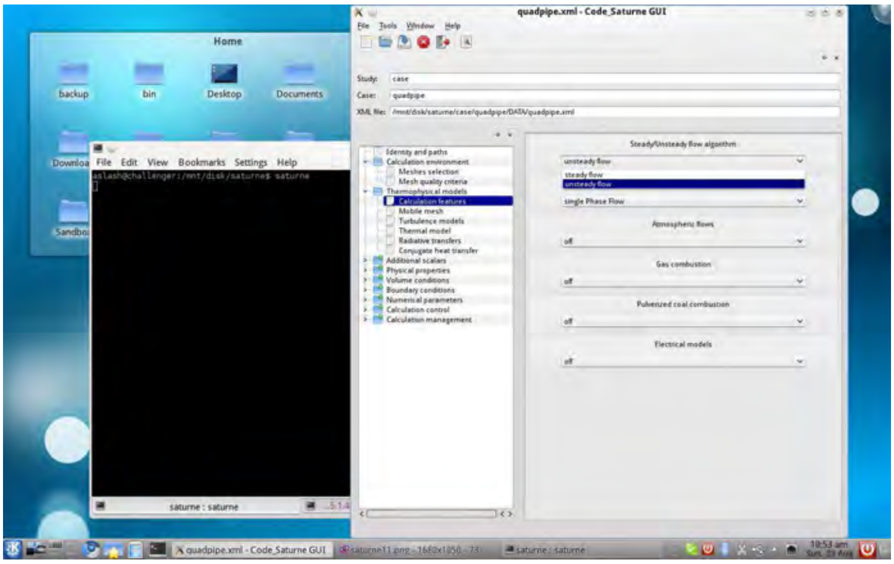
9. If we are asked to save the log file, it means that the check was successful. We can use `listpre.0` as filename.



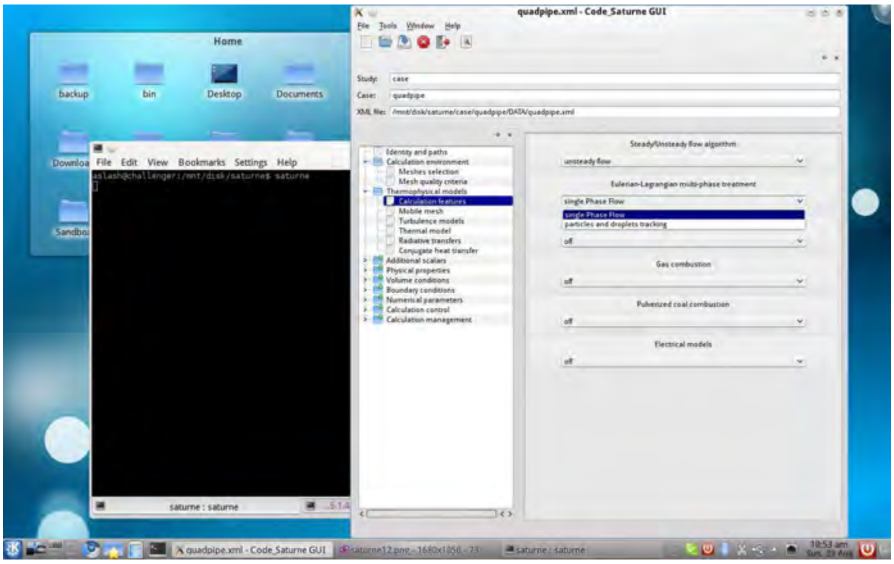
10. After the saving, we can check the log to see if all the data are correct (see the file `preprocessor_output` Section 3.3.3)



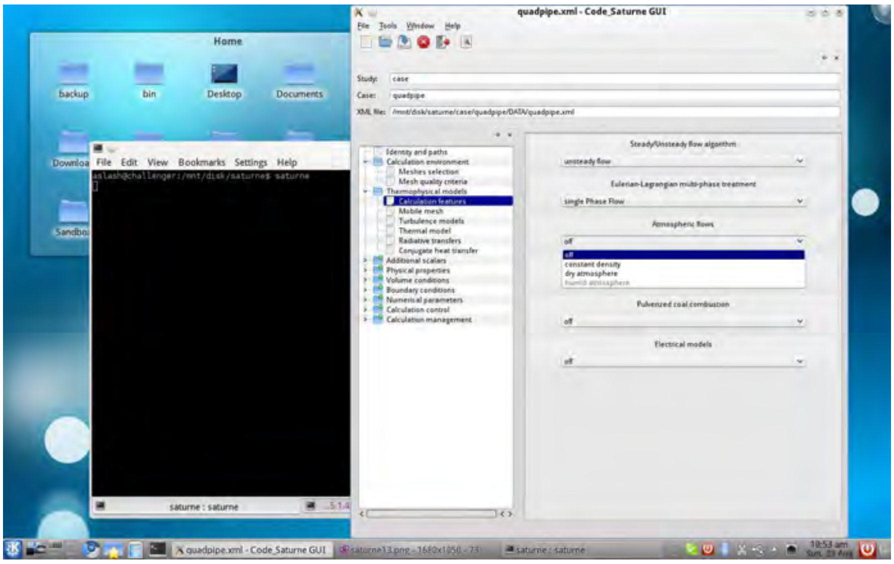
11. We go to the $\boxed{\textsf{Thermophysical properties}}$ directory. The first tab is $\boxed{\textsf{Calculation features}}$. We select in the first menu $\boxed{\textsf{Unsteady flow}}$.



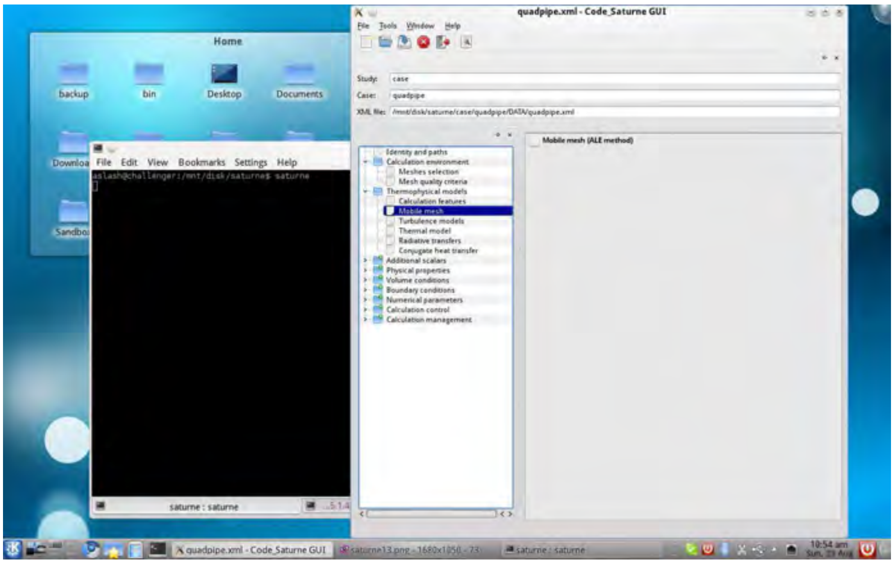
12. We select $\boxed{\textsf{Single phase}}$ flow in the second menu.



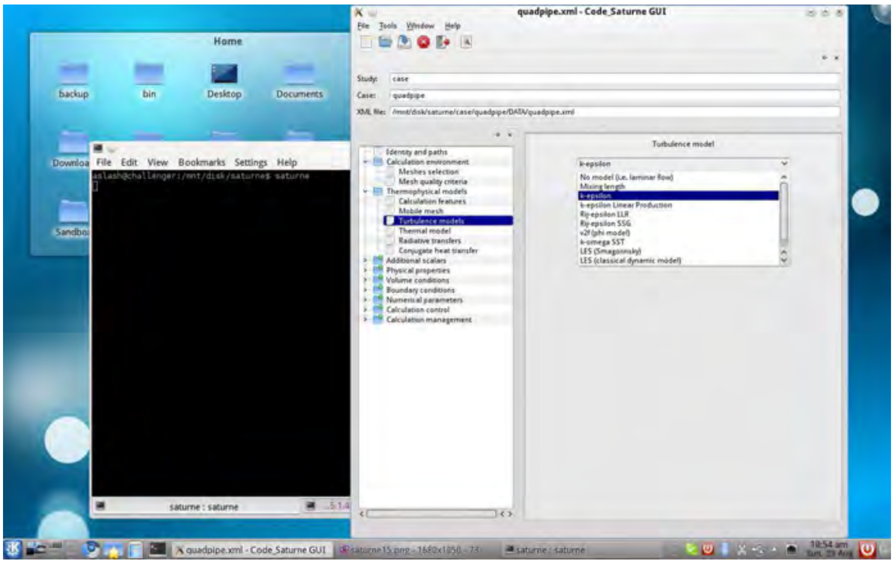
13. We check that the $\boxed{\text{Atmospheric flows}}$ is set to off.



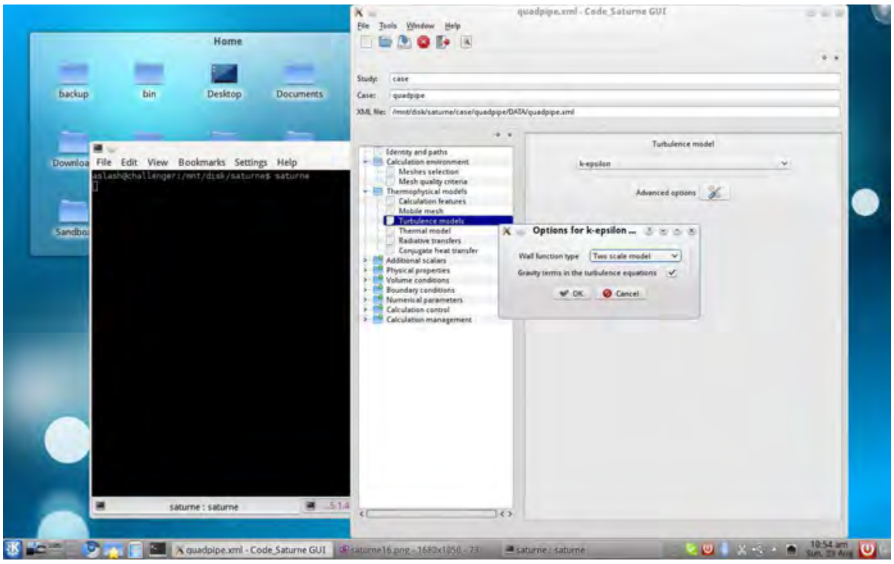
14. In the $\boxed{\text{Mobile mesh}}$ tab, we check that the $\boxed{\text{ALE method}}$ is not checked.



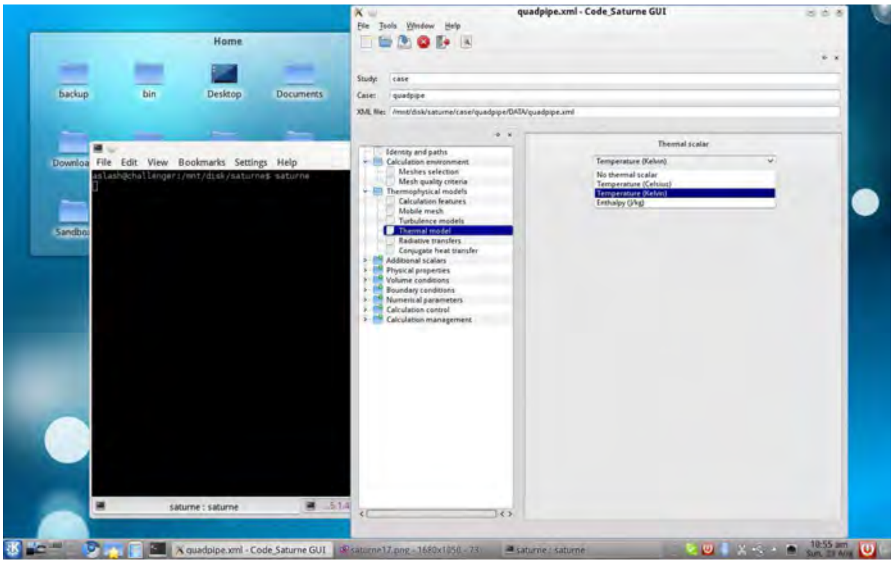
15. In the Turbulence models tab, we select the k-epsilon model.



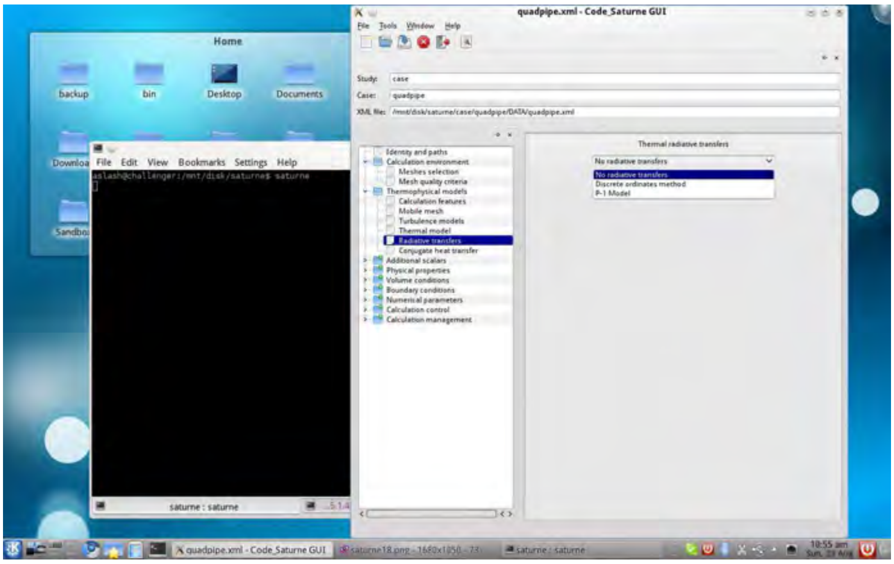
16. In the Advanced options panel, we select the Two scale model.



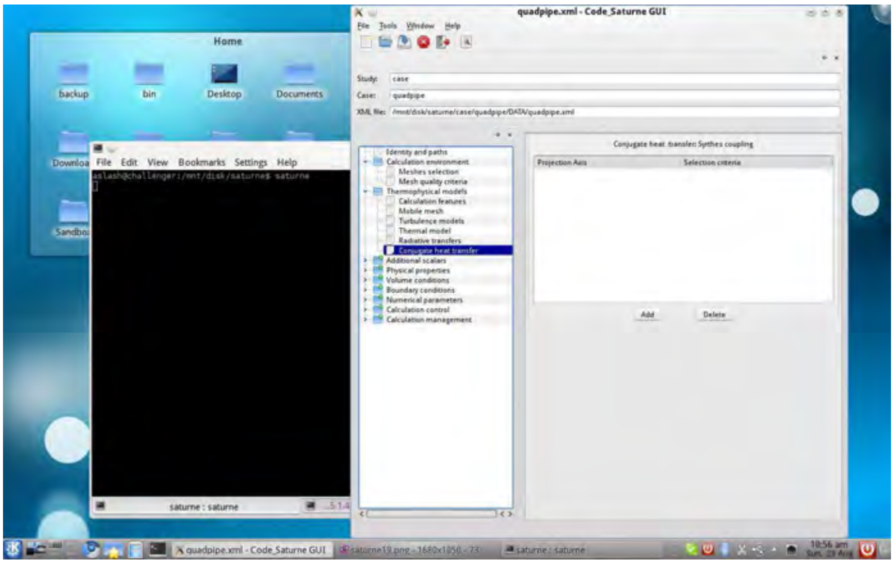
17. In the Thermal model tab, we select the Temperature (Kelvin) option.



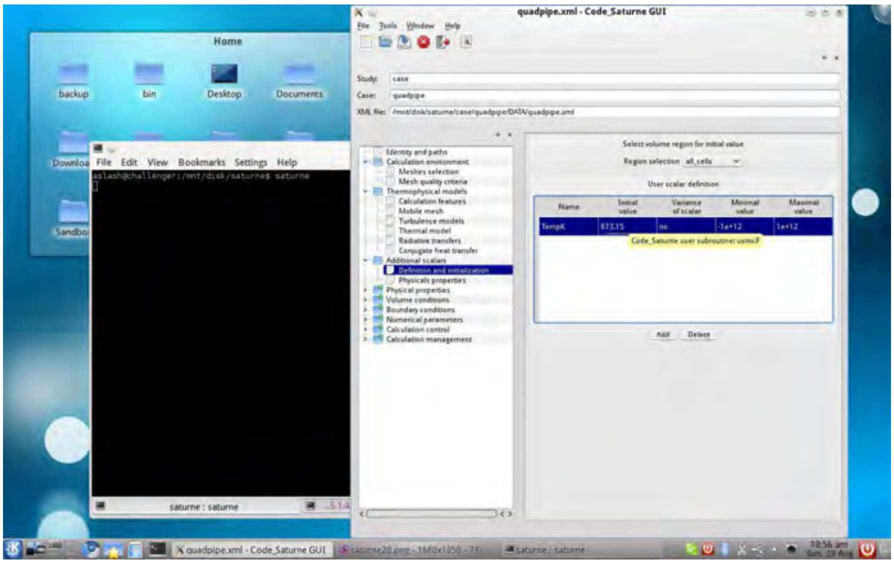
18. In the Radiative transfers tab, we select the No radiative transfers option.



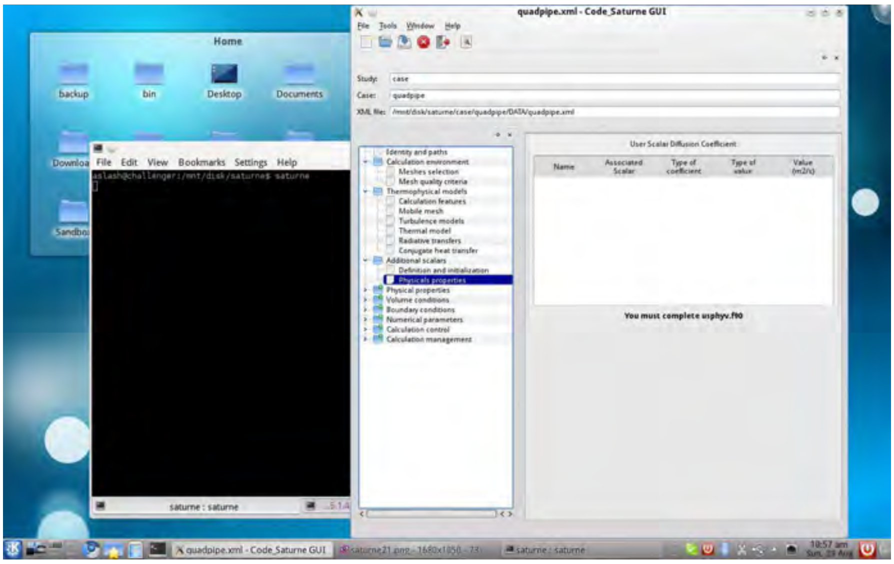
19. We check that in the Conjugate heat transfer tab the list is empty. This tab is used to couple SATURNE with the Syrthes code for heat transfer in solids.



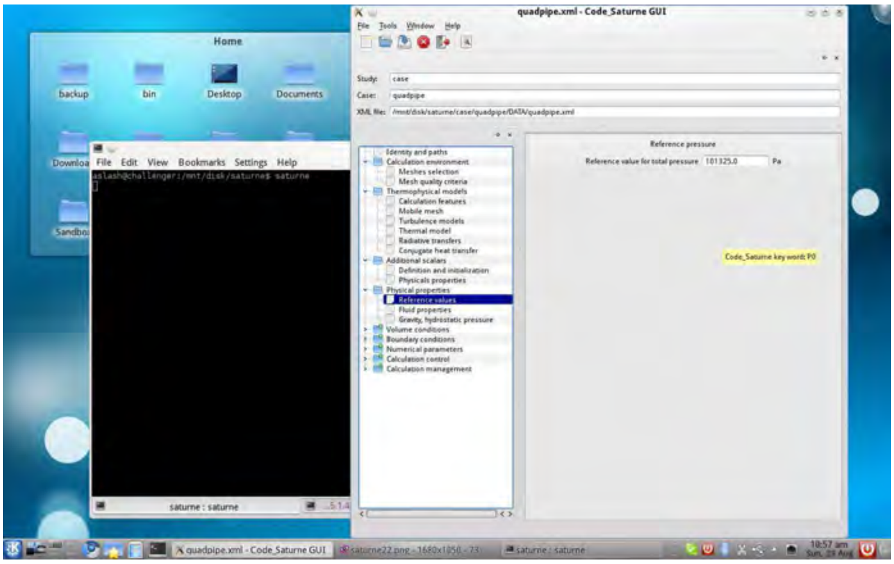
20. We go to the Additional scalars directory. The first tab is Definition and initialization, where we set the Temperature initial value at 673.15, as in Tab. 3.1.



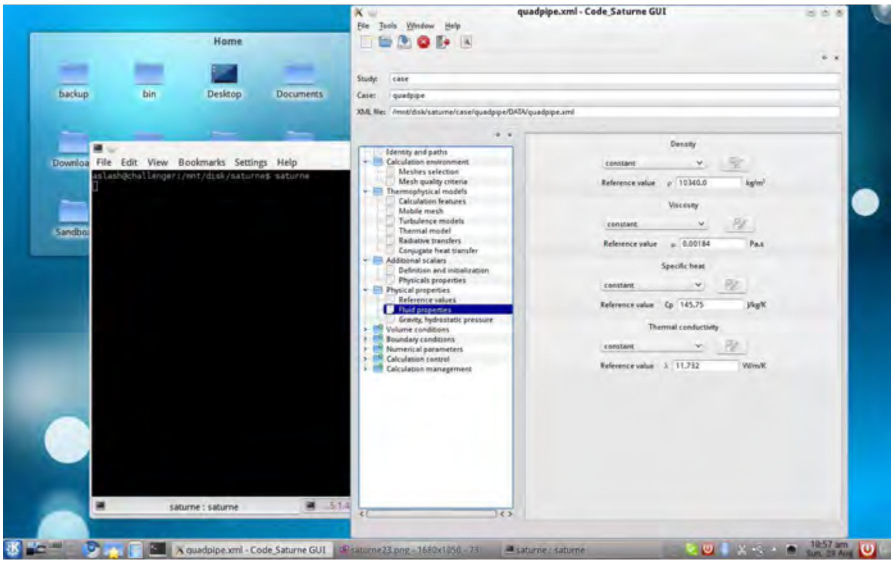
21. In the Physical properties tab, the list must be empty.



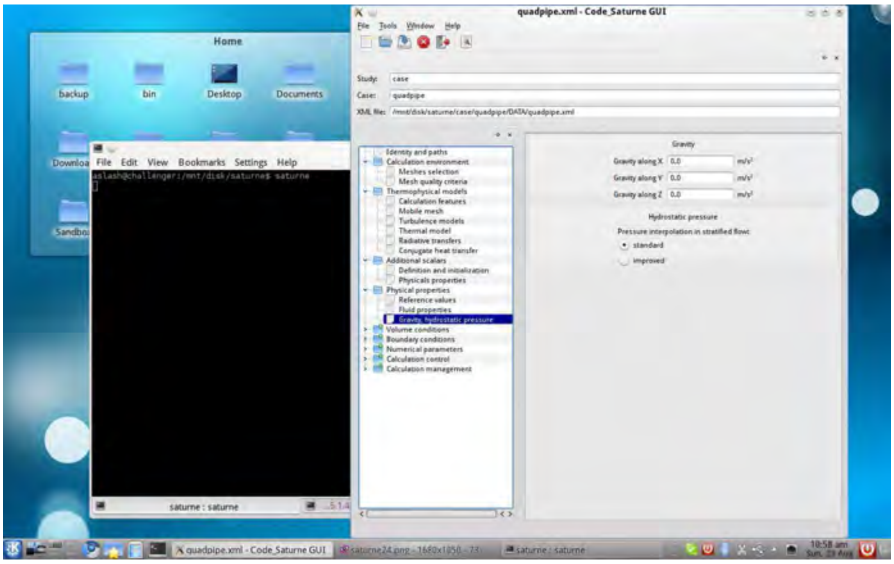
22. The Reference values tab in the Physical properties directory is used to set the reference pressure. We keep the default value (atmospheric pressure).



