

EDF R&D



FLUID DYNAMICS, POWER GENERATION AND ENVIRONMENT DEPARTMENT
SINGLE PHASE THERMAL-HYDRAULICS GROUP

6, QUAI WATIER
F-78401 CHATOU CEDEX

TEL: 33 1 30 87 75 40
FAX: 33 1 30 87 79 16

APRIL 2013

Code_Saturne documentation

***Code_Saturne* version 2.0.4 tutorial**

contact: saturne-support@edf.fr



EDF R&D	<i>Code_Saturne</i> version 2.0.4 tutorial	<i>Code_Saturne</i> documentation Page 2/ 120
---------	--	---

TABLE OF CONTENTS

I	INTRODUCTION	7
1	Introduction	8
II	SIMPLE JUNCTION TEST CASE	9
1	General description	10
1.1	OBJECTIVE	10
1.2	DESCRIPTION OF THE CONFIGURATION	10
1.3	CHARACTERISTICS	10
1.4	MESH CHARACTERISTICS	11
2	CASE 1: Basic calculation	11
2.1	CALCULATION OPTIONS	11
2.2	INITIAL AND BOUNDARY CONDITIONS	12
2.3	PARAMETERS AND USER ROUTINES	13
2.4	RESULTS	13
III	FULL DOMAIN	14
1	General description	15
1.1	OBJECTIVE	15
1.2	DESCRIPTION OF THE CONFIGURATION	15
1.3	CHARACTERISTICS	15
1.4	MESH CHARACTERISTICS	16
1.5	SUMMARY OF THE DIFFERENT CALCULATIONS	16
2	CASE 2: Passive scalar with various boundary conditions and output management	17
2.1	CALCULATION OPTIONS	17
2.2	INITIAL AND BOUNDARY CONDITIONS	17
2.3	PARAMETERS AND USER ROUTINES	18
2.4	OUTPUT MANAGEMENT	19
2.5	RESULTS	19

3	CASE 3: Time dependent boundary conditions and variable fluid density . . .	22
3.1	CALCULATION OPTIONS	22
3.2	INITIAL AND BOUNDARY CONDITIONS	22
3.3	VARIABLE DENSITY	23
3.4	PARAMETERS	23
3.5	USER ROUTINE	23
3.6	OUTPUT MANAGEMENT	24
3.7	CALCULATION RESTART	25
3.8	RESULTS	25
4	CASE 4: Head loss, parallelism and spatial average	28
4.1	CALCULATION OPTIONS	28
4.2	INITIAL AND BOUNDARY CONDITIONS	28
4.3	VARIABLE DENSITY	29
4.4	HEAD LOSS	29
4.5	PARAMETERS	30
4.6	USER ROUTINES	30
4.7	OUTPUT MANAGEMENT	31
4.8	RESULTS	31
	 IV STRATIFIED JUNCTION	 34
1	General description	35
1.1	OBJECTIVE	35
1.2	DESCRIPTION OF THE CONFIGURATION	35
1.3	CHARACTERISTICS	35
1.4	MESH CHARACTERISTICS	36
2	CASE 5: Stratified junction	36
2.1	CALCULATION OPTIONS	36
2.2	INITIAL AND BOUNDARY CONDITIONS	37
2.3	VARIABLE DENSITY AND DYNAMIC VISCOSITY	37
2.4	PARAMETERS	37
2.5	OUTPUT MANAGEMENT	38
2.6	USER ROUTINES	38
2.7	RESULTS	39
	 V STEP BY STEP SOLUTION	 42
1	SOLUTION FOR CASE 1	43

2	SOLUTION FOR CASE 2	80
3	SOLUTION FOR CASE 3	98
4	SOLUTION FOR CASE 4	105
5	SOLUTION FOR CASE 5	109

Part I

INTRODUCTION

1 Introduction

Code_Saturne is a system designed to solve the Navier-Stokes equations in the cases of 2D, 2D axisymmetric or 3D flows. Its main module is designed for the simulation of flows which may be steady or unsteady, laminar or turbulent, incompressible or potentially dilatable, isothermal or not. Scalars and turbulent fluctuations of scalars can be taken into account. The code includes specific modules, referred to as “specific physics”, for the treatment of lagrangian particle tracking, semi-transparent radiative transfer, gas, pulverized coal and heavy fuel oil combustion, electricity effects (Joule effect and electric arcs) and compressible flows. The code also includes an engineering module, *Matisse*, for the simulation of nuclear waste surface storage.