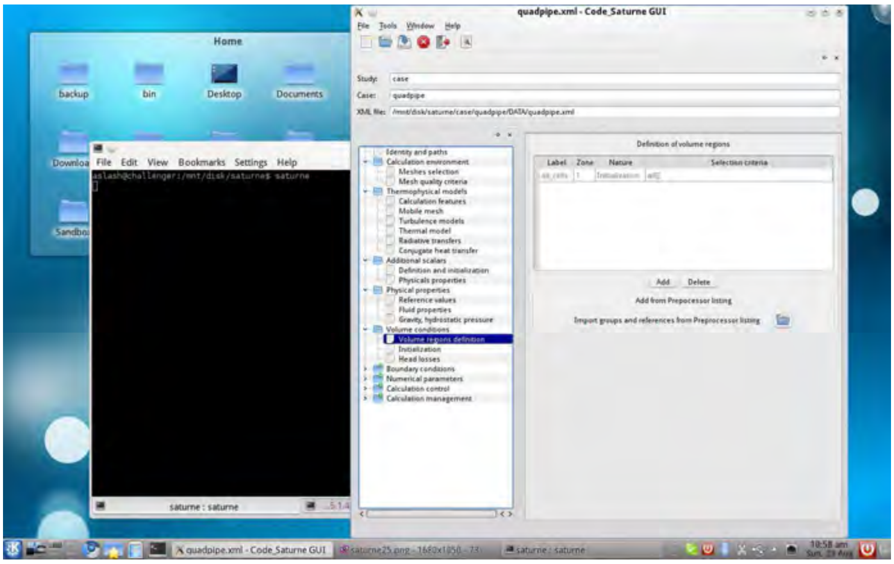
23. In the Fluid properties tab, we set the values from Tab. 3.1. The constant option means that the properties do not depend on temperature.



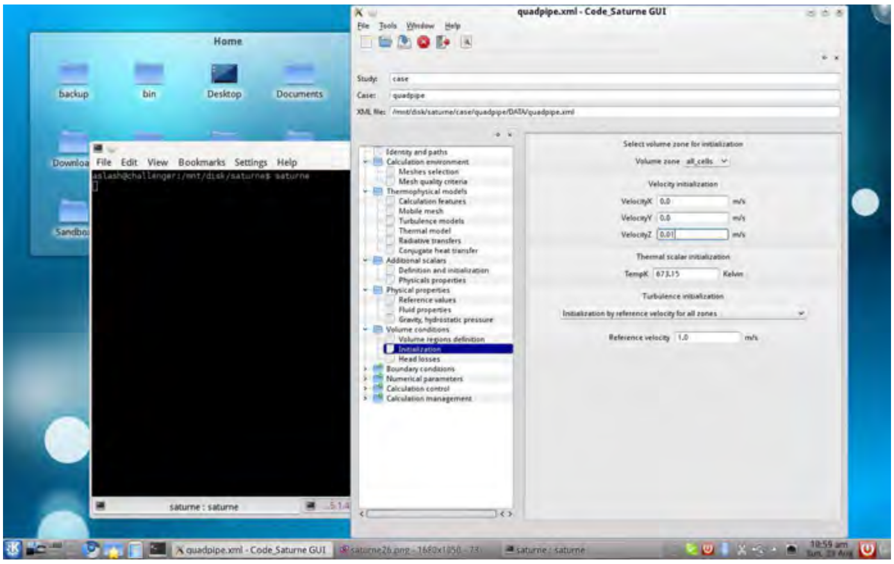
24. In the Gravity, hydrostatic pressure tab we set to 0 all gravity components.



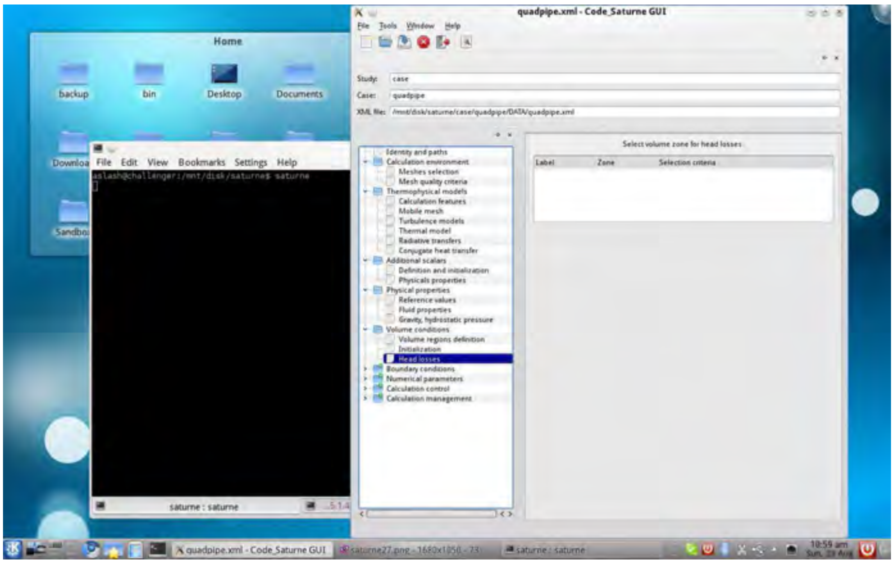
25. We go to the Volume conditions directory, Volume and regions definition tab. The list must contain only one region labeled `all_cells`.



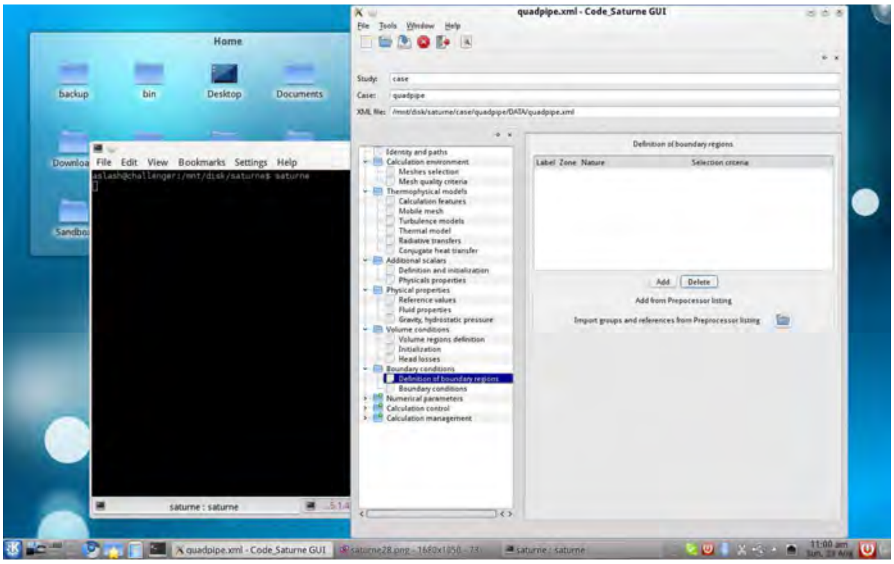
26. In the Initialization tab, we set the z-component of the velocity to 0.01. The temperature value should be already set to the 673.15 value. For turbulence, we select
initialization by reference velocity for all zones, with a velocity value of 0.01.



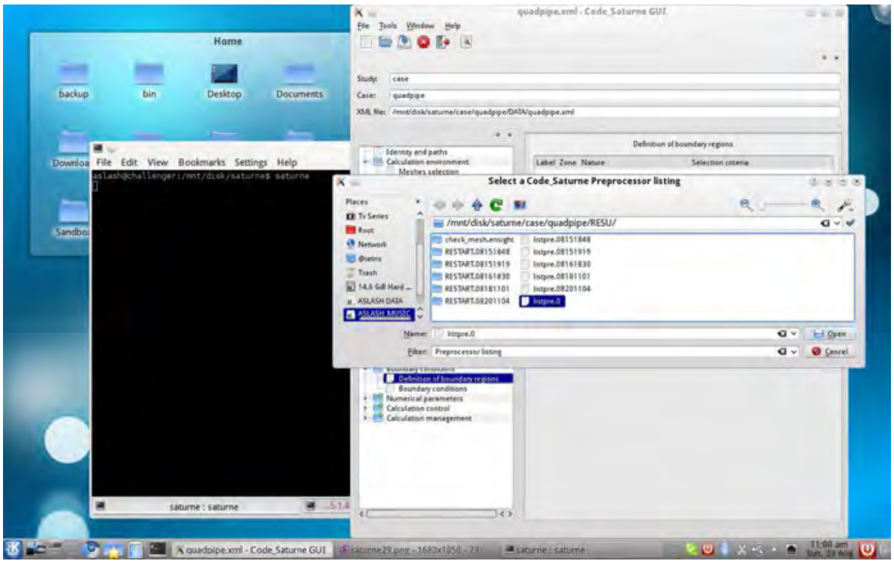
27. In the Head losses tab, the list must be empty.



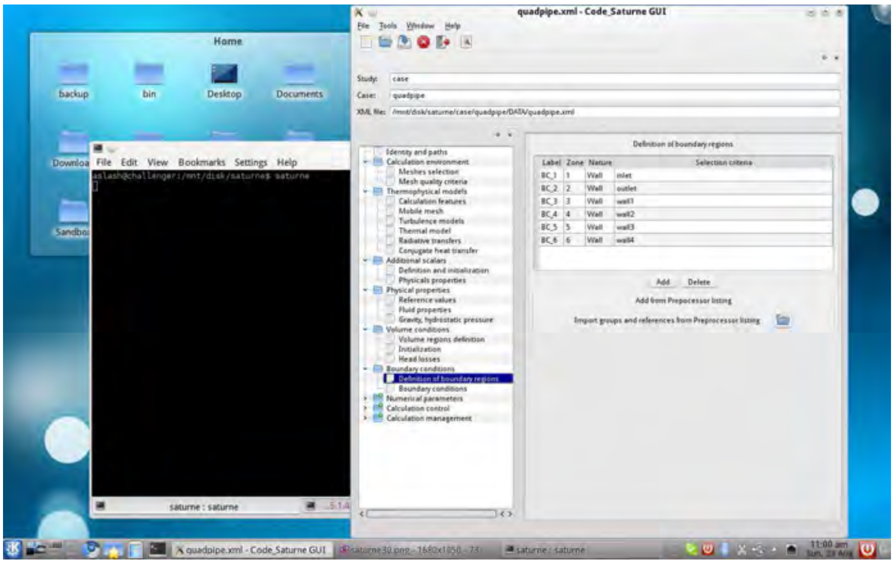
28. In the Boundary conditions directory, we first create the regions in the Definition of boundary region tab using the pre-processing log file.



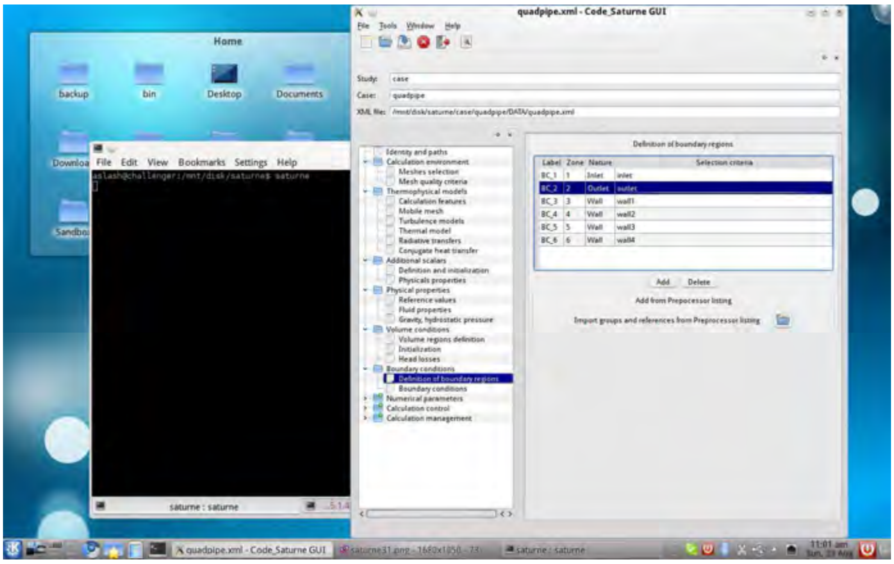
29. We select the previously saved `listpre.0` and click on Open.



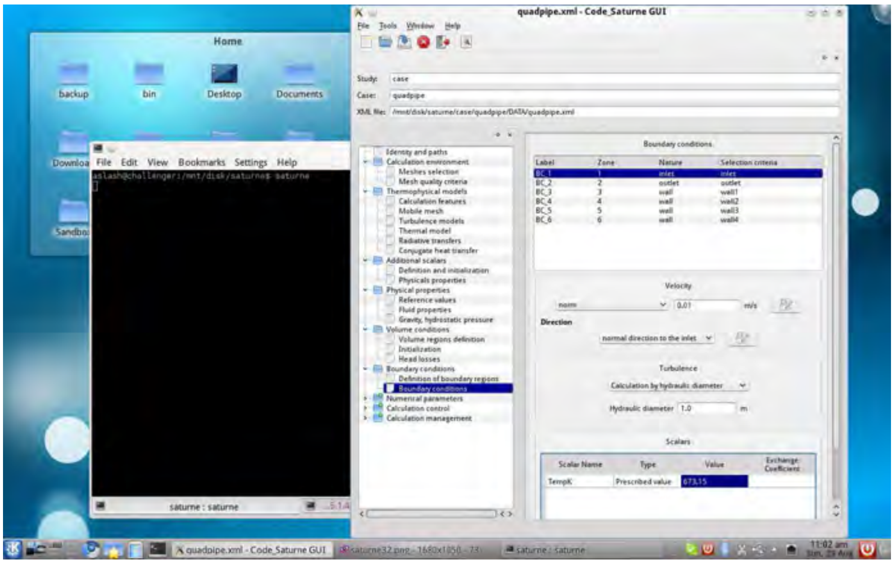
30. The list should report the six sides of the domain.



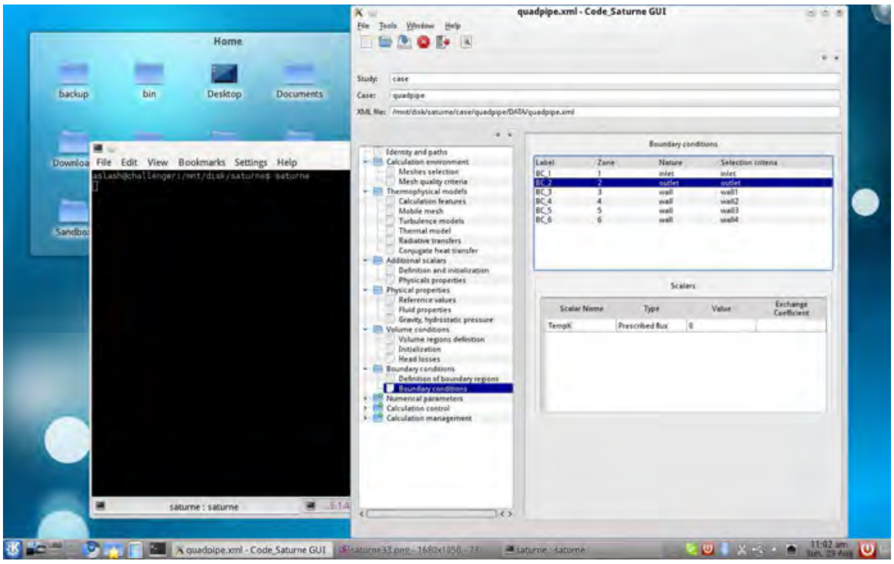
31. The default value for the `Nature` column is Wall. We must change it in the `inlet` and `outlet` regions.



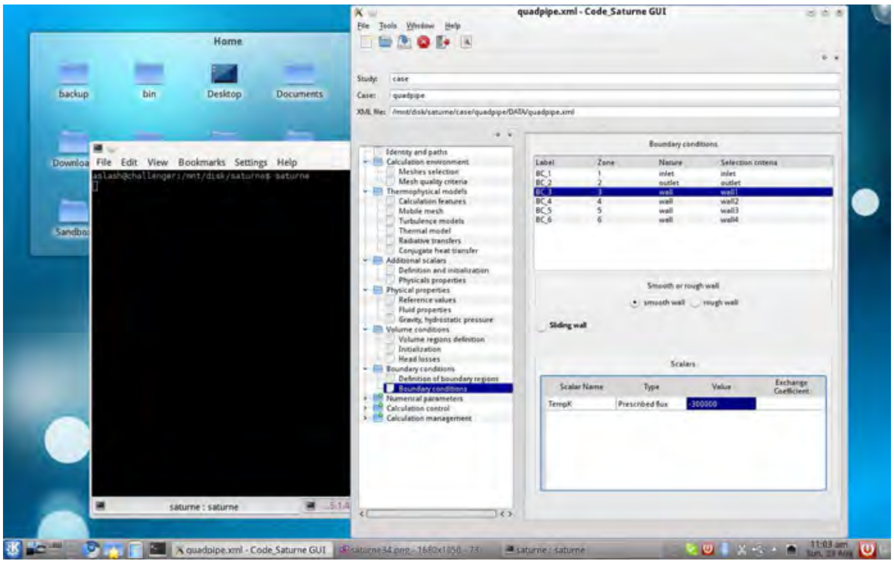
32. In the Boundary conditions tab we set the values in each region. In the `inlet` region, the velocity must be norm to the boundary and equal to 1.0. The turbulence value is set with the Calculation by hydraulic diameter option, with an Hydraulic diameter equal to 0.01. For the temperature, we select a Prescribed value of 673.15.



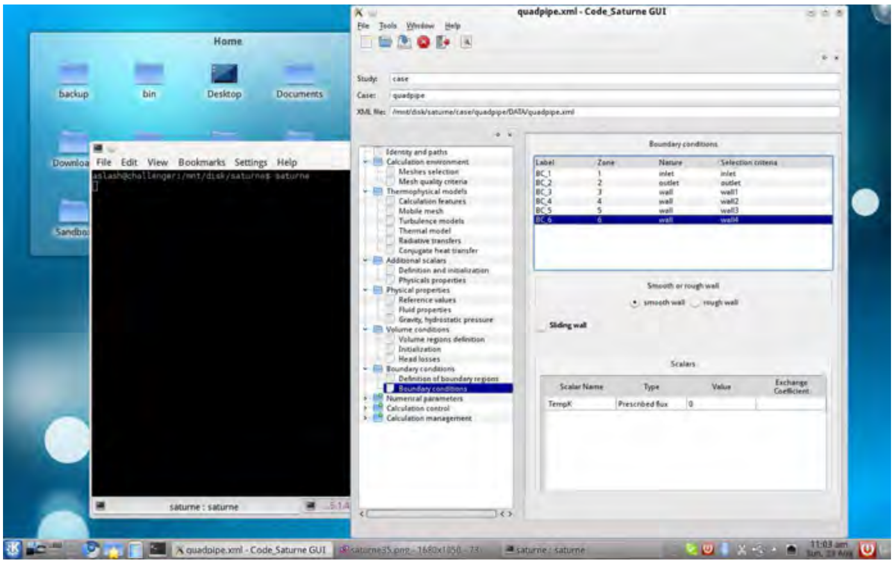
33. In the `outlet` region, we set the Prescribed flux option to 0.



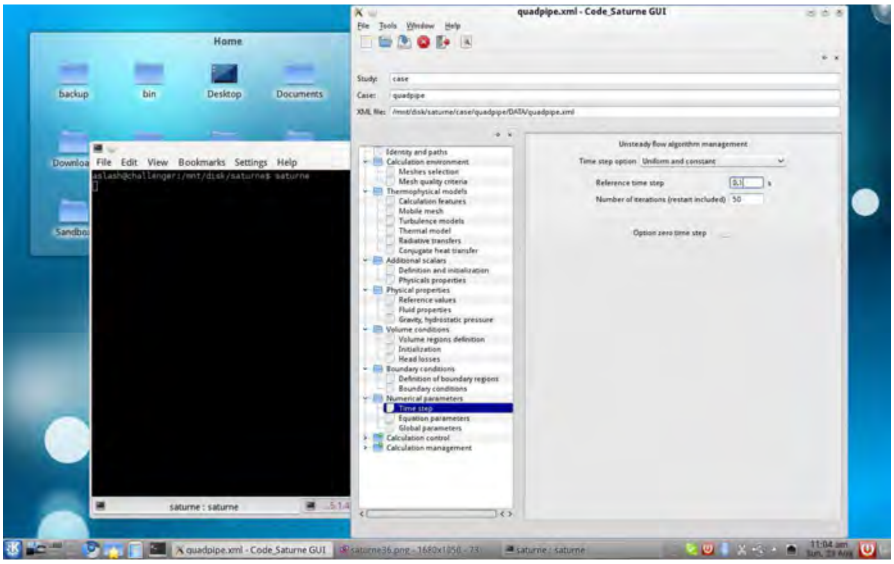
34. We set a flux that heats the fluid from the `wall1` region. We set the value of the Prescribed flux to $-3 \cdot 10^5$ (the minus sign means that the heat goes from the wall to the fluid).



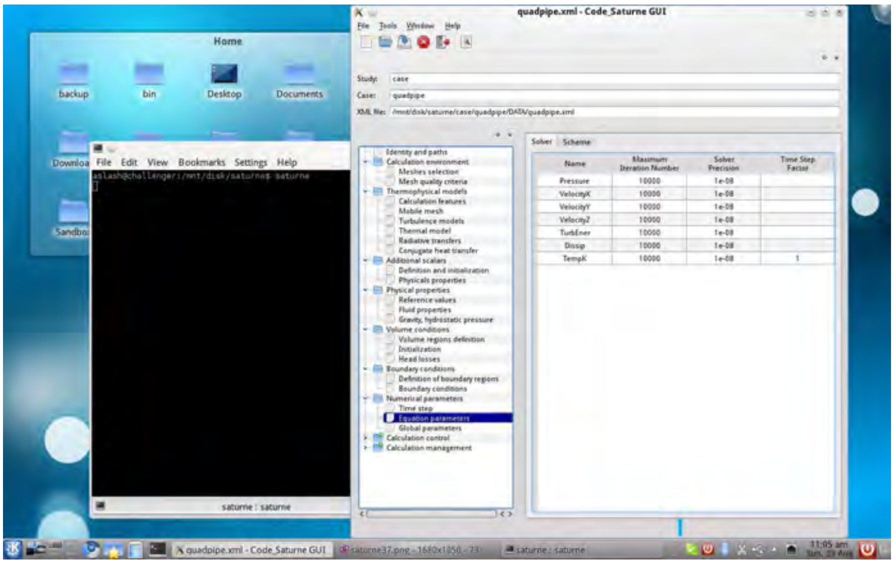
35. All other wall region are adiabatic.