Code_Saturne relies on a finite volume discretization and allows the use of various mesh types which may be hybrid (containing several kinds of elements) and may have structural non-conformities (hanging nodes).

The present document is a tutorial for *Code_Saturne* version 2.0.4. It presents five simple test cases and guides the future *Code_Saturne* user step by step into the preparation and the computation of the cases.

The test case directories, containing the necessary meshes and data are available in the **examples** directory.

This tutorial focuses on the procedure and the preparation of the *Code_Saturne* computations. For more elements on the structure of the code and the definition of the different variables, it is highly recommended to refer to the user manual.

Code_Saturne is free software; you can redistribute it and/or modify it under the terms of the GNU General Public License as published by the Free Software Foundation; either version 2 of the License, or (at your option) any later version. *Code_Saturne* is distributed in the hope that it will be useful, but WITHOUT ANY WARRANTY; without even the implied warranty of MERCHANTABILITY or FITNESS FOR A PARTICULAR PURPOSE. See the GNU General Public License for more details.

Part II

SIMPLE JUNCTION TEST CASE

1 General description

1.1 Objective

The aim of this case is to train the user of *Code_Saturne* on an oversimplified 2D junction including an inlet, an outlet, walls and symmetries.

1.2 Description of the configuration

The configuration is two-dimensional.

It consists of a simple junction as shown on figure II.1. The flow enters through a hot inlet into a cold environment and exits as indicated on the same figure. This geometry can be considered as a very rough approximation of the cold branch and the downcomer of the vessel in a nuclear pressurized water reactor. The effect of temperature on the fluid density is not taken into account in this first example.

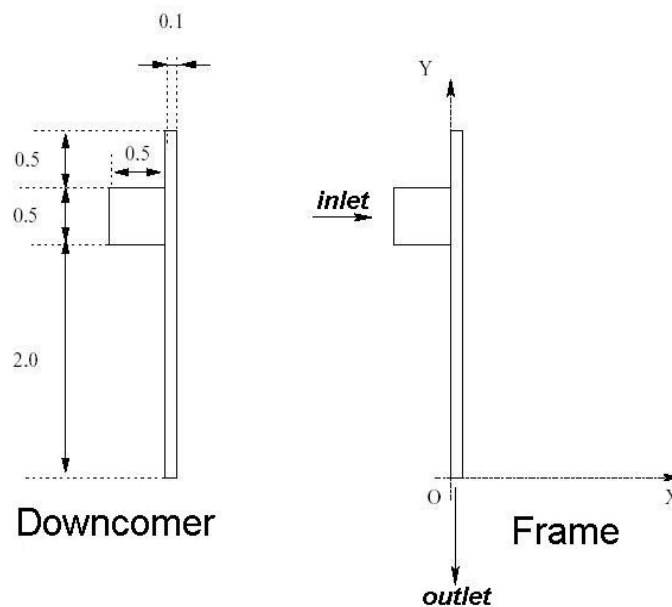


Figure II.1: Geometry of the downcomer

1.3 Characteristics

Characteristics of the geometry and the flow:

Height of downcomer	$H = 3.00 \text{ m}$
Thickness of downcomer	$E_d = 0.10 \text{ m}$
Diameter of the cold branch	$D_b = 0.50 \text{ m}$
Inlet velocity of fluid	$V = 1 \text{ m.s}^{-1}$

Physical characteristics of fluid:

The initial water temperature in the domain is equal to 20°C. The inlet temperature of water in the cold branch is 300°C. Water characteristics are considered constant and their values taken at 300°C and $150 \times 10^5 \text{ Pa}$:

- density: $\rho = 725.735 \text{ kg.m}^{-3}$

- dynamic viscosity: $\mu = 0.895 \times 10^{-4} \text{ kg.m}^{-1}.\text{s}^{-1}$
- specific heat: $C_p = 5483 \text{ J.kg}^{-1}.\text{°C}^{-1}$
- Thermal Conductivity = $0.02495 \text{ W.m}^{-1}.\text{K}^{-1}$

1.4 Mesh characteristics

Figure II.2 shows a global view of the downcomer mesh. This two-dimensional mesh is composed of 700 cells, which is very small compared to those used in real studies. This is a deliberate choice so that tutorial calculations run fast.