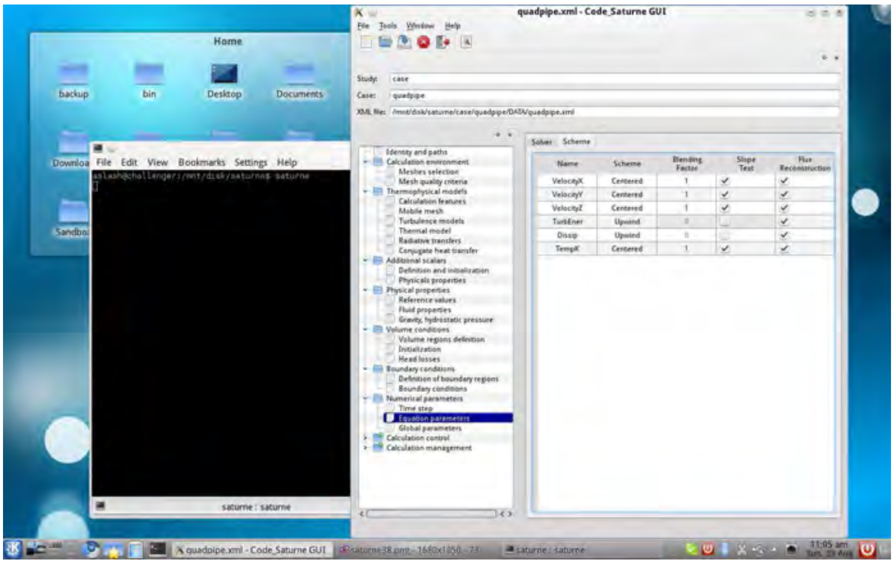
36. We go to the Numerical parameters directory. In the Time step tab, we set an Uniform and constant time step, with a reference reference value of 0.1 and 50 iterations.



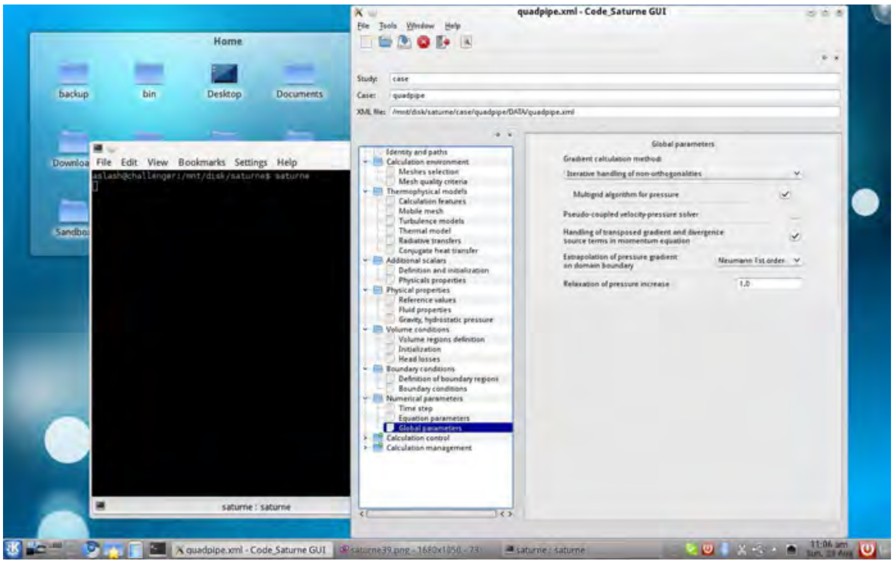
37. In the equation parameters tab we can see the `Solver precision` settings. We keep the default values.



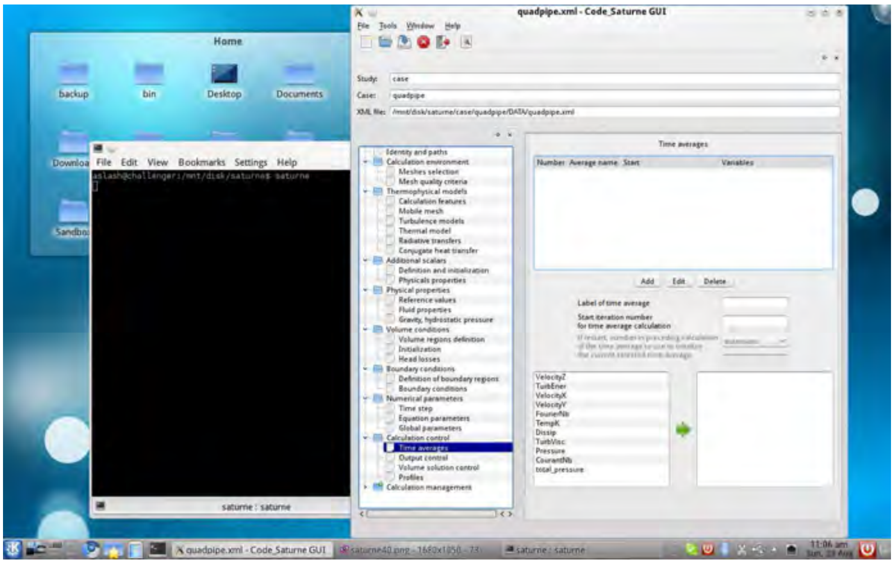
38. In the Scheme sub-tab, we can see the numerical configuration of the solver. Also in this case we keep the default values.



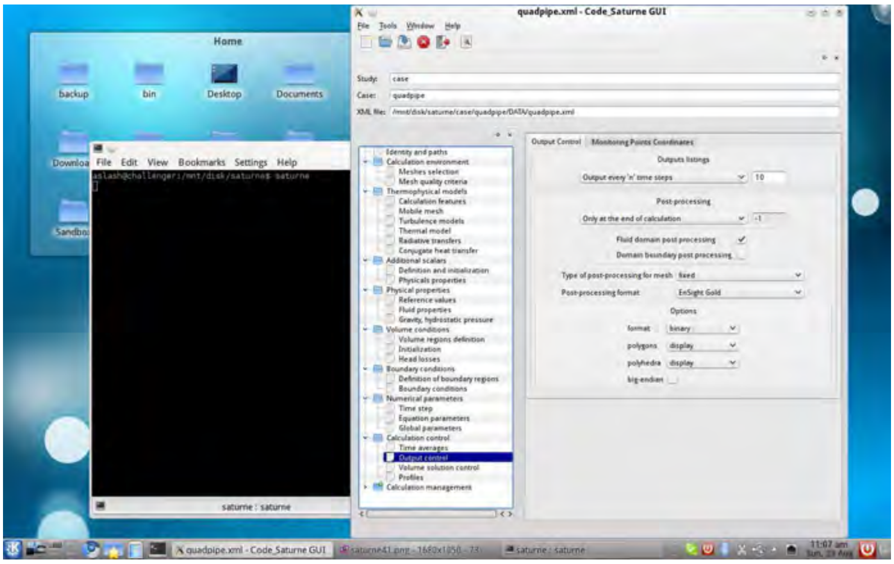
39. The Global parameters tab has some more numerical configurations. These values must be changed only for some peculiar application.



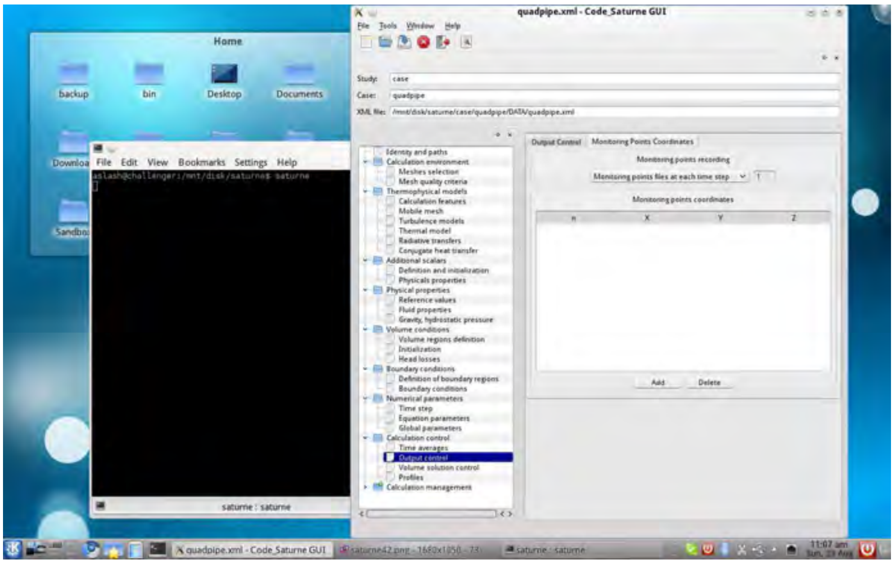
40. We go to the Calculation control directory, Time averages tab and check that the list is empty.



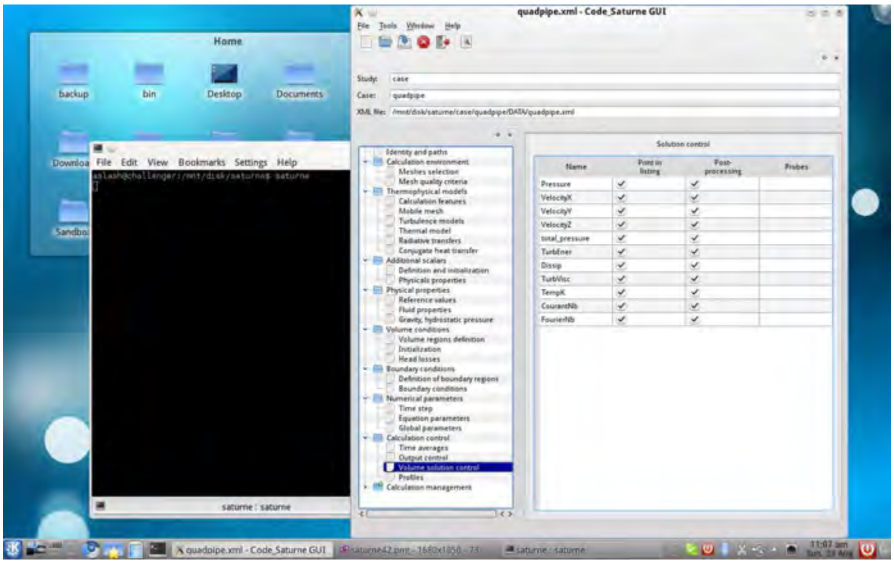
41. In the Output control tab, we keep the default options. Be sure that Post-processing format is set to Ensight Gold.



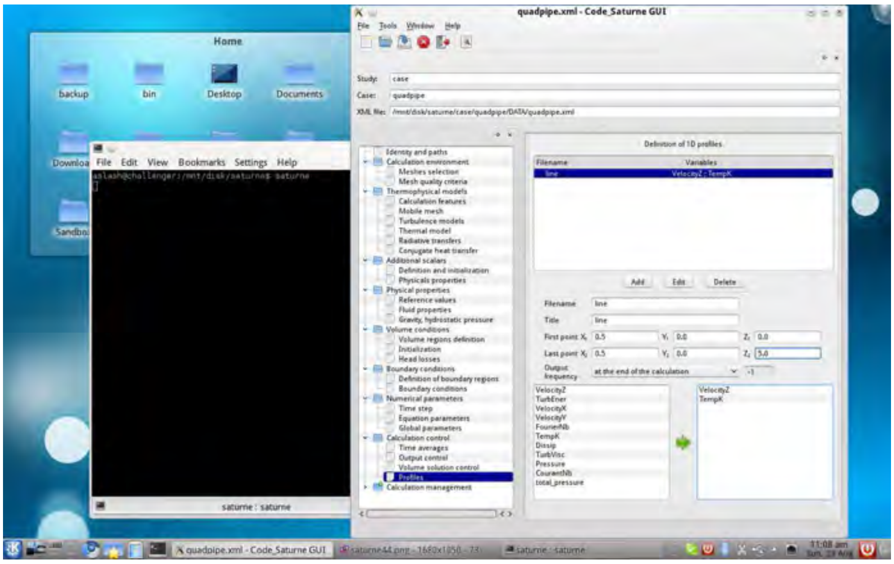
42. In the Monitoring Points Coordinates sub-tab the list should be empty.



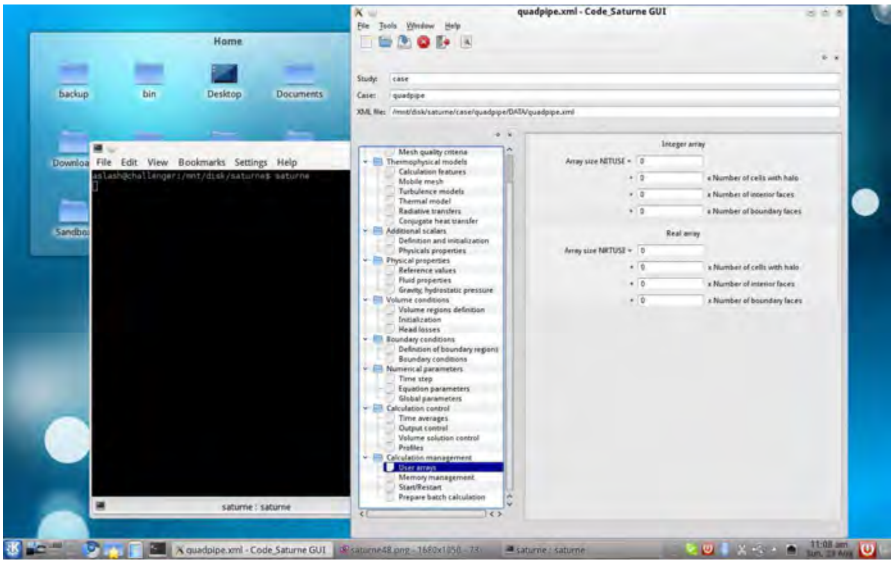
43. We keep default options also in the Volume solution control tab. In this way, all variables will be printed in the post-processing file.



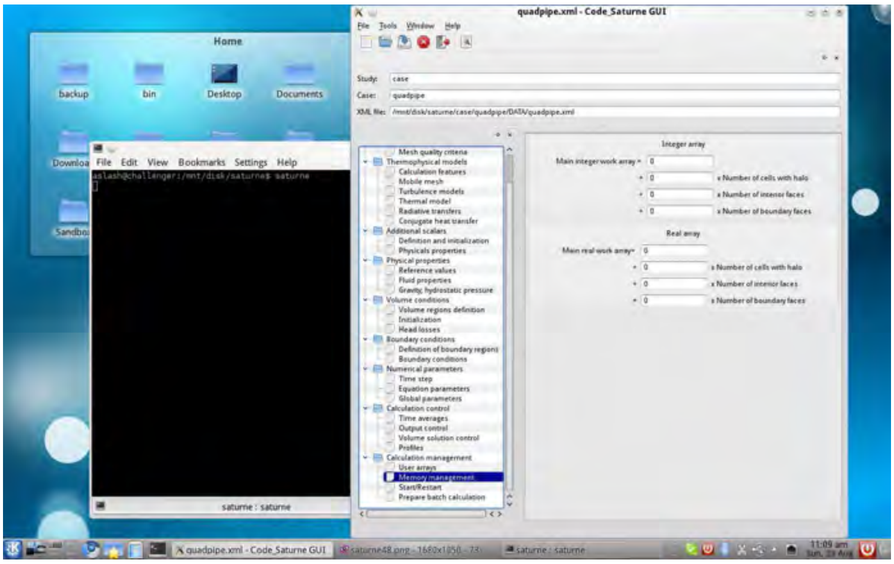
44. In Profiles we can set put an extra output over a line. An example in shown in the screenshot.



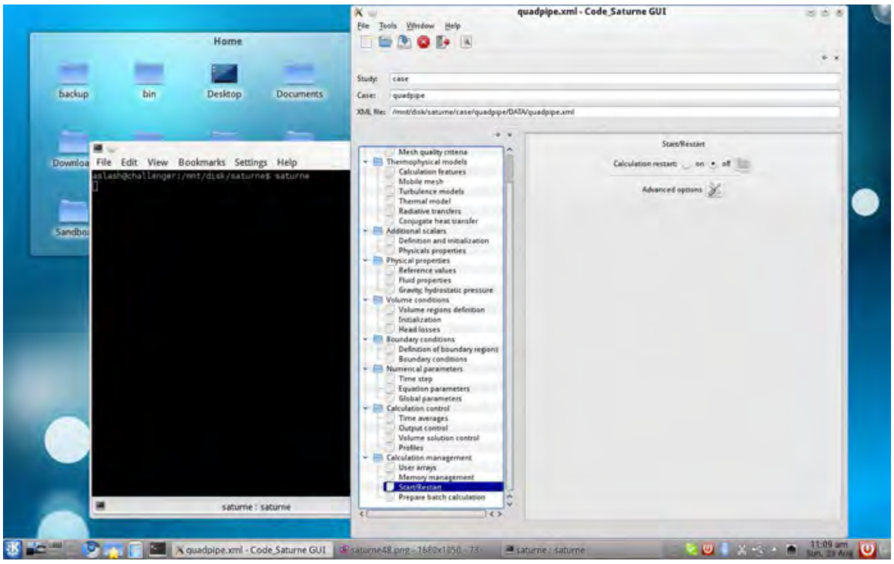
45. We jump to the $\boxed{\text{Calculation management}}$ directory, $\boxed{\text{User Arrays}}$ tab. Also in this case, we do not need to change any option.



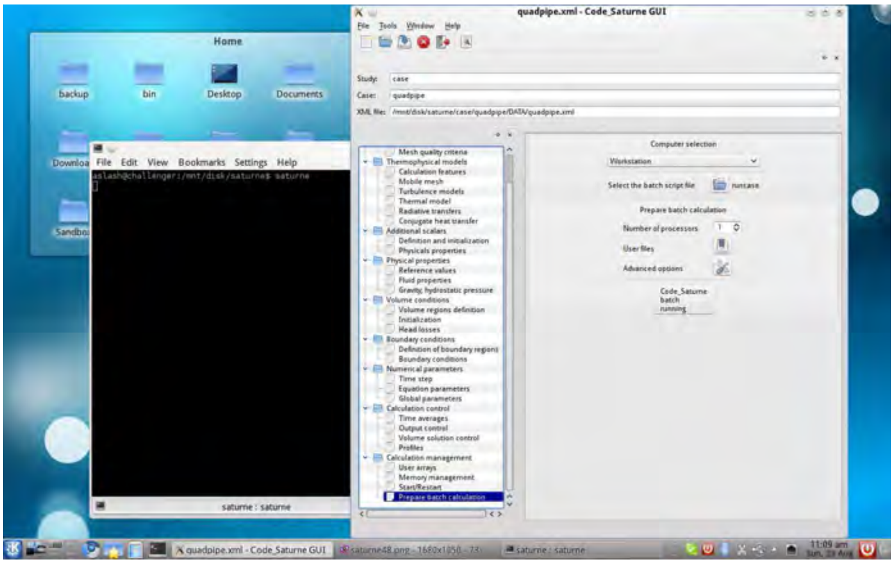
46. The $\boxed{\text{Memory management}}$ tab is treated in the same way as the previous one.



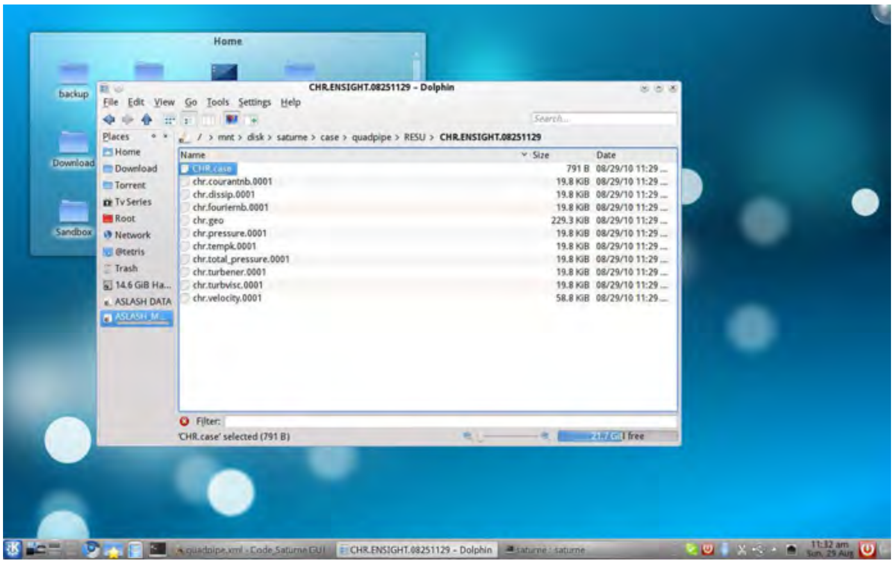
47. The Start/Restart tab controls if we want to start from scratch or from a previously calculated solution. We select off.



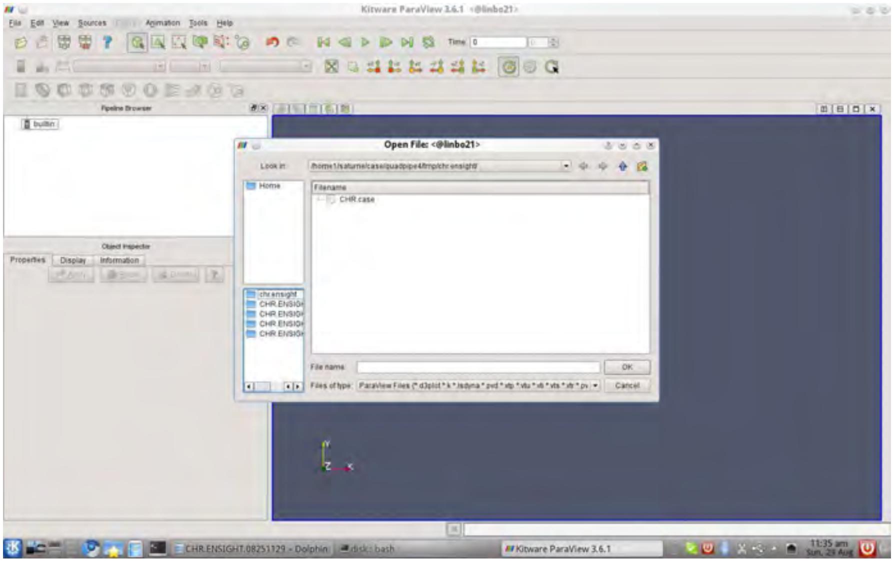
48. We start the calculation from the Prepare batch calculation tab. For a direct calculation (without submission to a queue), we select the Workstation option. A generic batch script file named `runcase` is already configured. We can choose any number of processors and start the calculation with the Batch running button.



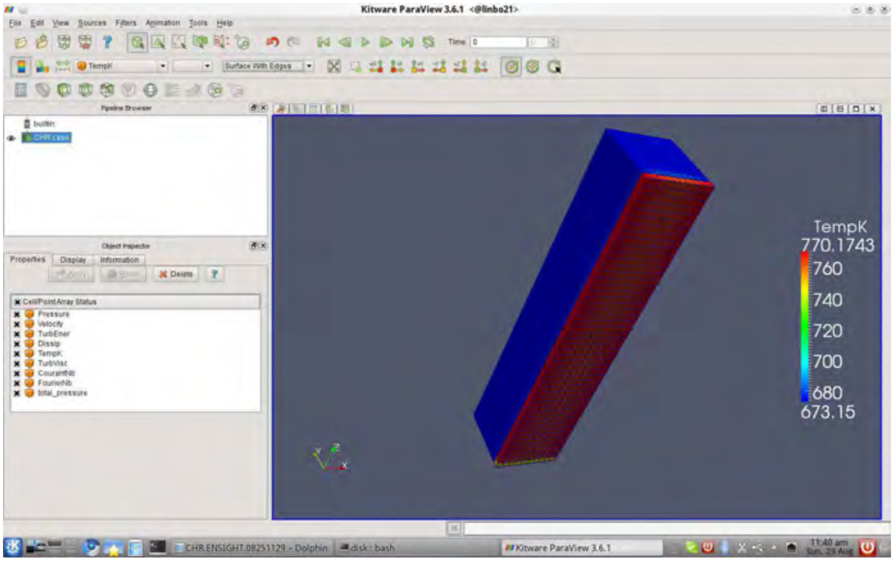
49. the results are stored in the `RESU` directory. There is a sub-directory named `CHR.ENSIGHT` followed by the date/time of execution.



50. Form PARAVIEW one should select the `chr.case` file.



51. The solution of the tutorial gives the temperature distribution shown in the screenshot.



Chapter 4

TRIO_U

4.1 Introduction

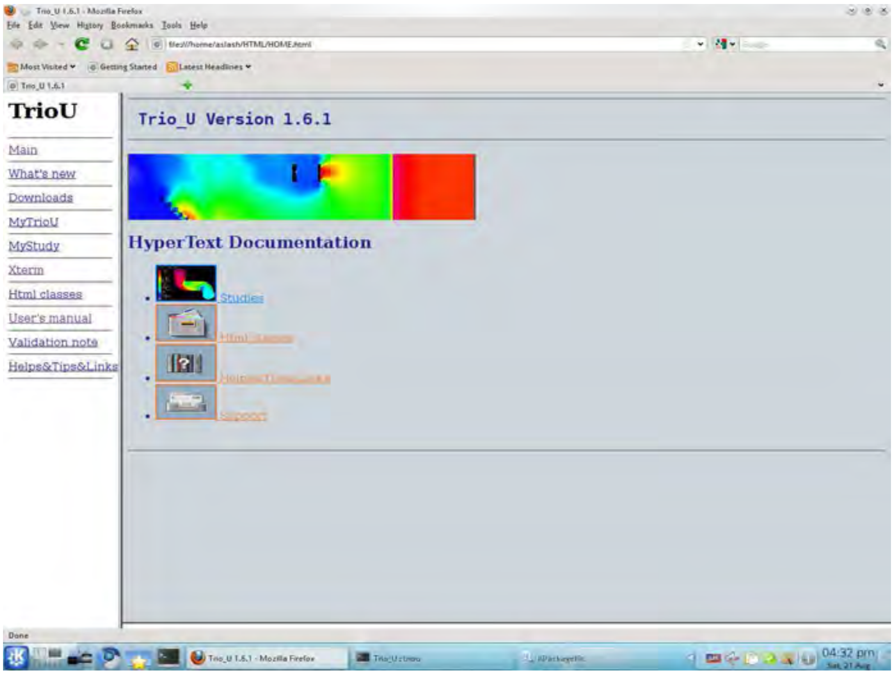


Figure 4.1: TRIO_U graphical user interface.

4.1.1 Code development

Developer(s)	CEA
Stable release	1.61 / June, 2010;
Operating system	Linux
License	not free (use only under written agreement)
Website	http://www-trio-u.cea.fr

4.1.2 Location on CRESCO-ENEA GRID

CRESCO-ENEA GRID:	
executable:	`triou`
install directory:	`/afs/enea.it/project/fissicu/soft/Triou`

4.1.3 TRIO_U overview

Trio_U, developed at the Laboratory of Modeling and Software Development of the Directorate of Nuclear Energy of the CEA, is a project that aims to develop numerical simulation software for fluid dynamics. This project starts as an object-oriented, parallel code dedicated to scientific and industrial applications in the nuclear field. The variety of physical models and numerical methods implemented in this code allow to simulate various problems ranging from the local two-phase flow simulations to turbulent flows in industrial facilities or in components of nuclear reactors.

Inside the code two modules are available: a VDF module (finite difference volume) and a VEF module (finite element volume not to be confused with the finite element method). The VDF and VEF modules are designed to process the 2D or 3D flow of Newtonian, incompressible or slightly incompressible fluids where the density is a function of a local temperature and concentration values (Boussinesq approximation). Non-Newtonian fluid by using the Otswald law are possible [16, 17, 18].

It is planned to interface Trio_U with other simulation software supported or developed by the CEA. In particular the SALOME platform may be used for different stages of the Trio_U calculation: creation of CAD and mesh editing of the data set [15].

4.2 TRIO_U on CRESCO-ENEA GRID

The TRIO_U platform is located on CRESCO-ENEA GRID on the directory

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

The TRIO_U application can be run in two ways:
a) from console
b) from FARO website

4.2.1 How to start TRIO_U from console

From console one must first set the access to the bin directory

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

by executing the script

```
$ source pathbin.sh
```

The script `pathbin.sh` must be in the home directory. One must copy the template script `pathbin.sh` from the directory

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

and then execute the script to add the bin directory to the `PATH`. If the `pathbin.sh` script is not available one must enter the `bin` directory to run the program.

Once the bin directory is on your own `PATH` all the programs of the platform can be launched. The command needed to start the TRIO_U application is

```
$ triou
```

The script `triou` consists of two commands: the environment setting and the start command. The environment script sets the environment of TRIO_U calling the script `bin/Init_Trio_U`. The start command is a simple command that launches the `TrioU` command calling the TRIO_U command Trio_U.

4.2.2 How to start TRIO_U from FARO

From FARO web application it is possible to access the TRIO_U platform with remote accelerated graphics. Once FARO has been started (see Section 1.2.2) one must open an xterm. In the xterm console one must follow the same procedure as before. First, set the access to the bin directory

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

by executing the script

```
$ source pathbin.sh
```

TRIO_U starts with the command

```
$ triou
```

The graphical interface of TRIO_U is based on FIREFOX application.

4.2.3 How to interrupt TRIO_U

In order to interrupt TRIO_U one must enter the value 1 in the `case.stop` file whereas case is the name of the case. When the calculation is started, Trio_U enters the value 0 in the stop file.

4.3 Mesh, dataset and output files

4.3.1 Mesh File

A mesh file may be created for Trio_U by using one of the following software:
a) Xprepro mesh generator (inside the Trio_U directory) for Cartesian 2D/3D domain
b) Gmsh freeware mesh generator(download at http://www.geuz.org/gmsh) for VEF 2D/3D domain
c) Trio_U mesh generator for simple geometries
d) ICEM,IDEAS,SIMAIL mesh generator for VEF 3D domains
f) Use a format translator to translate the mesh from Gambit to Trio_U meshing format

Xprepro mesh format

Xprepro is a new tool for Trio_U calculation which can create very complex 2D, 3D VDF meshes. You can run Xprepro either from a study opened with the GUI of Trio_U through a button named Mesh, either by running the command line Xprepro.

Gmsh mesh format

Gmsh is a freeware to build 2D/3D unstructured meshes with tetrahedral or hexahedral meshes. Meshes generated by Gmsh must be translated to Trio_U format by a converter located in `$TRIO_U_ROOT/Gmsh` directory. It can also be run from the GUI of Trio_U using the button Gmsh.

Tgrid/Gambit mesh format

An instruction in the data set is available to reread meshing issued by Gambit/Tgrid (tools from Fluent) using Trio_U. This instruction is as follows:

```
Lire_Tgrid dom nom_fichier_maillage
```

where `dom` corresponds to the domain name, `nom_fichier_maillage` corresponds to the file containing the mesh. 2D (triangles or quadrangles) and 3D (tetra or hexa elements) meshes, may be read by Trio_U. The template for the Gambit/MED converter can be found in the directory

`/afs/enea.it/project/fissicu/soft/triou/data`

The file is as following

```
dimension 3
Domaine dom
Lire_tgrid dom mesh.msh
ecrire_med dom mesh.med
Fin
```

SALOME MED format

An instruction in the data set is available to read MED mesh issued for example from SALOME. This instruction is as follows

```
Lire_Med [vef][fam_name_from_gr_name] mesh_name filename.med dom_name
```

The `dom_name` corresponds to the domain name, `filename.med` corresponds to the file (written in format MED) containing the mesh named `mesh_name`. Option `vef` is obsolete and is kept for backward compatibility. The option `fam_names_from_gr_name` uses the group names instead of the family names to detect the boundaries into a MED mesh.

4.3.2 Dataset file

The dataset file must be labeled with the extension `data` and contains all the parameter values and all the options. The options are introduced in the code through key words. For example consider the `Lire` key word. The interpreter allows the key`Lire` object to be read (defined) in various ways:
a) with bracket

```
Lire object1
{
....
}
```

In this case this keyword provides the object `object1` defined between the braces. b) simple line command

```
Lire_fichier object1 namefile
```

The keyword `Lire_fichier` is to read the object object1 contained in the file `namefile`. This is notably used when the calculation domain has already been meshed and the mesh contains the file `namefile` c) with bin

```
Lire_fichier_bin object1 namefile
```

for an unformatted file.

For all the keyword one can see the TRIO_U tutorial inside the doc directory which is located in

```
/afs/enea.it/project/fissicu/soft/Triou/doc
```

4.3.3 Output files

There are different output file formats:

- name.lml: standard storage files for post-processing. The lml format files allow the results to be viewed with Data Visualizer or AVS Express

- name.lata: which is similar to lml format but comprises several files;
- name.ijk format which outlets the results in tables;
- name.tv format to use the file using the freeware viewing tool: VisIt. - name.son: standard storage files for physical values measured by probes integrated into the calculation domain by the user. This file can be read by the gnuplot application.

4.4 TRIO_U tutorial for the obstacle test example

This examples is taken by the list of examples that comes with TRIO_U. The study is called `obstacle` and it consists of two files: `obstacle.dat` and `obstacle.geo`. The `obstacle.dat` is the dataset file while `obstacle.geo` is the mesh file written with the internal format.

4.4.1 How to run the obstacle test example

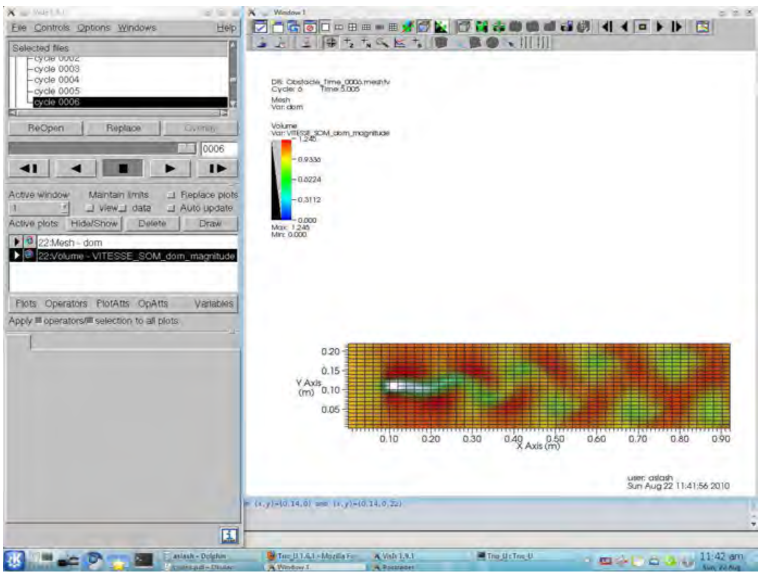
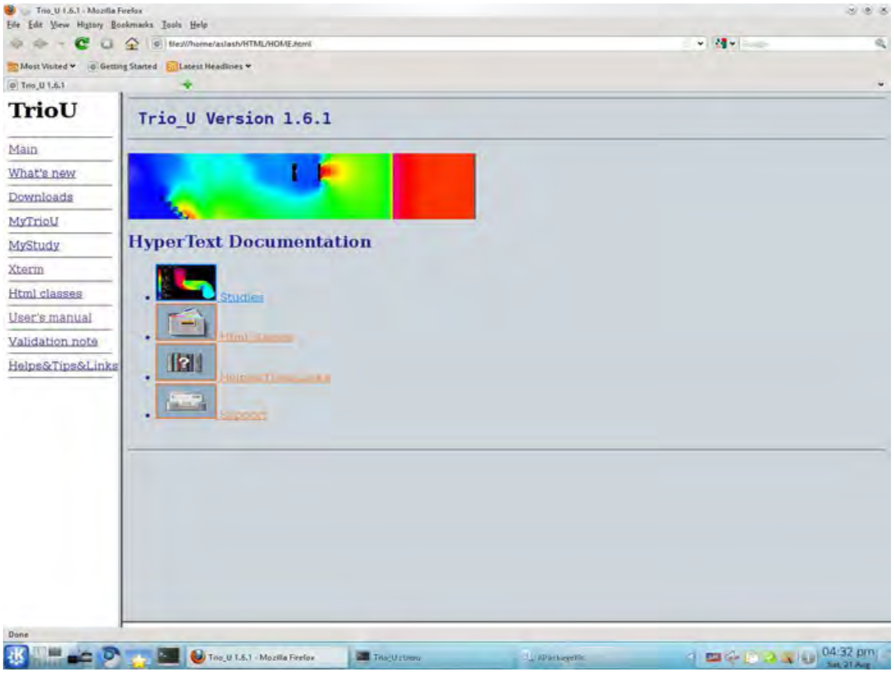
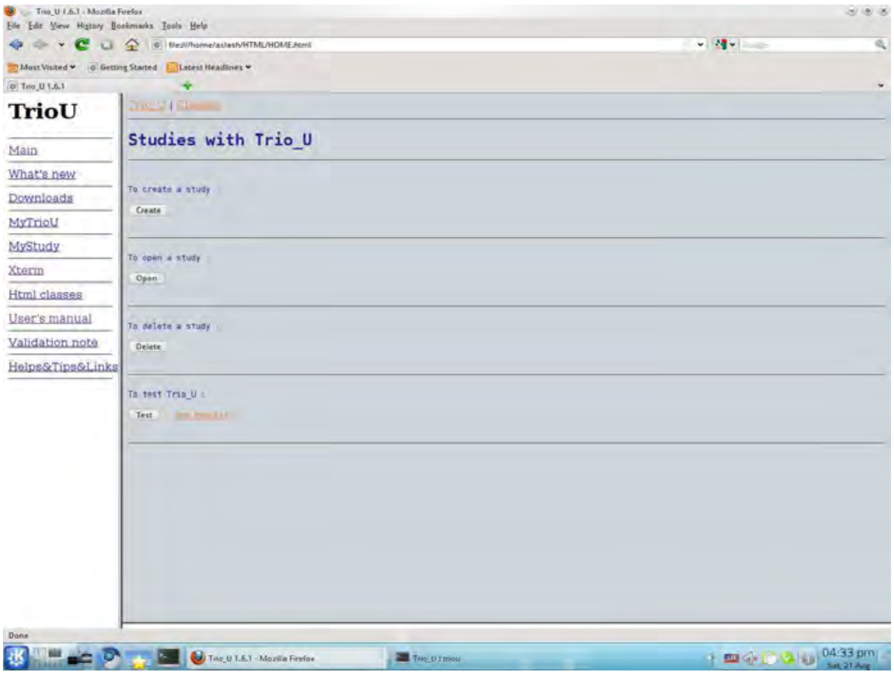


Figure 4.2: The obstacle test

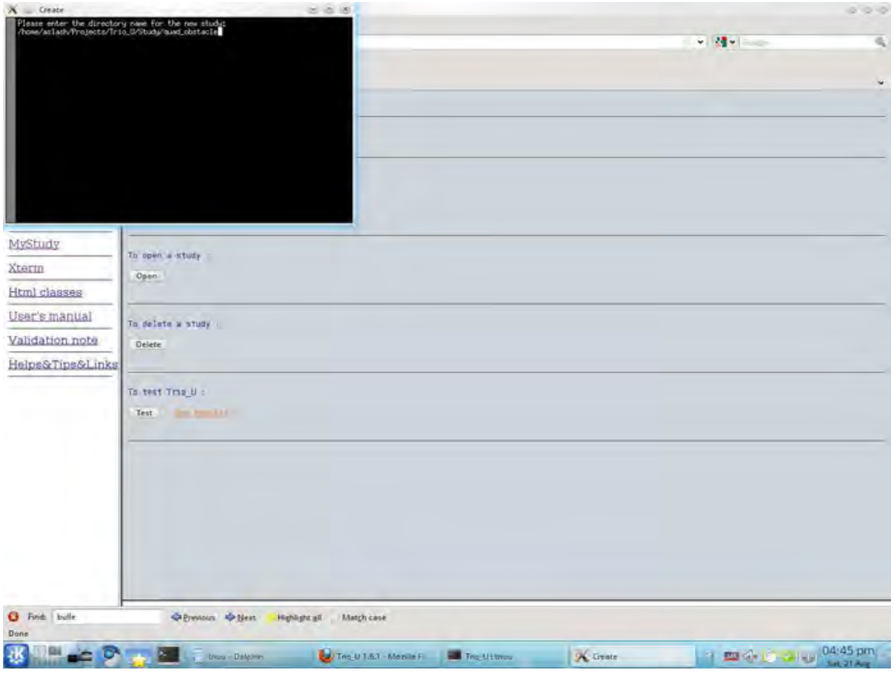
1. We run `triou` from the command line. TRIO_U graphical interface is managed through a web browser. The default case will open Firefox. To start a new project we click on the Studies link.



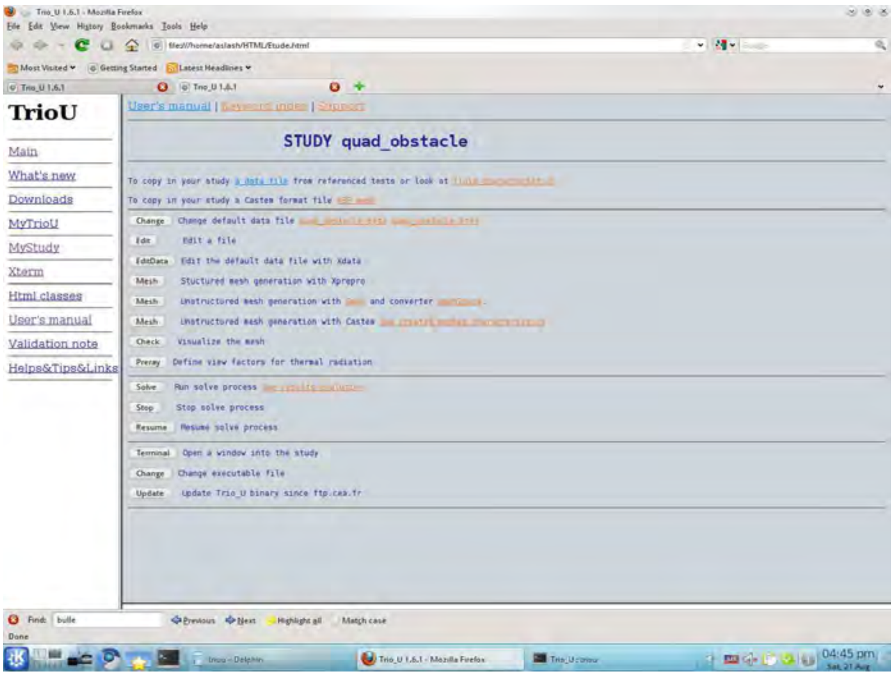
2. In the new screen we can push the Create button to start a new study.



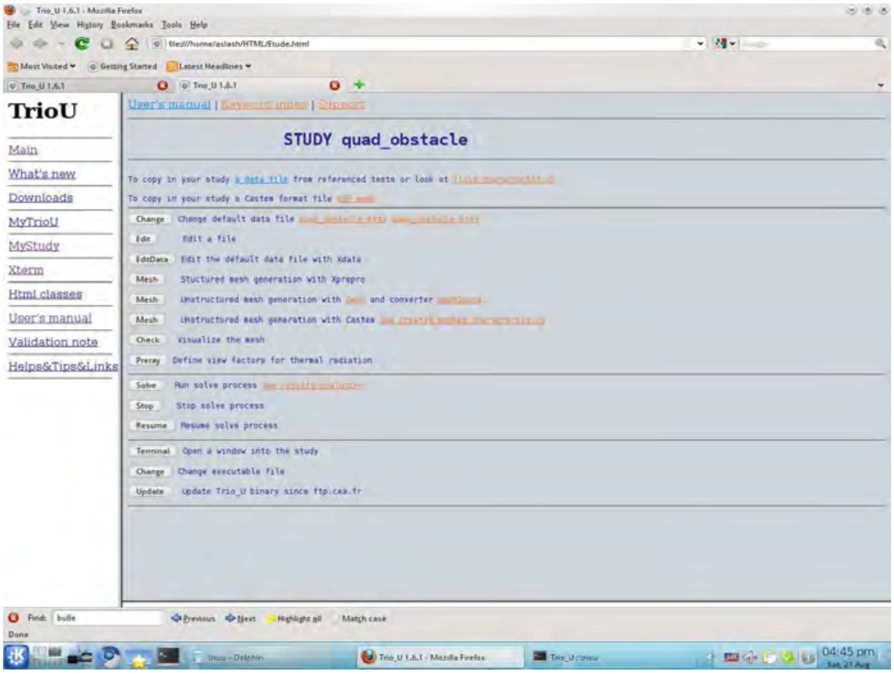
3. In the appearing shell, we can insert the path for the new study. We use `Study/quad_obstacle` inside the TRIO_U directory.



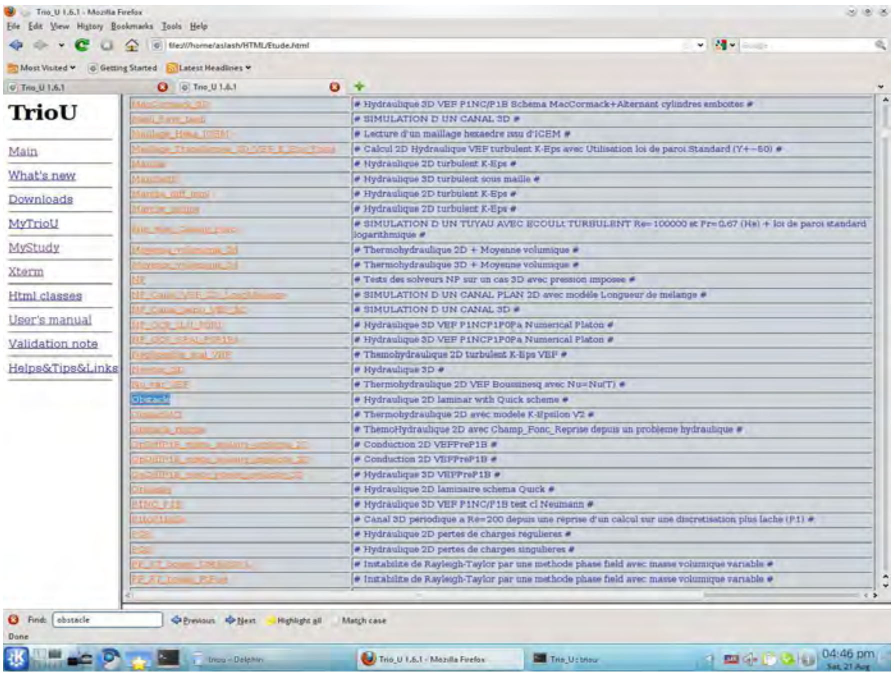
4. We reach the main window for the study. The name is clearly visible in the title.



5. In order to generate our study, we click on the a data file button to copy the configuration file from a test case.



6. We search for the Obstacle test and click it.



7. the first file we need is the data file. We click on the Copy button besides it.

8. We use the name `quad_obstacle.data` in the terminal.

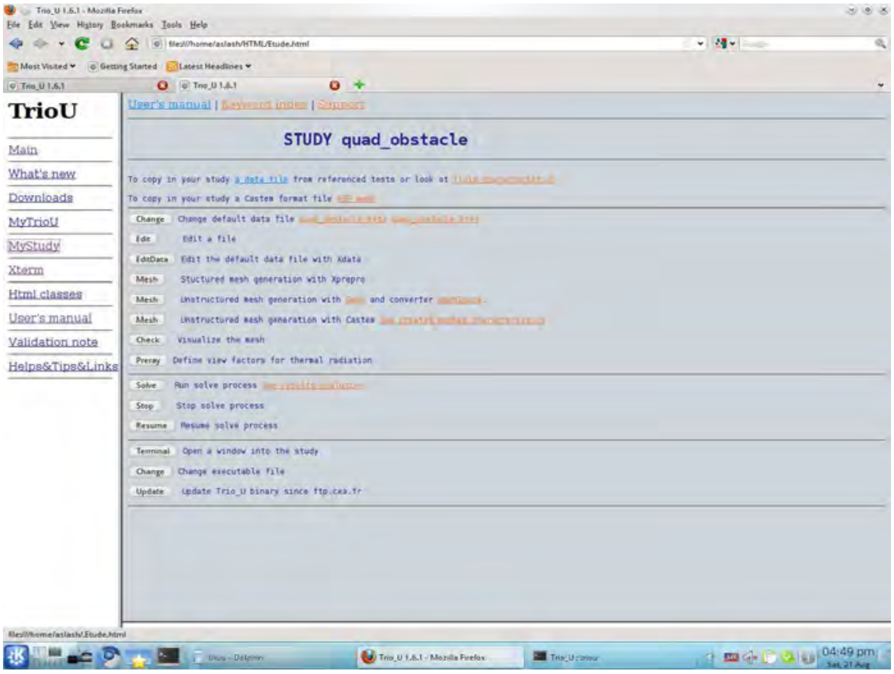
9. The file is opened for editing. Details on the content are given in Section 4.3.2.

10. The only edit we need is the name of the mesh file: we insert `quad_obstacle.geo` instead of `Obstacle.geo`.

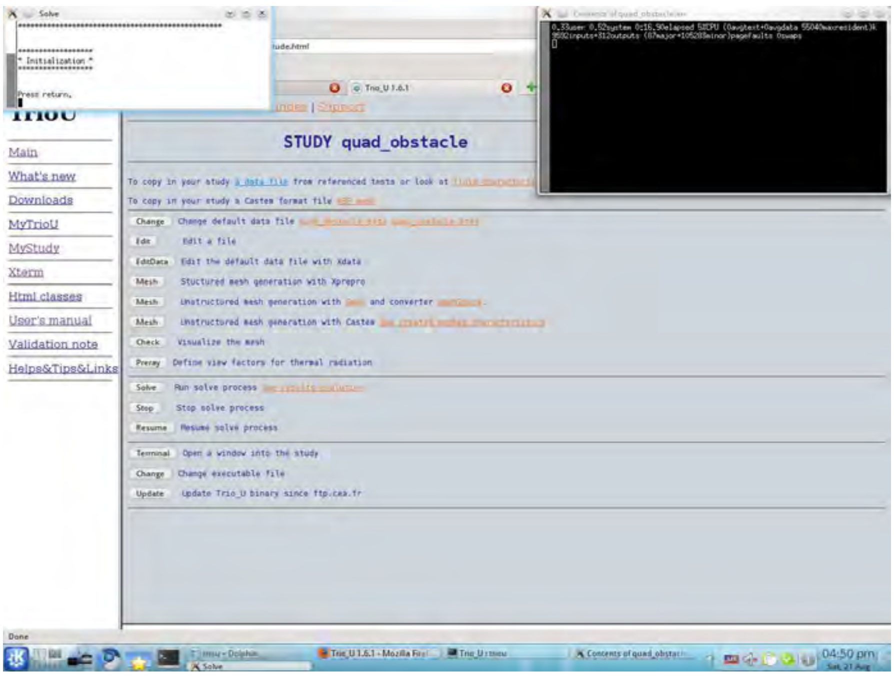
11. We can now copy the mesh file. We must use the name we have already put in the data file, `quad_obstacle.geo`.

12. The file is opened for edit. We do not make any modification. In this case, the internal generator is used to create the mesh.

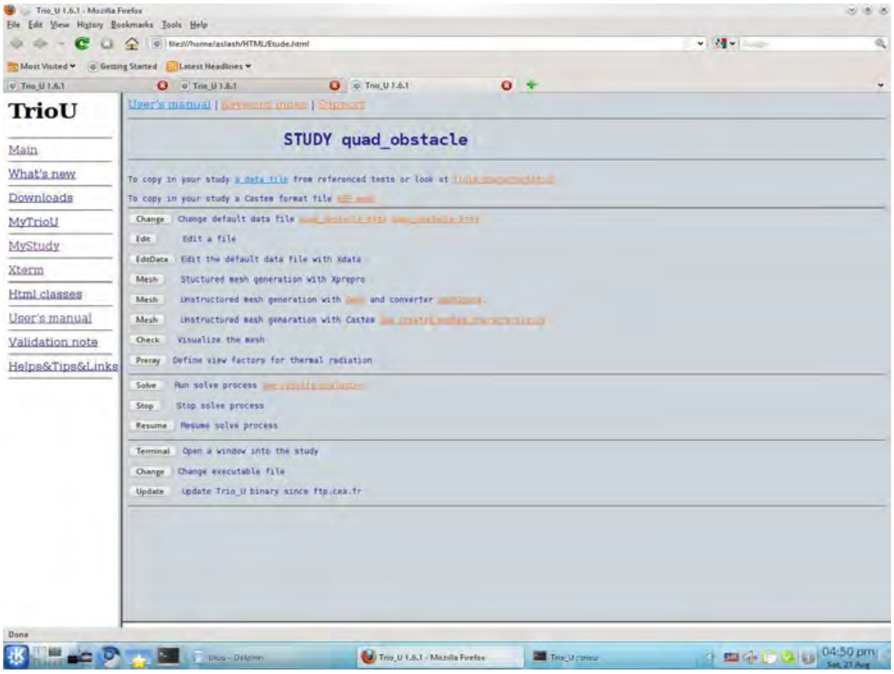
13. We go back to the study main page. We are ready to click on the Solve button to start the calculations.



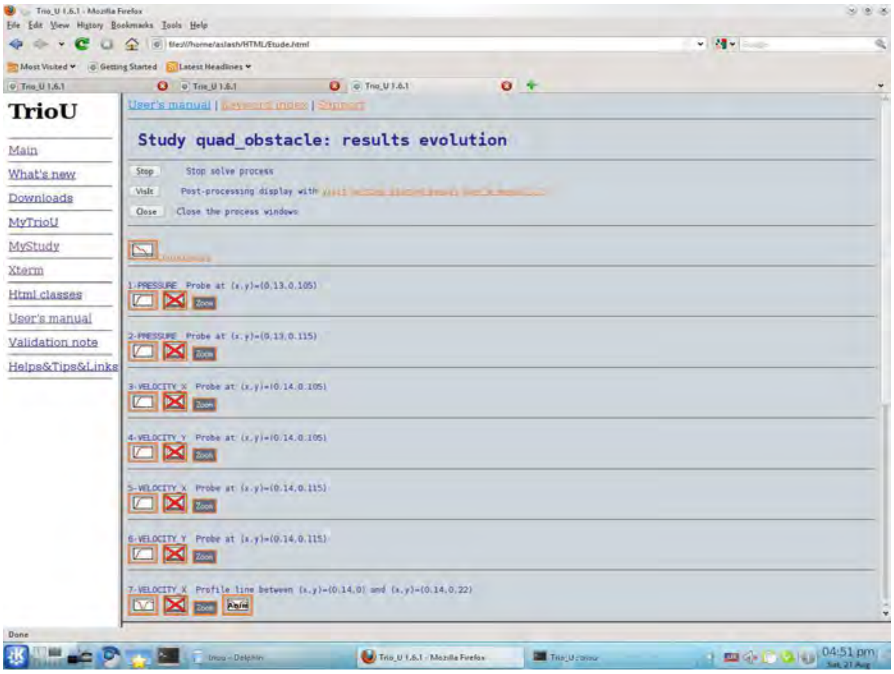
14. The windows on the top left will report the advance of the calculation, while in the top right we can see if there are errors.



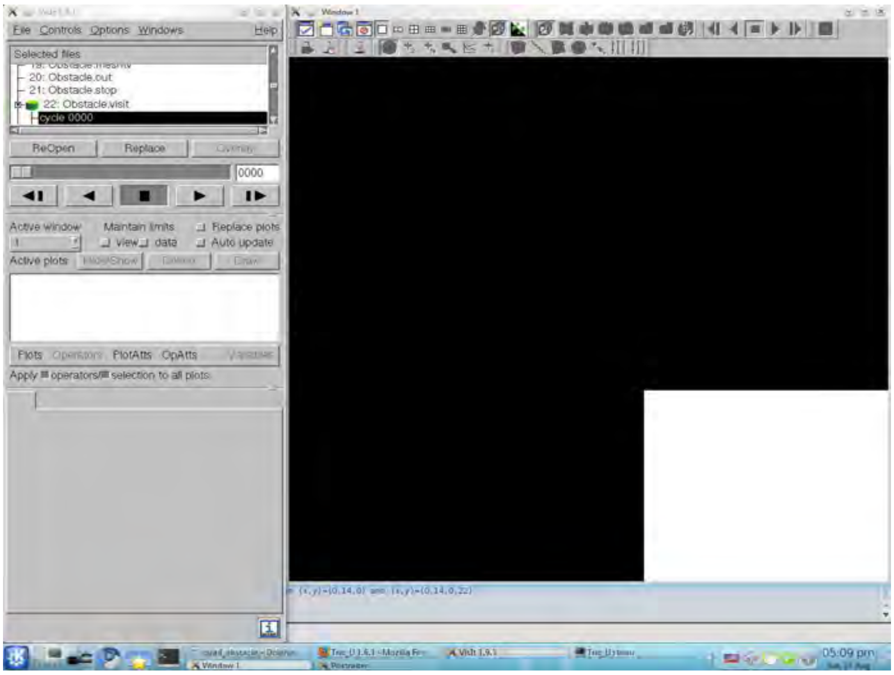
15. Once the calculation are finished, we can click on the $\boxed{\text{See results evolutions}}$ on the right of the $\boxed{\text{Solve}}$ button.



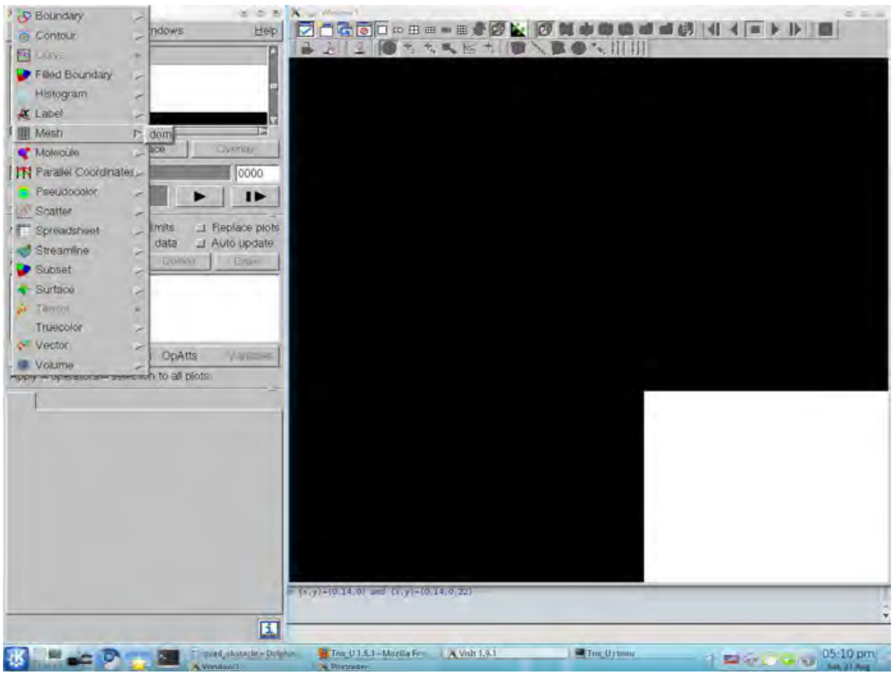
16. We can launch $\boxed{\text{VisIt}}$ directly with the dedicated button.



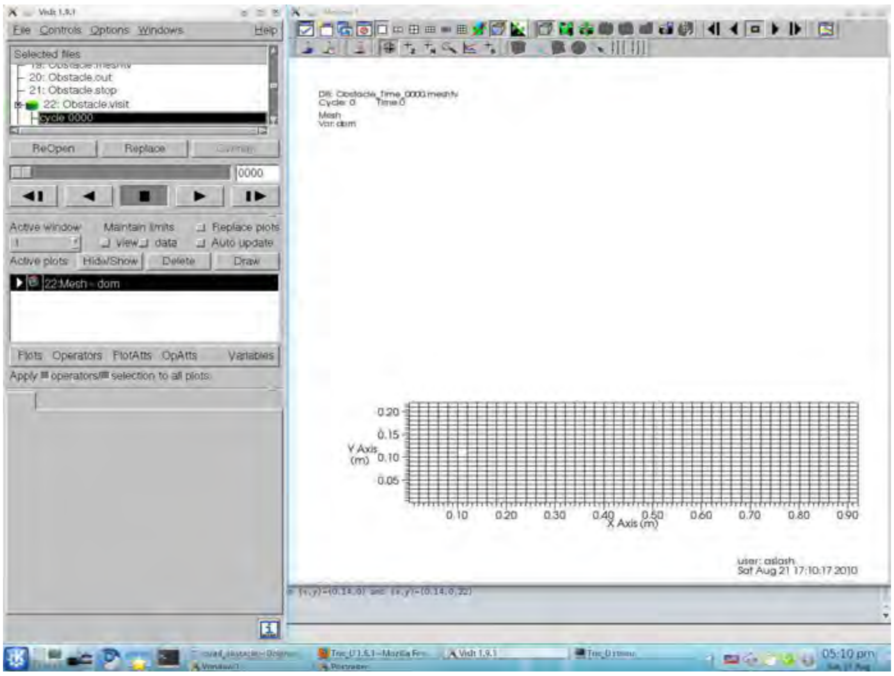
17. The main window of VisIt appears. The file browser is already configured inside the study directory.



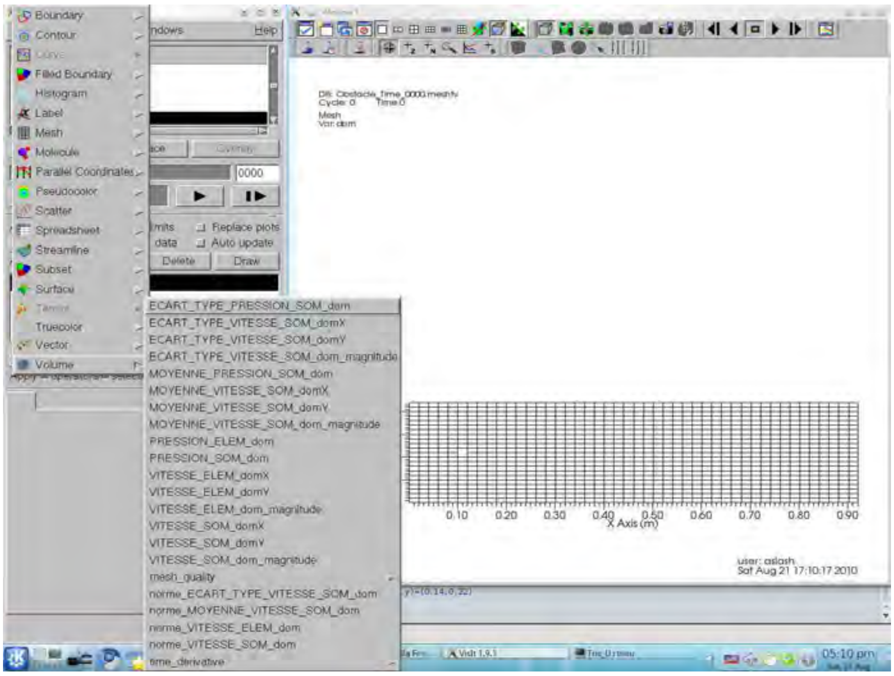
18. All the drawable elements can be accessed via the $\boxed{\text{Plots}}$ menu. We start by visualizing the computational domain with $\boxed{\text{Plots -> Mesh -> dom}}$.



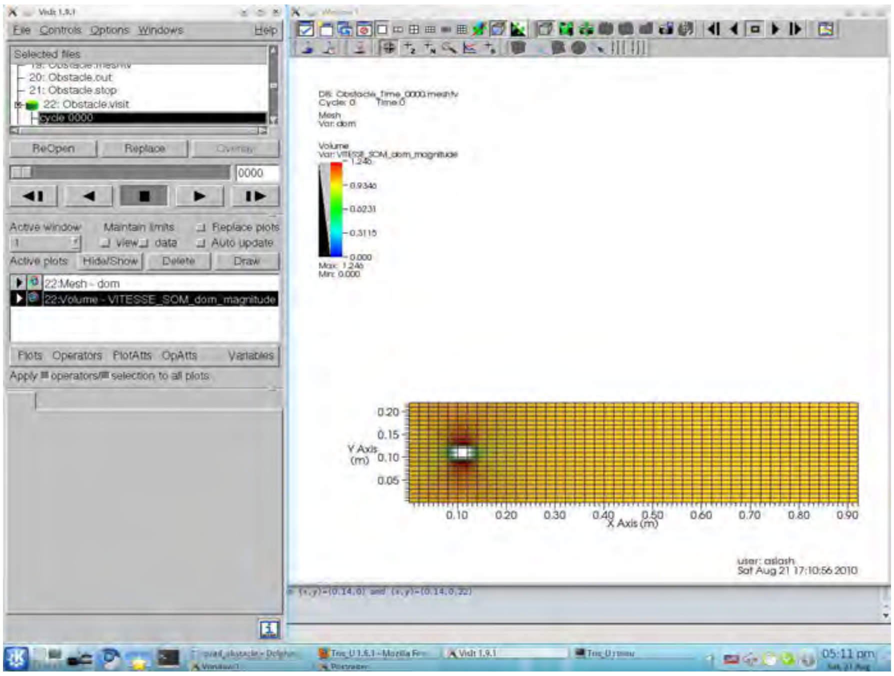
19. The visualization becomes effective when we click on the $\boxed{\text{Draw}}$ button.



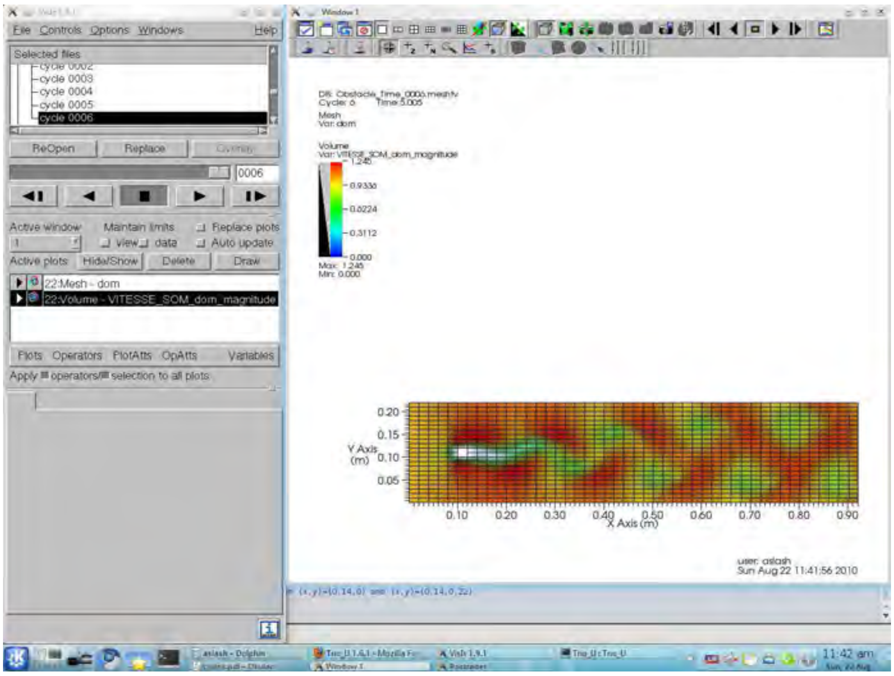
20. We can now visualize the velocity magnitude. We select it via $\boxed{\text{Plots -> Volume -> VITESSE\_SOM\_dom\_magnitude}}$.



21. Clicking on the Draw button the velocity will appear in the main window.



22. The Play button can be used to visualize the successive time steps of the simulation.



Chapter 5

NEPTUNE

5.1 Introduction

Figure 5.1: Neptune graphical user interface.

5.1.1 Code development

Developer(s)	EDF
Stable release	June 7, 2010;
Operating system	Linux and Cross-platform
License	not free (use under NURISP written agreement)
Website	no website

5.1.2 Location on CRESCO-ENEA GRID

CRESCO-ENEA GRID:	
executable:	`neptune`
install directory:	`/afs/enea.it/project/fissicu/soft/Neptune`

5.1.3 NEPTUNE overview

The NEPTUNE project is a joint research and development program between EDF and CEA for nuclear reactor simulation tools. The project provides a two-phase flow thermal hydraulics software for multiscale and multidisciplinary calculations. The code may perform three-dimensional computations of the main components of the reactors: cores, steam generators, condensers, and heat exchangers. NEPTUNE supports from one to twenty fluid fields (or phases) and includes thermodynamic laws for water/steam flows. It is based on advanced physical models (two-fluid equations combined with interfacial area transport and two-phase turbulence) and modern numerical methods (fully unstructured finite volume solvers). The code is based on the cell-centered type finite volume method which can use meshes with all types of cell and nonconforming connections. NEPTUNE uses co-localized gradients with reconstruction methods to compute face values and supports distributed-memory parallelism by domain splitting. NEPTUNE is

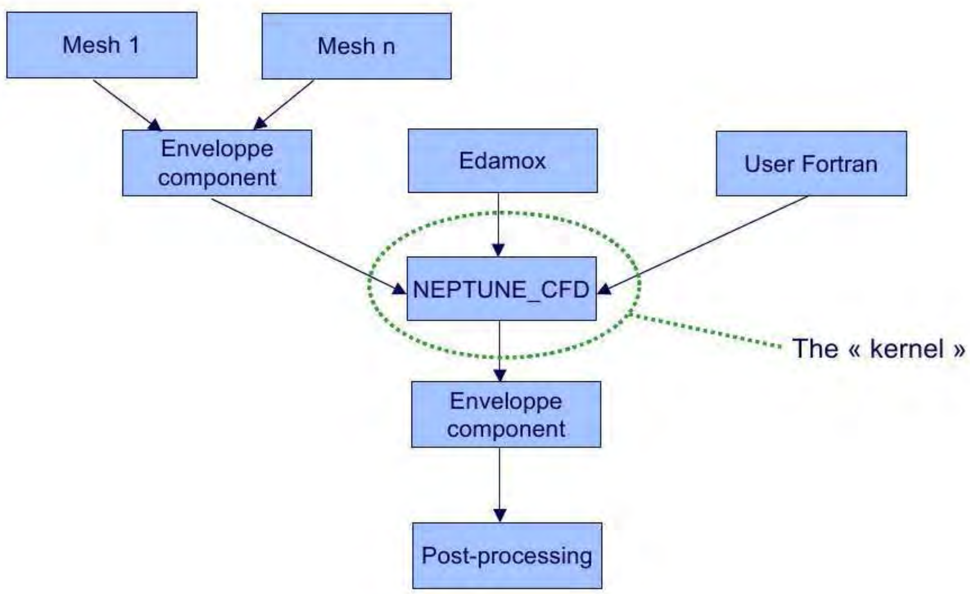


Figure 5.2: Modules of the NEPTUNE CFD

written in Fortran and organized in modules as shown in Figures 5.2. The `enveloppe` component manages the pre-processing and the post-processing functions, while `edamox` is the graphical user interface. One can introduce user functions by using the `user Fortran` module. The kernel of the calculation is implemented in the `Neptune_CFD` module [10, 11, 12, 13, 14].

5.2 NEPTUNE on CRESCO-ENEA GRID

5.2.1 Graphical interface

The NEPTUNE code is located on CRESCO-ENEA GRID in the directory

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

Once the `PATH` is set for the directory

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

by executing the script

```
$ source pathbin.sh
```

as it is explained in Section 1.2.3, the NEPTUNE GUI starts with the command

```
$ neptune
```

Remark. Not all libraries are yet available at the moment for the CRESCO architecture. We suggest to run NEPTUNE GUI on a personal workstation.

The GUI is used to set up the simulation creating a `param` file. The solution of the case must be run in command line mode or in batch mode as explained in the next section.

5.2.2 Data structure

NEPTUNE requires a specific structure for the configuration and input files. Each simulation is denoted as *case*. We can therefore create a `cases` directory and put all NEPTUNE simulations inside.

Inside this directory, each case will have its own directory (for example `case1`, `case2`) and there must be a `MESH` directory, where all the meshes are stored.

```
cases
+-- case1
+-- case2
...
+-- MESH
```

Inside each case directory, we have to create the four sub-directories

- `DATA`, where the XML configuration file is stored;

- RESU, that is used for the outputs;
- SCRIPTS, that hosts the execution scripts;
- SRC, in which we can put some additional source file.

To create a folder tree for the study case1, it is available a script

```
$ buildcase_nept -study case1
```

This generates the correct directory structure.

During the execution, NEPTUNE will generate some temporary files that are by default stored in the tmp_NEPTUNE directory in the user directory. This directory must be periodically cleaned by hands, there is no automatic procedure.

5.2.3 Command line execution

In order to execute the application in a shell we must first set up the environment using the script

```
neptune_env
```

that is located in the directory

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

Remark. The neptune_env script consists of the following lines

```
#! /bin/bash
export NEPTHOME=/afs/enea.it/por/arcproj/fissicu/soft/Neptune\
/package_neptcfd-1.0.8/NEPTUNE_CFD/neptcfd-1.0.8-r844/bin
source $NEPTHOME/neptcfd_profile
export NEPTMPI=/afs/enea.it/por/arcproj/fissicu/soft/Neptune\
package_neptcfd-1.0.8/opt/lam-7.1.1/arch/Linux_x86_64/bin/
```

The recommended way to run NEPTUNE from command line is to use the runcase script. There is a template available inside the directory

```
/afs/enea.it/project/fissicu/soft/Neptune/data
```

One has to navigate to the SCRIPTS directory inside the case in analysis and run

```
$ ./runcase
```

5.2.4 Batch running

On the top of the `runcase` template there are the configuration options for LSF. This is the template file for queue submission using LSF on CRESCO-ENEA

```
...
# BSUB -J JOBNAME
# BSUB -n NPROC
# BSUB -oo stdout_file
# BSUB -eo errout_file
....
```

where the options `-J` sets the job name, `-n` the number of processors, `-oo` the files for the standard output and `-eo` the error output. There is a space between the `#` and `BSUB` to be erased in order to run in batch mode. Once the script is ready the command

```
$ bsub < runcase
```

starts the batch execution.

Further information on batch commands are available in Section 1.2.4.

5.3 NEPTUNE dataset and mesh files

NEPTUNE requires a specific structure for the configuration and input files. Each simulation is denoted as *case*. One must therefore create a `case` directory and put all NEPTUNE simulations inside. For details on NEPTUNE file structure see Section 5.2.2.

NEPTUNE requires a dataset file (named `param`) and a mesh file (with extension `med`) with the mesh geometry.

5.3.1 NEPTUNE mesh file

The mesh file must be in MED format. For MED format file one can see Section 1.3.1 and for mesh generation the SALOME section 2.5.

5.3.2 NEPTUNE `param` file

The `param` file is a dataset file which is in the case directory (subdirectory DATA). There are two different ways to generate this dataset file:
a) Using the NEPTUNE GUI
b) editing the `param` file directly

The `param` file consists of several sections. As shown in Figure 5.3 the NEPTUNE GUI opens a window which is divided into two main panels: the menu bar and the selection panel. As we can see, the selection panel for the data structure is composed by 9 modules

- Special modules

Figure 5.3: NEPTUNE GUI interface (Edamox).

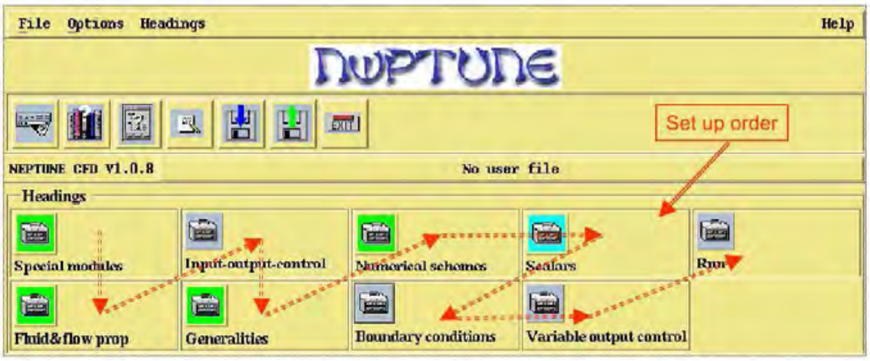


Figure 5.4: Suggested parameter order.

- Fluid&flow properties
- Input-output control
- Generalities
- Numerical schemes
- Boundary conditions
- Scalars
- Variable output control
- Run

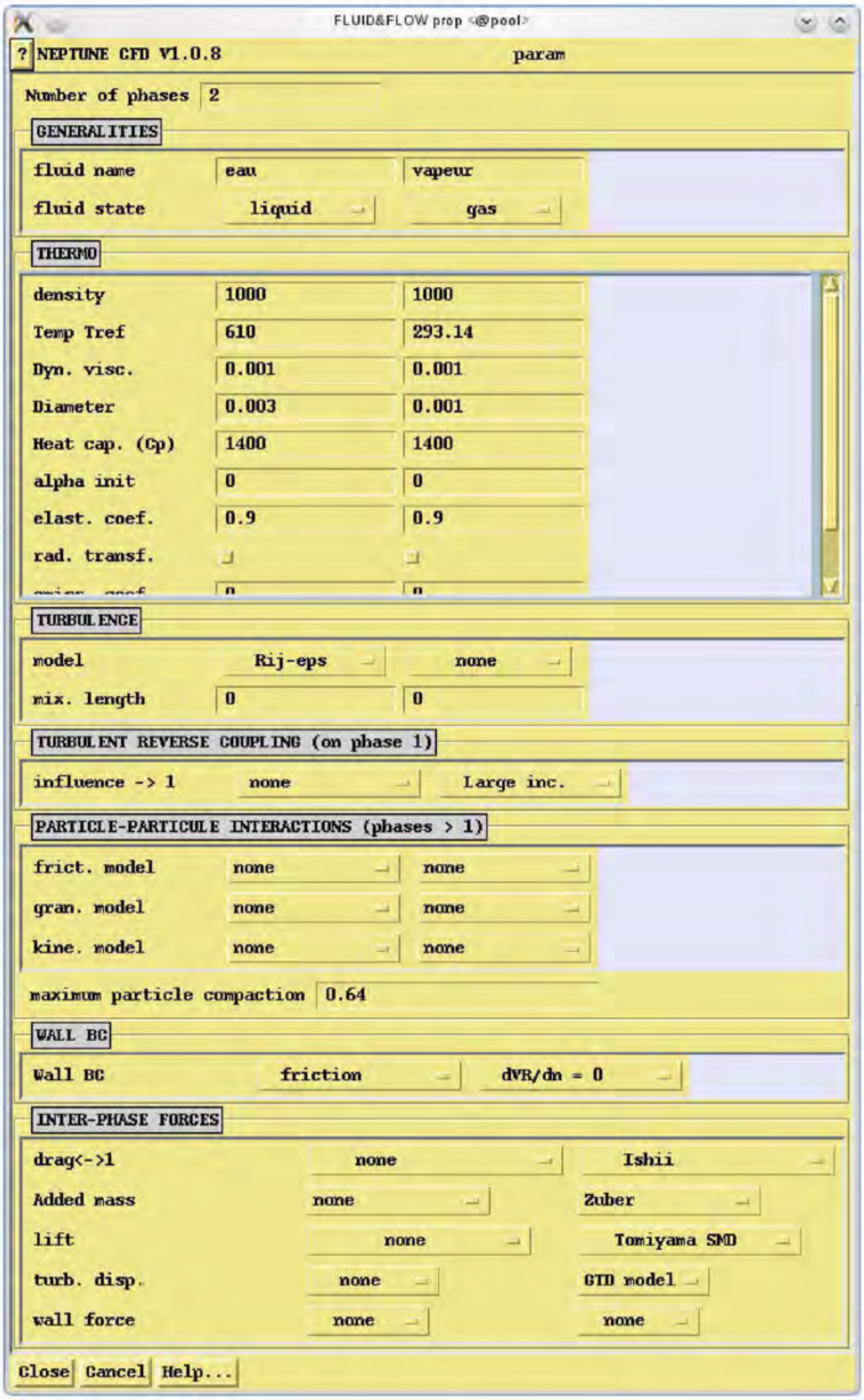


Figure 5.5: Fluid and flow properties

In order to insert the parameters of the case it is preferable to follow the order shown in Figure 5.4.

In the menu `Options` it is possible to set the level of the users. There are three different level, User, Expert, Programmer. The User Level contains less parameters respect to the Expert Level.

Special Modules

The module Special Modules allows to enable special features of the two-phase flow. The options are

- the option none for the separate phases
- the option water/steam module
- the option water/non-condensable module

Fluid&flow properties

In the `Fluid&flow properties` one can find the number of fluids and the fluid name options. All the physical properties and the turbulence models are defined in this module

Input-output control

In the input-output control one set memory allocation, the mesh file, the time step and all input/output parameters

Numerical schemes

The numerical schemes module contains the options that coupled the different equations and lead to the iterative solution of each system

Scalar

In this section one can set the scalars. In particular, there are two scalars that are enabled automatically when the water/steam module is selected in Special modules, the two total enthalpies for each phase, water and steam. Other scalars must be defined by specifying total number of scalars. The possible data that define a scalar are

- Convection → selection of the convection phase of the scalar
- T-dep → time-dependent term in the scalar equation
- Effective Diffusion → diffusion term in the scalar equation
- Laminar Dynamic Coefficient → reference diffusion coefficient
- Turbulent Schmidt → turbulent Schmidt number

- Initialization Choice → scalar initialization choice
- Type → passive scalar or total enthalpy
- Initialization value and limit values

Boundary Conditions

In general, the Boundary Conditions module consists of several options to define Dirichlet or Neumann boundary conditions over the different boundary regions. For a more complete explanation see Section 5.4.

Variable output control

The `chrono` buttons select the output of variables in the chronological post-processing files. The listing buttons enable the variables to be tracked in the listing (i.e. textual output). The probes number fields are used to track the values of variables at the probes. The values given for this case mean that results are wanted at all the probes.

Subroutines

In this module one can set the use of user subroutine. To compile this subroutine it is necessary to copy it from the USERS directory in the SRC directory.

Run

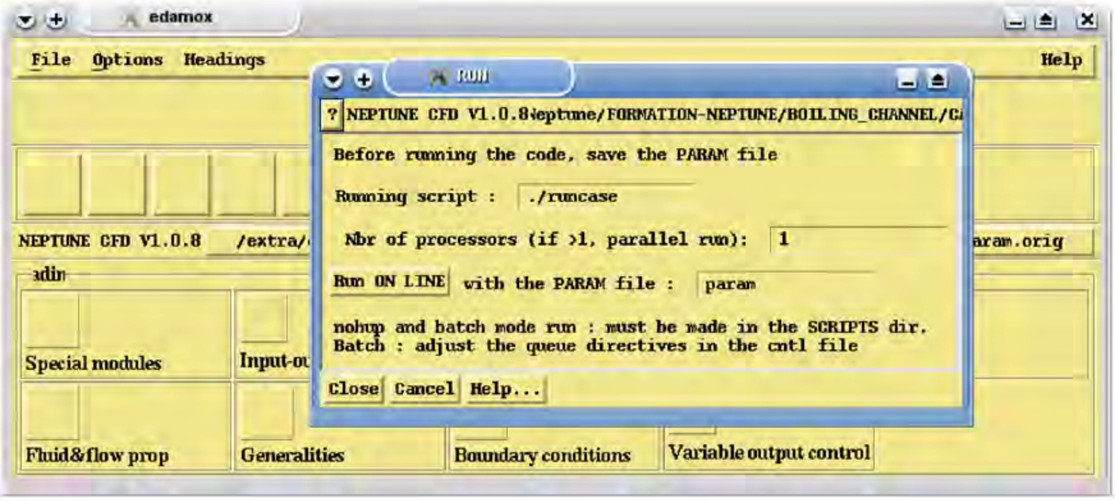


Figure 5.6: Run file

In the run module one can run the code and save the results. Before running the code, it is necessary to save the `param` file. In the module Run we set the number of processors for a parallel run and we launch the code on line with the button `Run on line`. If you decide to change the parameters of the `param` file it is necessary to re-save the file before launching the run.

`param` file

The NEPTUNE GUI generates a `param` file as

```
......
/Headings
/SPECIAL MODULES (1)
MODULE SPECIFIQUE = 1
/FLUID&FLOW prop (1)
NPHAS = 2
/GENERALITIES (2)
NOM FLUIDE =
eau;vapeur
ETAT FLUIDE =
0;1
/THERMO (2)
MASSE VOLUMIQUE =
1000;1000
TEMPERATURE REFERENCE =
610;293.14
VISCOSITE DYN =
0.001;0.001
 .......
/
/TURBULENCE (2)
/
ITURB =
2;-1
CNUTLO =
0;0
  ..............
/FLUID 1 (2)
/
UENT CONDL1 =
0;0;0;0;0
 ..............
HSTSCA =
' ';' '
/
/USER VARIABLES (2)
```

```
/
NUMUSE =
0
```

This file can also be generated directly by editing the file. The file is subdivided in various sections with characteristic key words. The same keys on the NEPTUNE GUI interface

5.4 NEPTUNE tutorial on boiling flow with interfacial area transport

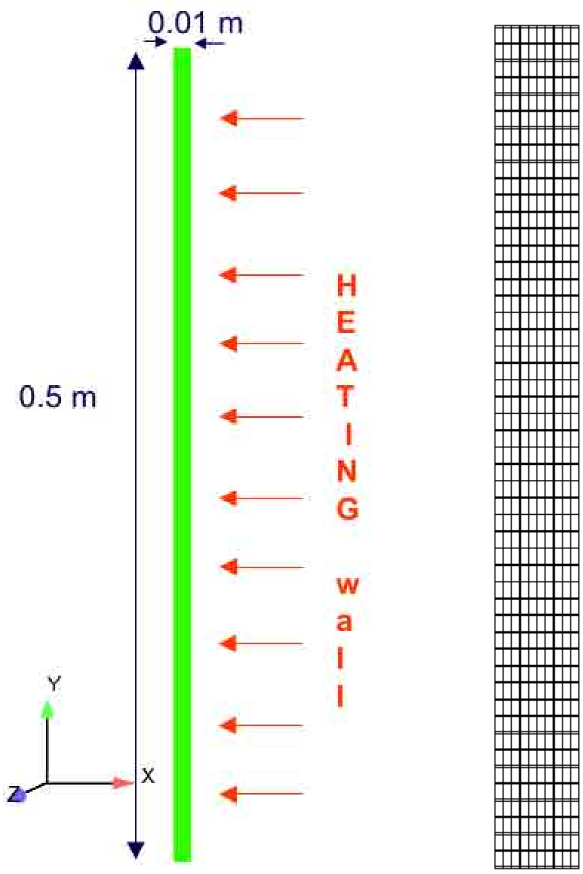
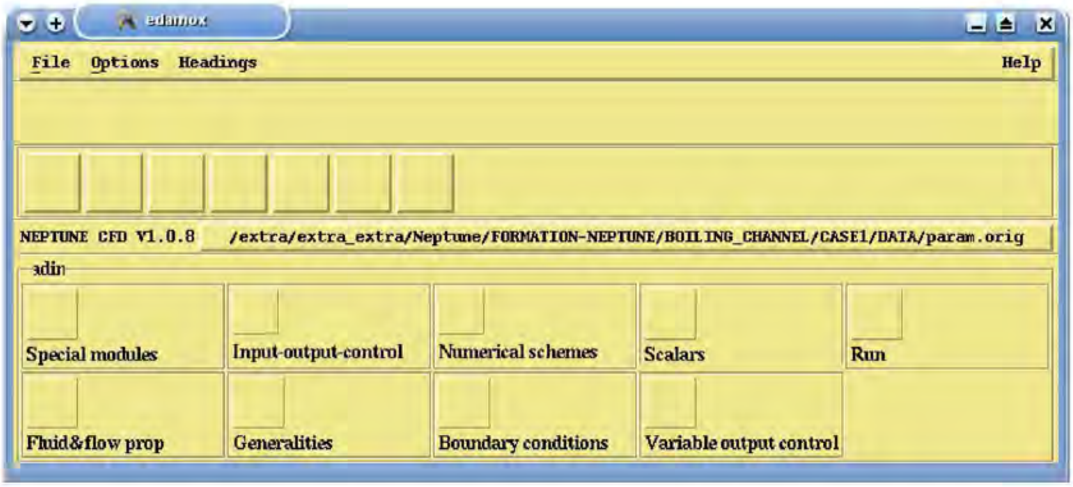


Figure 5.7: Geometry and mesh of the channel

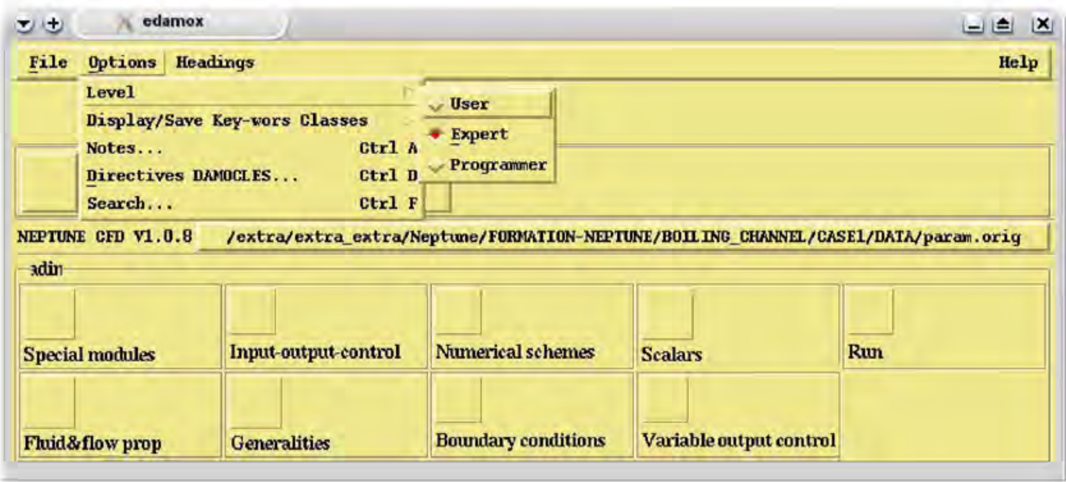
Now we present an example step by step. The case that we analyze is the standard boiling flow with interfacial area transport from NEPTUNE tutorial. For the simulation, we consider the mesh `m1.unv`. The geometry and the mesh chosen are show in Figure

5.7. As described in the previous section, we create the tree structure of the current case. Then, we copy the file mesh `m1.unv` of our geometry in the MESH folder and we open the GUI, by launching the command `./edam` from the `bin` folder.

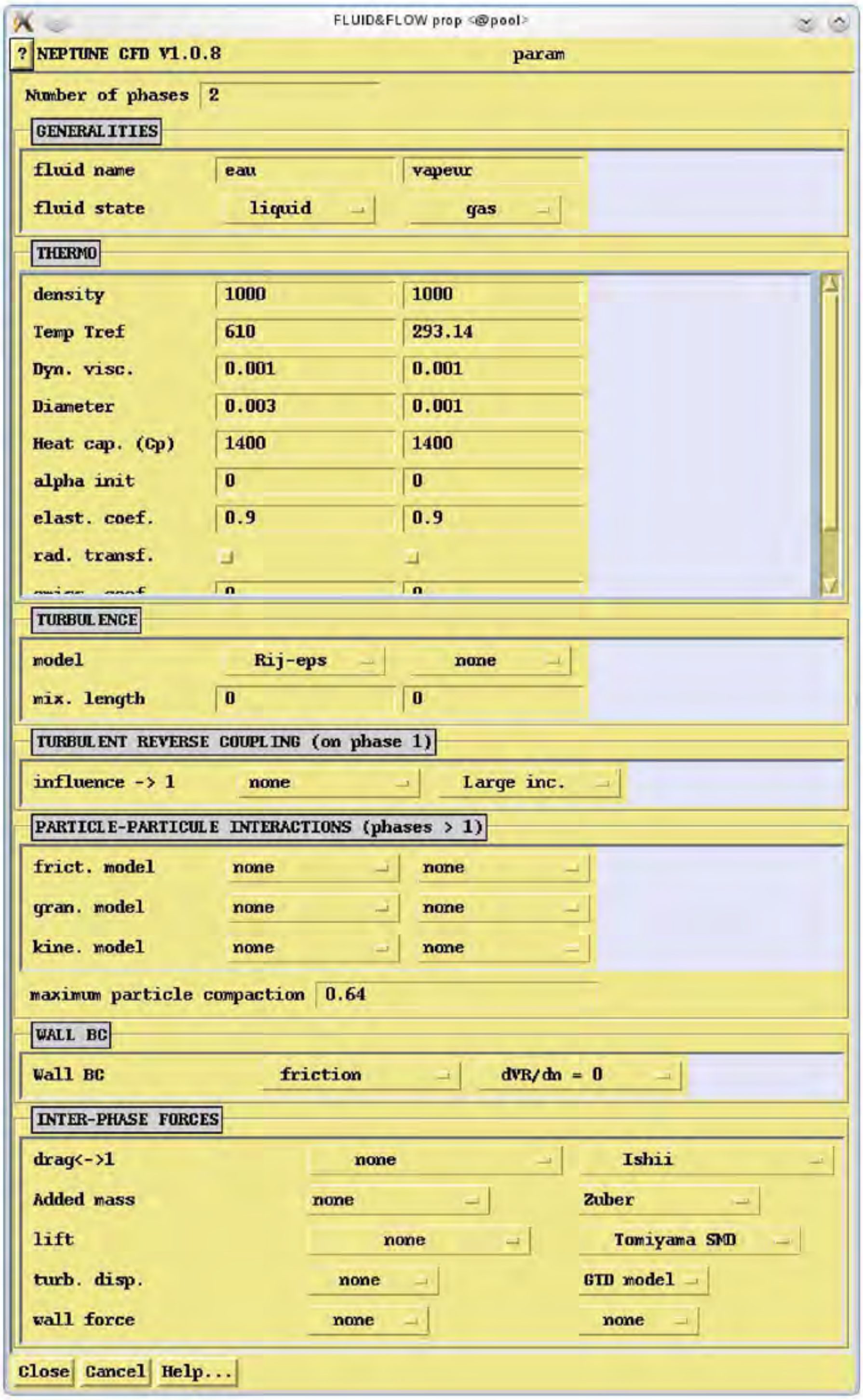
1. The GUI Edamox is open



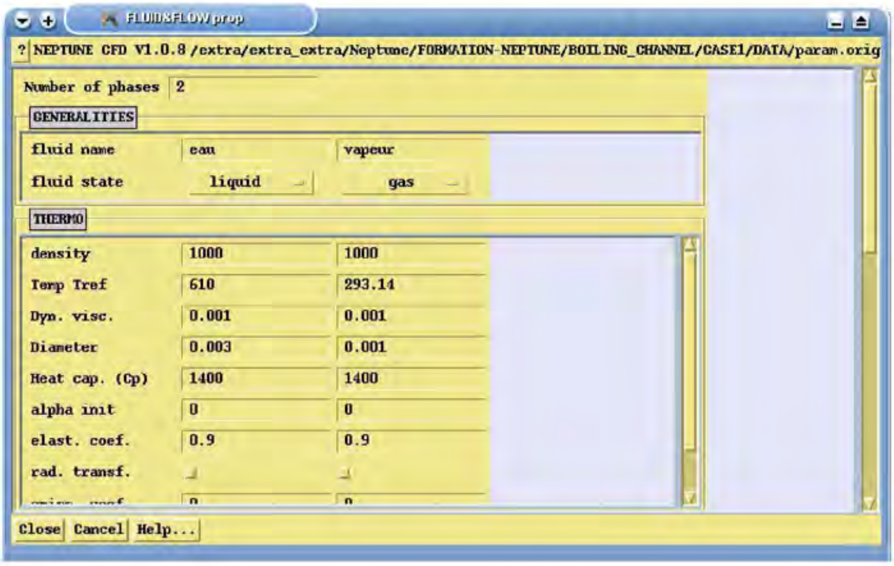
2. We must set the `expert level` in the menu Options, that allows to access to additional numerical options and activate the water/steam option



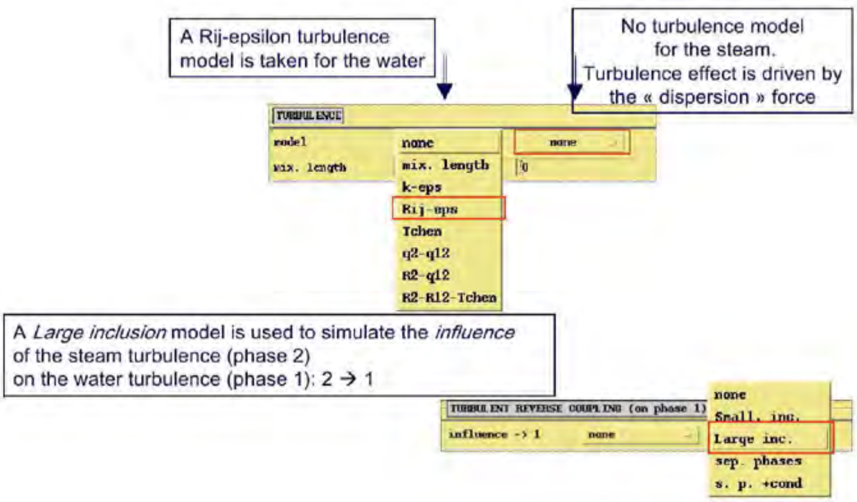
3. Open the `fluid and flow properties` panel



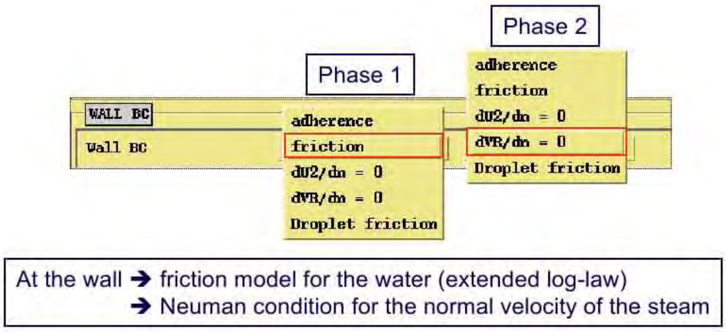
4. In this case, we have two phases, liquid and gas. Default bubble diameter is 1mm



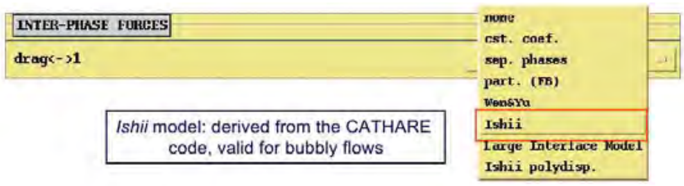
5. Specify the models chosen for the turbulence, both for the water and the steam

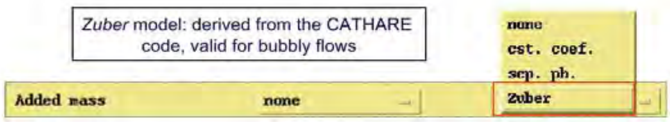


6. Set the wall boundary conditions

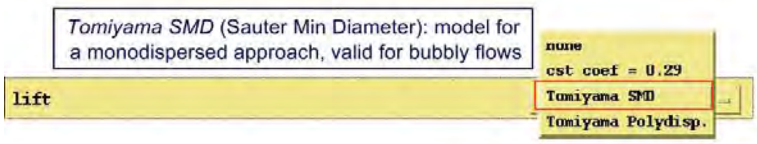


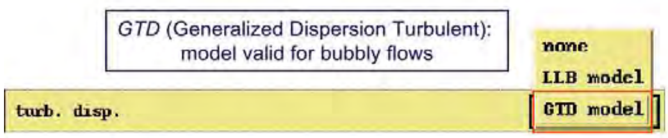
7. Set the inter-phase forces

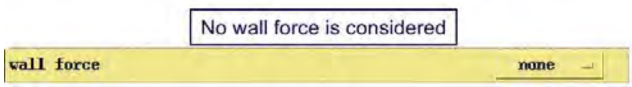




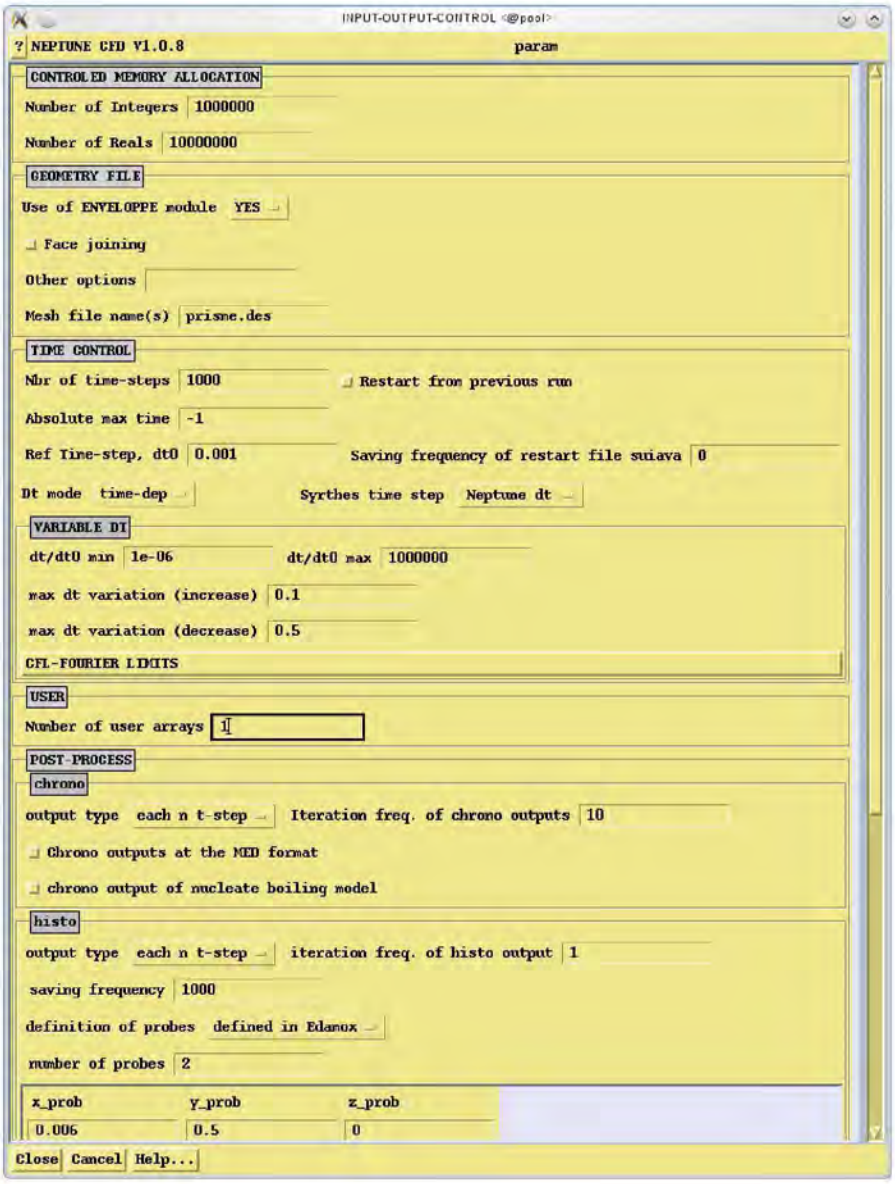
8. and also



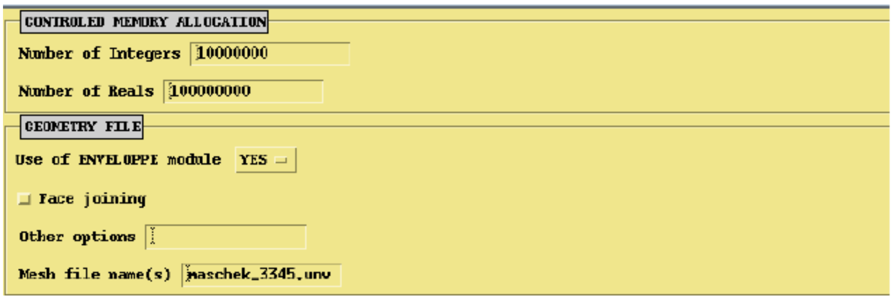




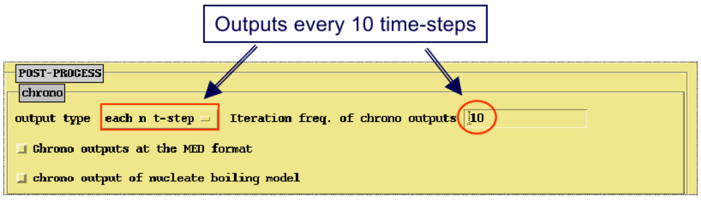
9. Open the `Input output control` panel



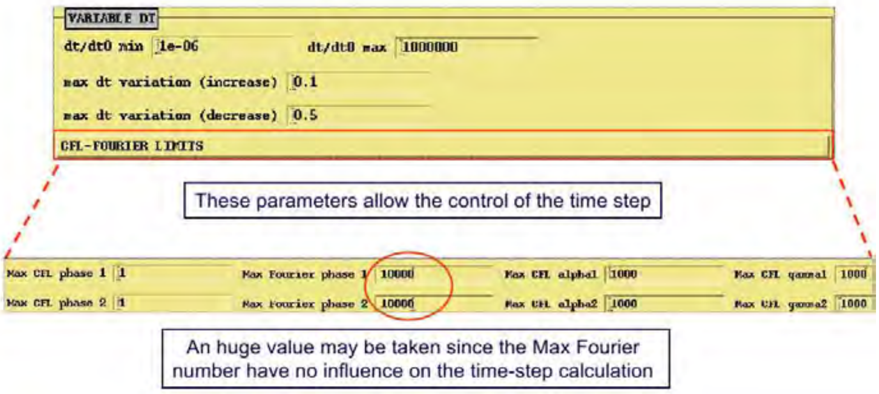
10. Set memory allocation and mesh file



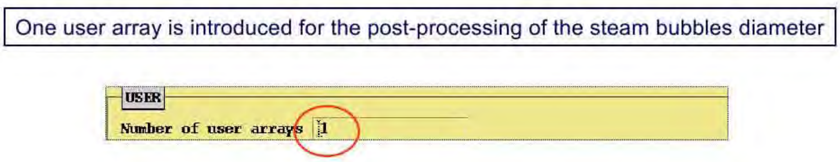
11. Set post-process output



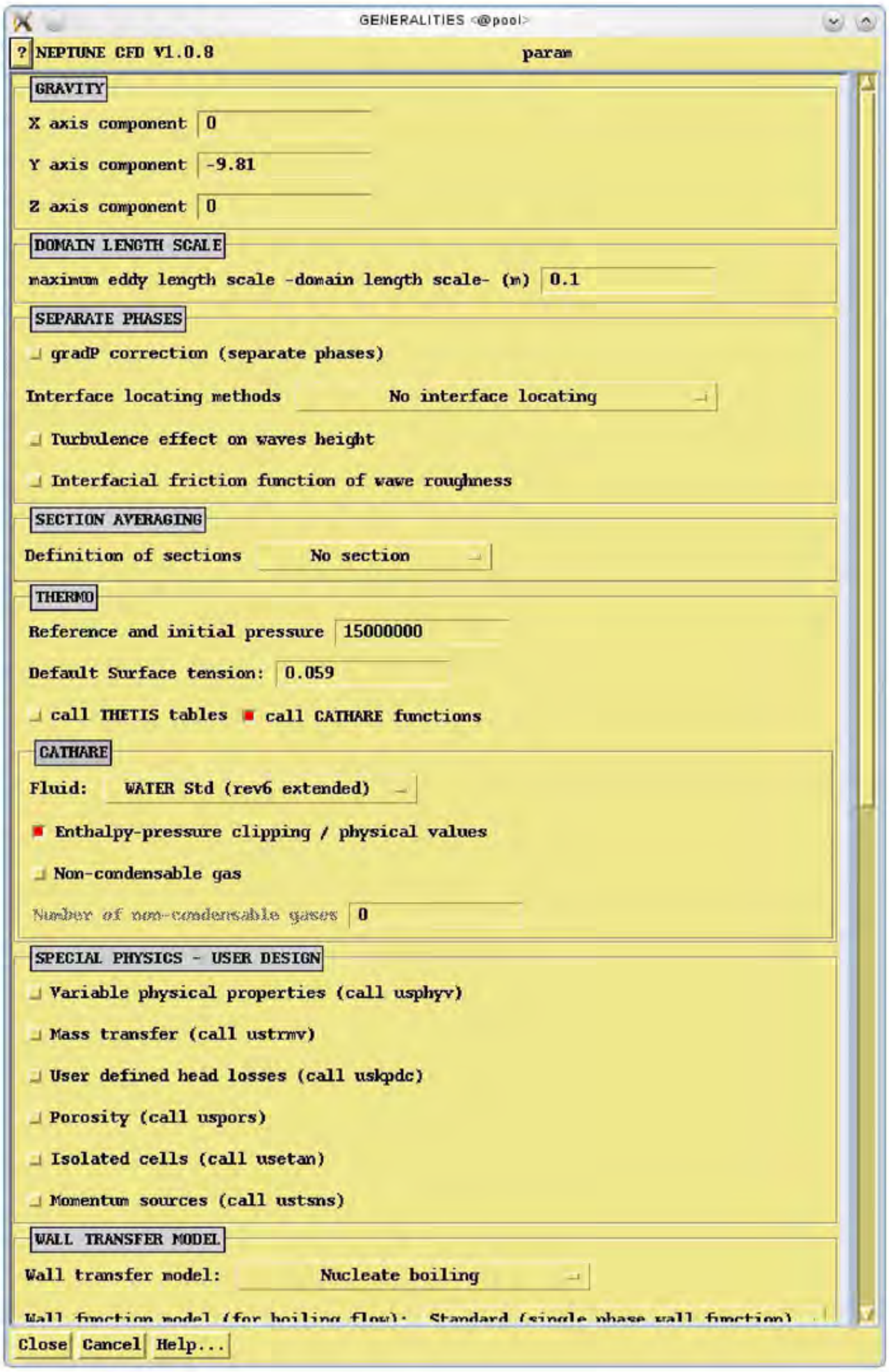
12. Set the time step `dt`



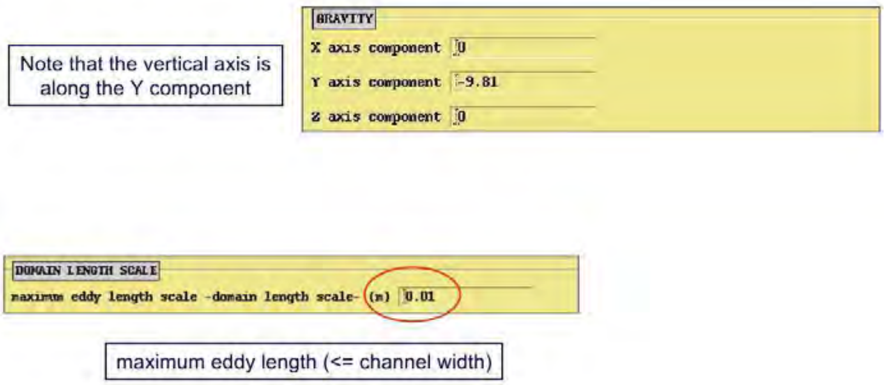
13. Set the number of user arrays



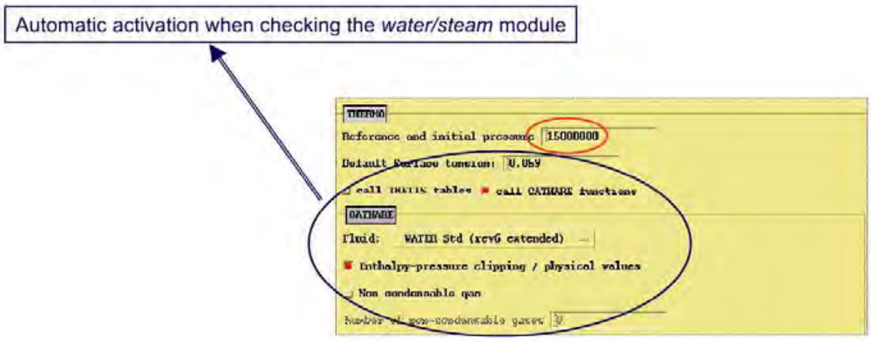
14. Open the `Generalities` panel



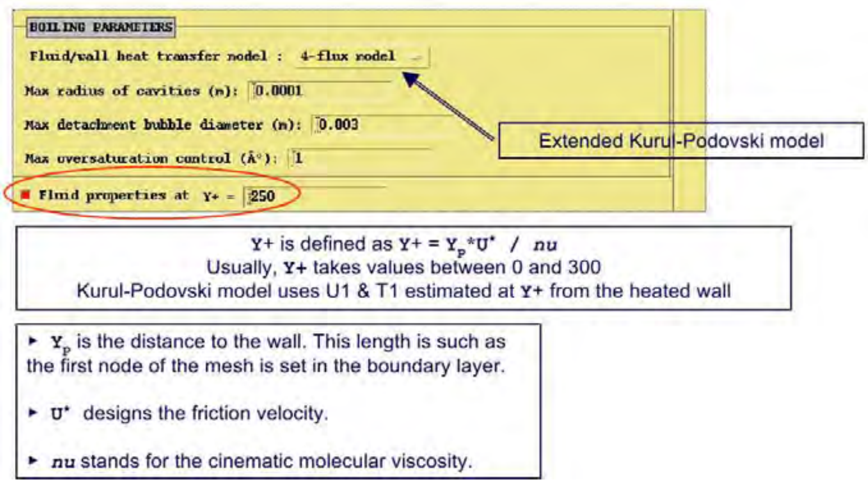
15. Set the gravity and domain length scale



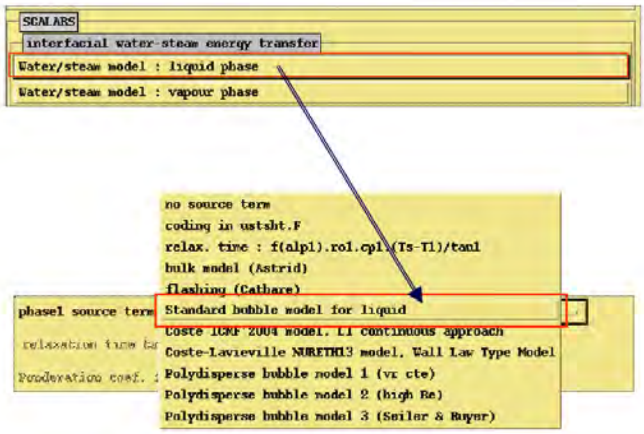
16. Set the thermodynamics and Cathare properties



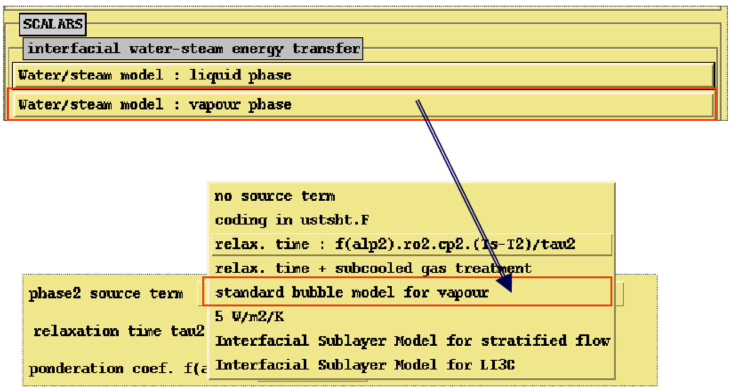
17. Set the boiling parameters



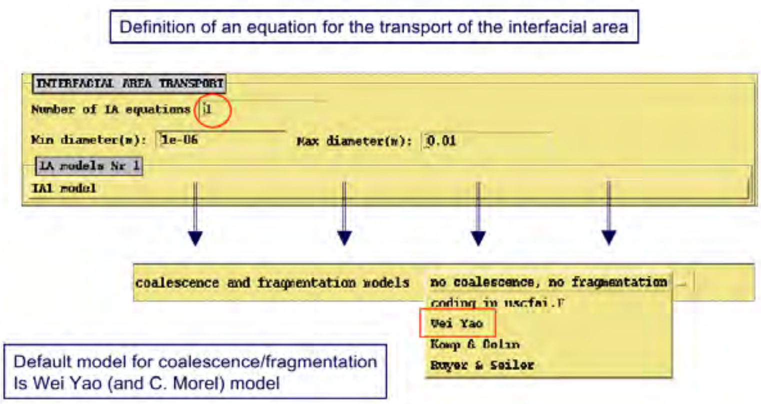
18. Set the interfacial water-steam energy transfer for the liquid face



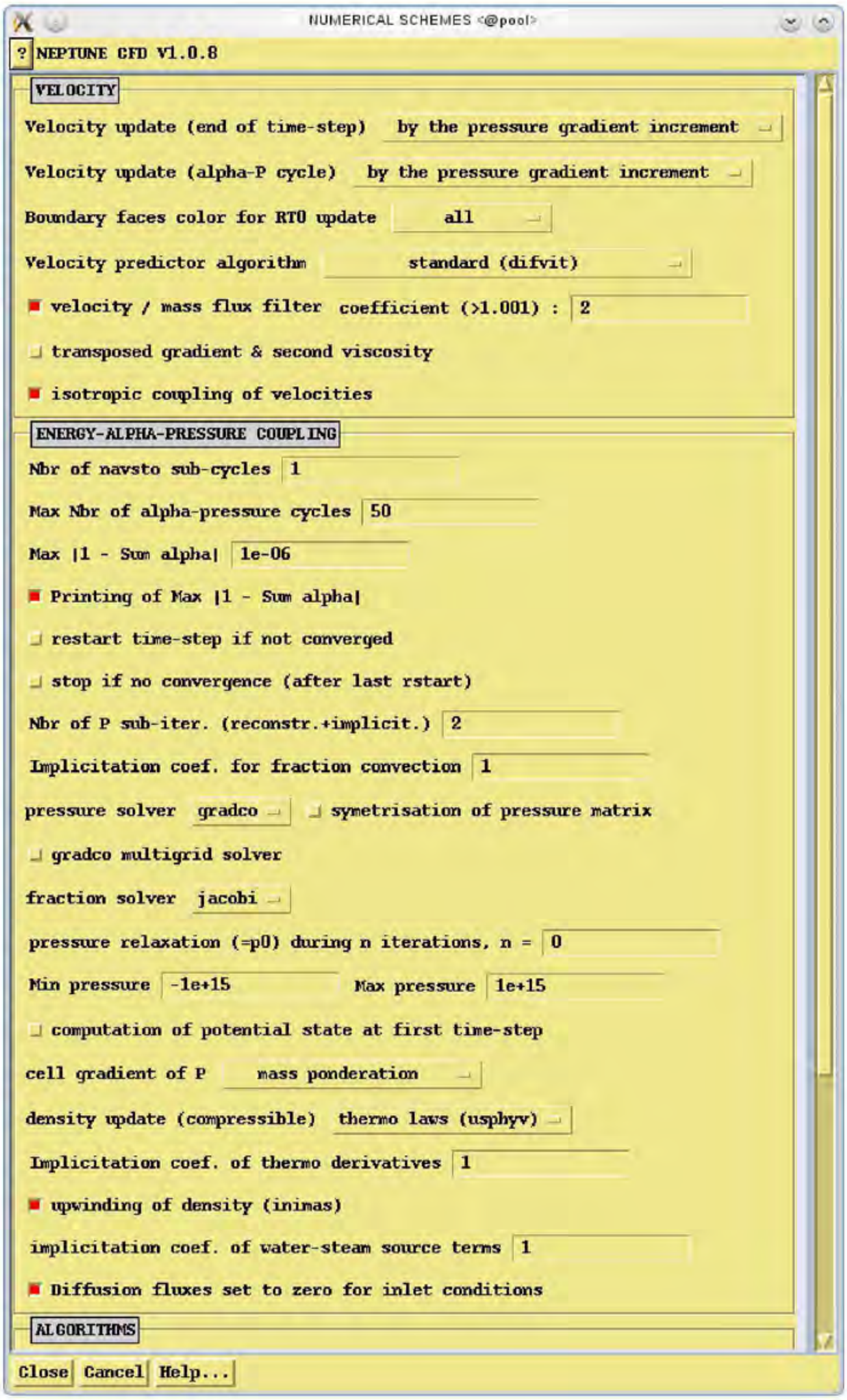
19. Set the interfacial water-steam energy transfer for the vapour face



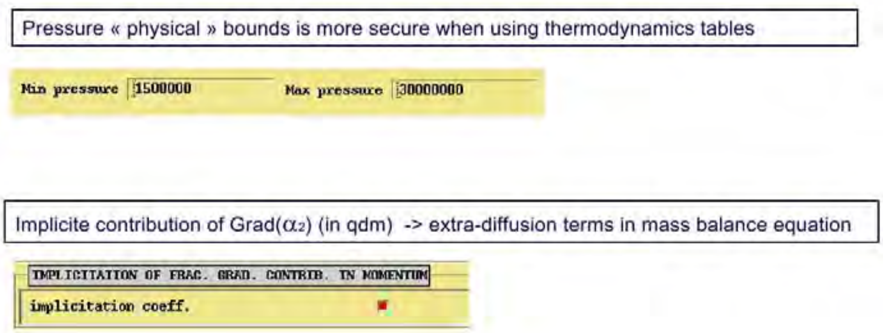
20. Set the interfacial area transport



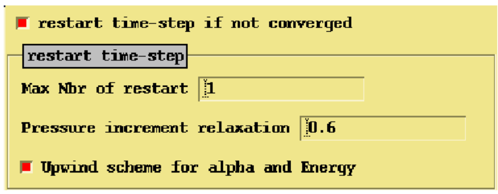
21. Open the `numerical schemes` panel



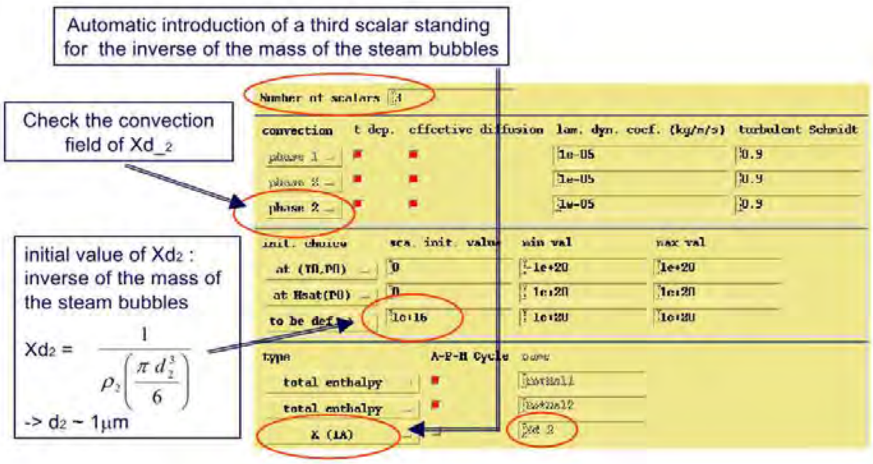
22. Set the pressure



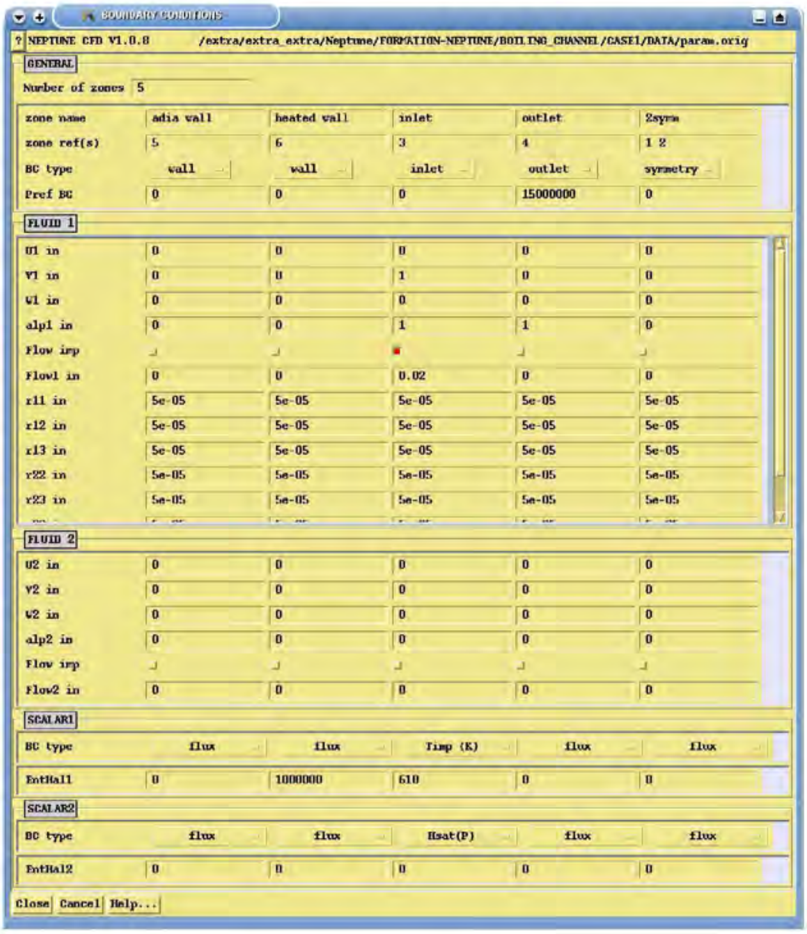
23. Set the restart time-step



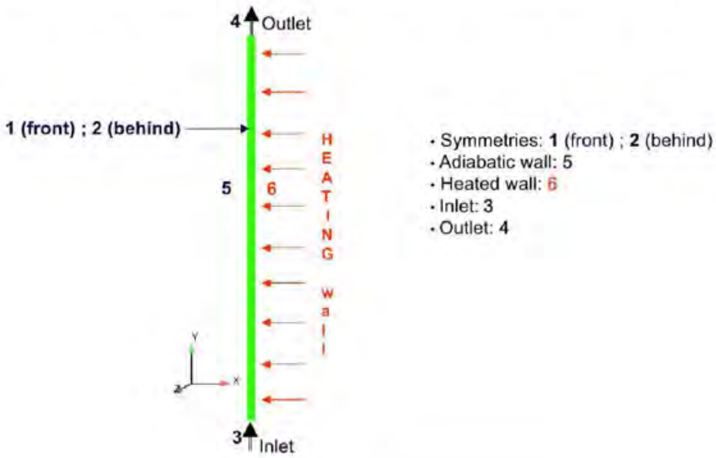
24. Open the `scalars` panel and set the scalar variables. In the current case we have three scalars, the ones settings automatically and a new scalar, that represents the inverse of the mass of the steam bubbles and then it is referred to the steam phase



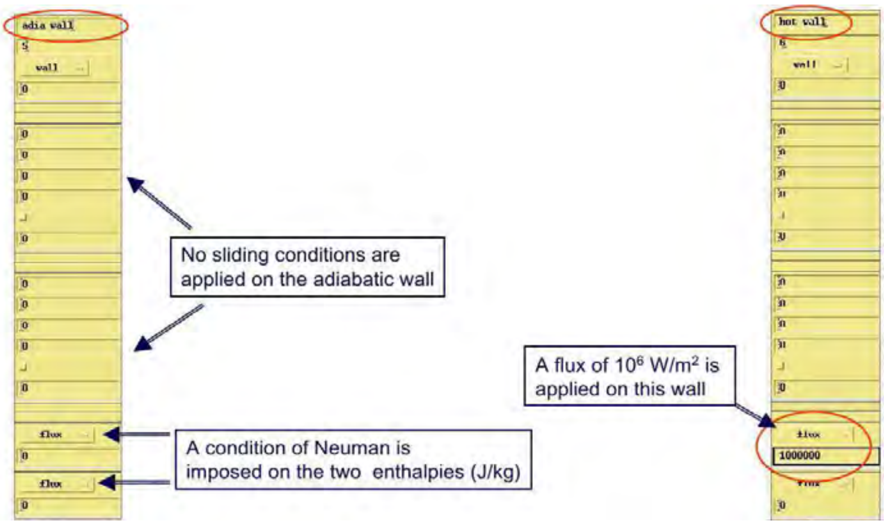
25. Open the `boundary conditions` panel



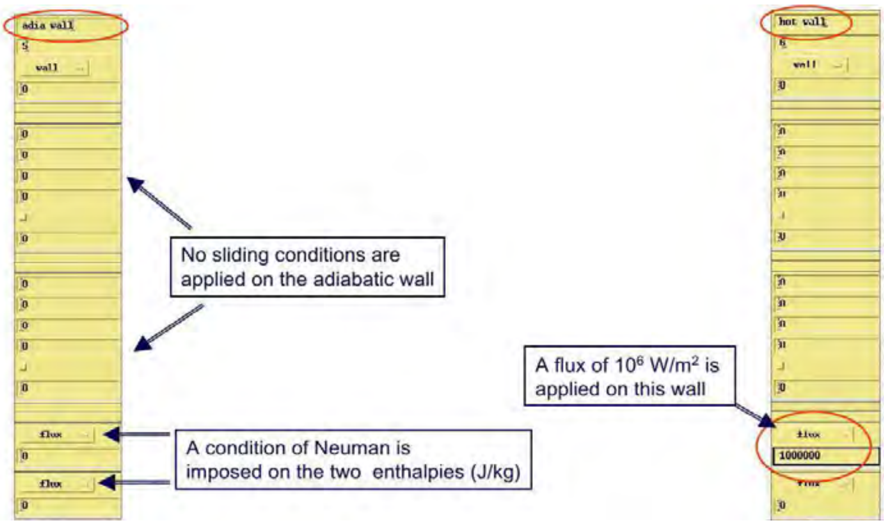
26. In this case, we set the following boundary conditions: symmetry for 1 and 2, adiabatic wall for 5, heated wall for 6, inlet for 3 and outlet for 4.



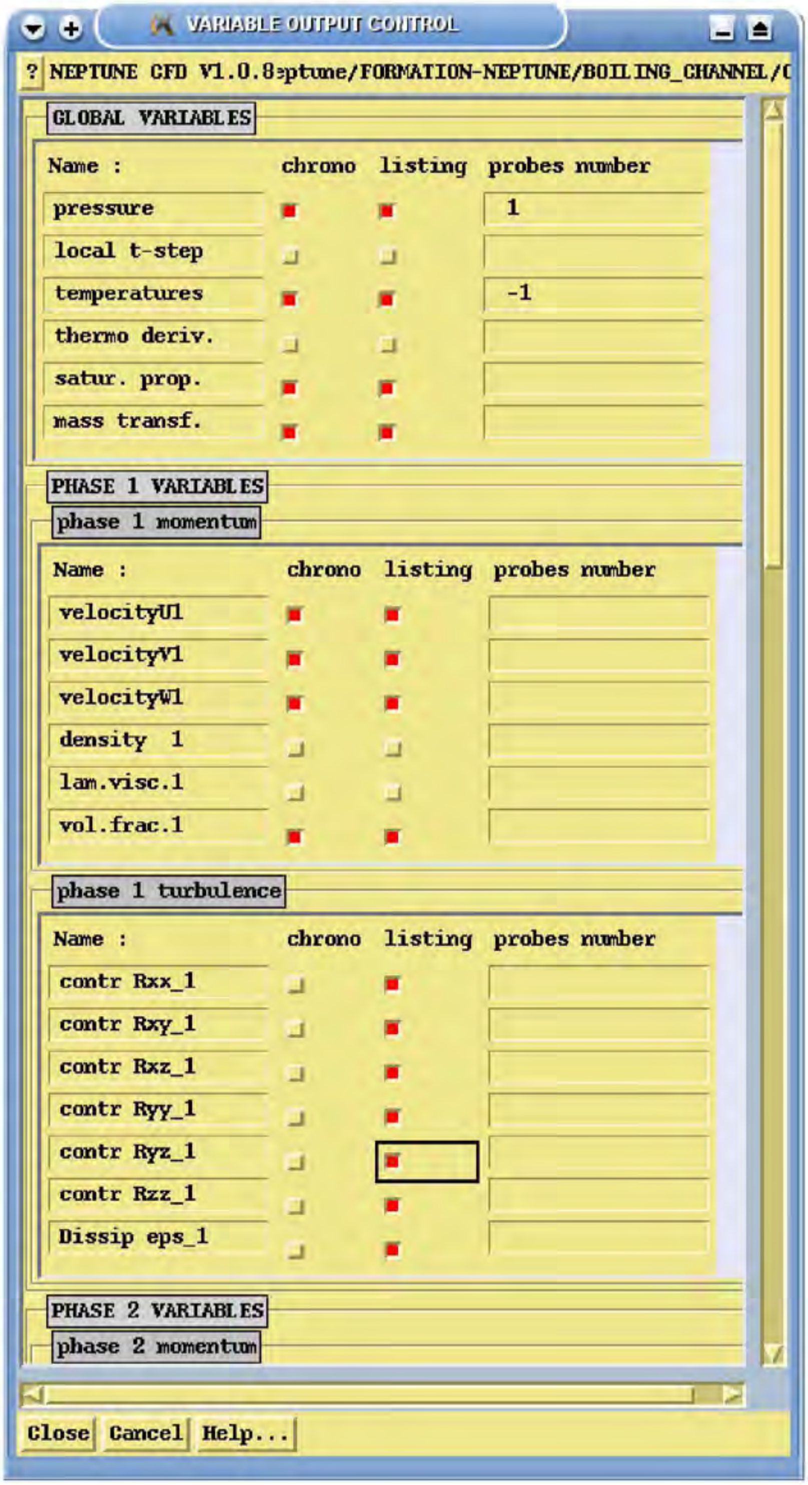
27. Set the adiabatic and heated conditions



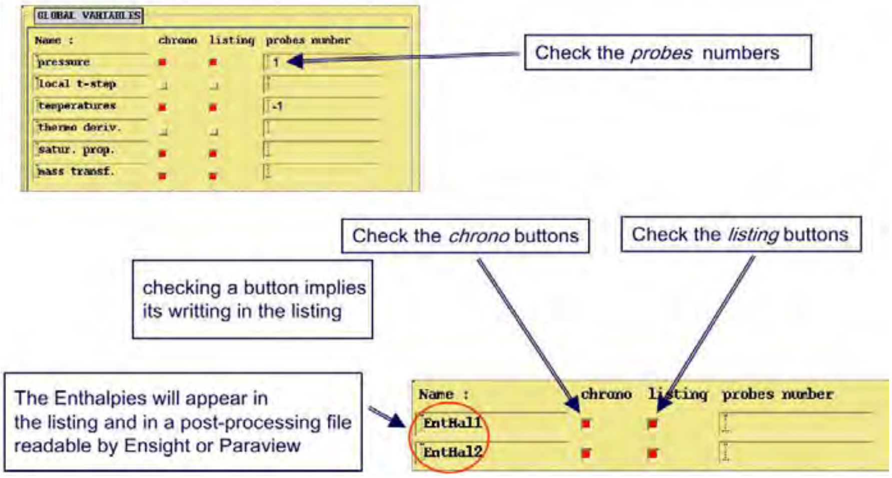
28. Set the inlet and outlet conditions



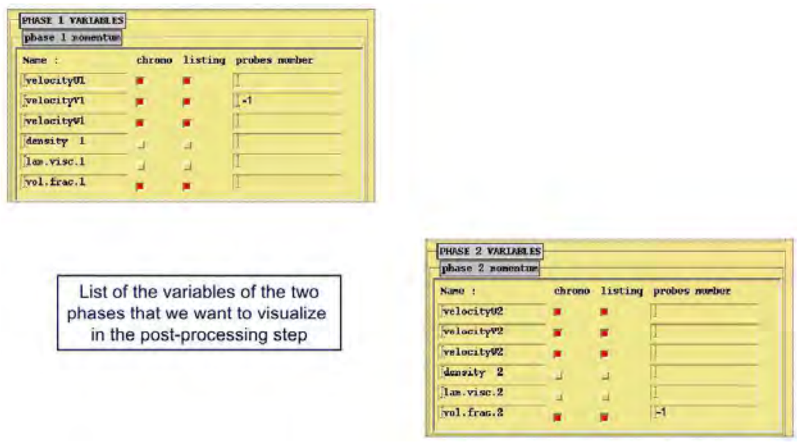
29. Open the `variable output control` panel



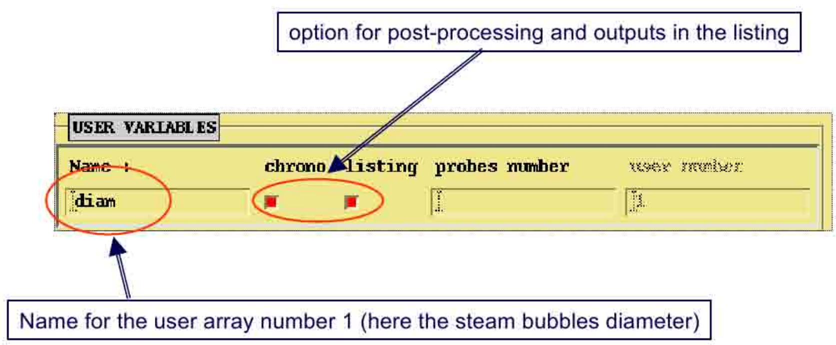
30. Set global variables



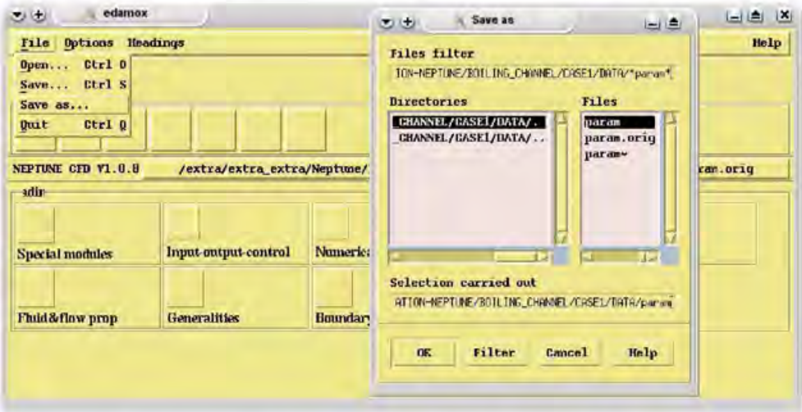
31. Set phase 1 and 2 variables



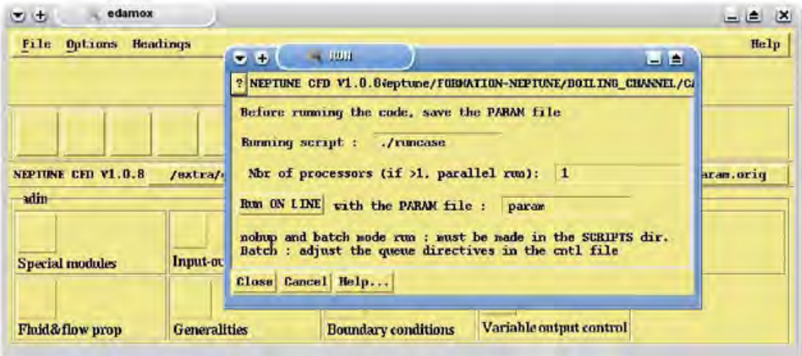
32. Set user variables



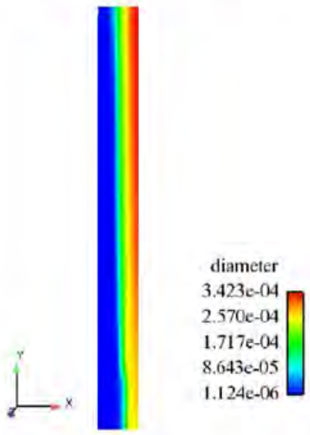
33. Enter the subroutine panel and use the subroutine `uscase.F`. To compile this subroutine it is necessary to copy it from the `USERS` directory in the `SRC` directory
34. Before running the code, it is necessary to save the `param` file

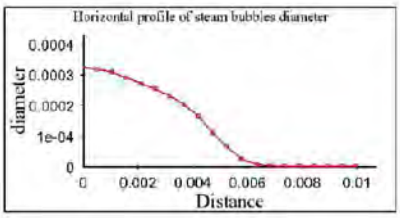


35. Set the number of processors and launch the code on line with the button `Run on line`



36. We can see the results for the steam bubbles diameter





Bibliography

[1] CRESCO-ENEA GRID Project: http://www.cresco.enea.it. 11

[2] SATURNE CFD software: http://www.code-saturne.org. 58

[3] F. Archambeau, N. Mehitoua and M. Sakiz, *Code SATURNE: A Finite Volume Code for Turbulent flows*, Int. J. Finite Volumes (2004) 58

[4] SALOME platform: http://www.salome-platform.org. 23, 30

[5] G. David, T.Chevalier and G. Meunier, *Unification of Physical Data Models. Application in a Platform for Numerical Simulation: SALOME* Magnetics IEEE Transactions, Volume: 43 (4), pp. 1661-1664 2007 30

[6] PARAVIEW visualization software: http://www.paraview.org. 27

[7] VTK visualization software: http://www.vtk.org. 26

[8] XDMF library: http://www.xdmf.org. 18

[9] HDF5 library: http://www.hdfgroup.org/HDF5/. 16

[10] R. F. Kulak and C. Fiala, *NEPTUNE: A System of Finite Element Programs for Three-Dimensional Nonlinear Analysis*, Nuclear Engineering and Design, 106, pp. 47-68 (1988) 112

[11] R.F. Kulak and C Fiala, *NEPTUNE: A system of finite element programs for three-dimensional nonlinear analysis*, Nuclear Engineering and Design, Vol. 106 (1), pp.47-68 (1988) 112

[12] D. Bestion and A. Guelfi, *Status and perspective of two-phase flow modelling in the NEPTUNE multi-scale thermal hydraulic platform for nuclear reactor simulation*, Nuclear Engineering and Technology, vol. 37 (6), (2005). 112

[13] J. Lavieville, E. Quemerais, S. Mimouni, and N. Mechitoua, NEPTUNE CFD V1.0 theory manual, EDF, 2006. 112

[14] Botjan Konar and Borut Mavko, *Simulation of Boiling Flow Experiments Close to CHF with the NEPTUNE CFD Code*, Hindawi Publishing Corporation Science and Technology of Nuclear Installations Volume 2008, Article ID 732158, 8 pages 112

[15] TRIO_U CFD software: http://www-trio-u.cea.fr. 94

[16] T. Hohnea, S. Kliema and U. Bieder, *Modeling of a buoyancy-driven flow experiment at the ROCOM test facility using the CFD codes CFX-5 and TRIO_U*, Nuclear Engineering and Design Volume 236, Issue 12, June 2006, Pages 1309-1325 94

[17] U. Biedera, and E. Graffardb, *Benchmarking of CFD Codes for Application to Nuclear Reactor Safety Qualification of the CFD code TRIO_U for full scale reactor applications*, Nuclear Engineering and Design Volume 238, Issue 3, March 2008, Pages 671-679 94

[18] U. Biedera, G. Faucheta, S. Betinb, N. Kolevc, and D. Popovd, *Simulation of mixing effects in a VVER-1000 reactor*, Nuclear Engineering and Design Volume 237, Issues 15-17, September 2007, Pages 1718-1728 94