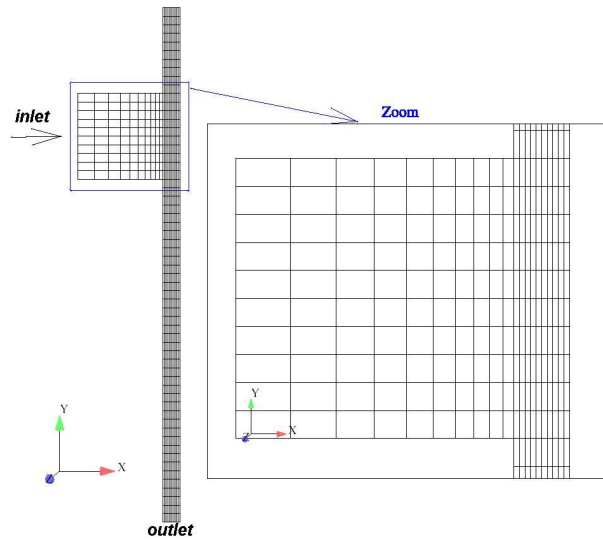


Figure II.2: Geometry of the downcomer

Note that here the case is two-dimensional but *Code_Saturne* always operates on three-dimensional mesh elements (cells). The present mesh is composed of a layer of hexahedrons created from the 2D mesh shown on figure II.2 by extrusion (elevation) in the Z direction. The virtual planes parallel to Oxy will have “sliding” (“symmetry”) conditions to account for the two-dimensional character of the configuration.

Type: structured mesh

Coordinates system: cartesian, origin on the edge of the main pipe at the outlet level, on the nozzle side (figure II.1)

Mesh generator used: SIMAIL

Color definition: see figure II.3. To specify boundary conditions on the boundary faces of the mesh, the latter have to be identified. It is commonly done by assigning an integer to each of them, characteristic of the boundary region they belong to. This integer is referred to as “color” or “reference”.

2 CASE 1: Basic calculation

2.1 Calculation options

Most of the options used in this calculation are default options of *Code_Saturne*.

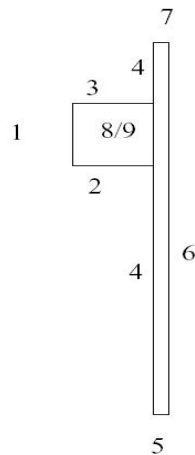


Figure II.3: Colors of the boundary faces

- Flow type: steady flow
- Turbulence model: $k - \epsilon$
- Scalar(s): 1 - temperature
- Physical properties: uniform and constant

2.2 Initial and boundary conditions

- Initialization: none (default values)

The boundary conditions are defined as follows:

- **Flow inlet:** Dirichlet condition, an inlet velocity of 1 m.s^{-1} and an inlet temperature of 300°C are imposed
- **Outlet:** default values
- **Walls:** default values

Figure [II.3](#) shows the colors used for boundary conditions and table [II.1](#) defines the correspondance between the colors and the type of boundary condition to use.

Do not forget to enter the value of the hydraulic diameter, adapted to the current inlet (used for turbulence entry conditions).

Colors	Conditions
1	Inlet
5	Outlet
2 3 4 6 7	Wall
8 9	Symmetry

Table II.1: Boundary conditions and associated references

2.3 Parameters and User routines

All parameters necessary to this study can be defined through the Graphical Interface without using any user Fortran files.

Calculation control parameters	
Number of iterations	30
Relaxation coefficient	0.9
Output period for post-processing files	1

2.4 Results

Figure II.4 presents the results obtained at different iterations in the calculation. They were plotted from the post-processing files, with EnSight.

Note: since the “steady flow” option has been chosen, the evolution of the flow iteration after iteration has no physical meaning. It is merely an indication of the rapidity of convergence towards the (physical) steady state.

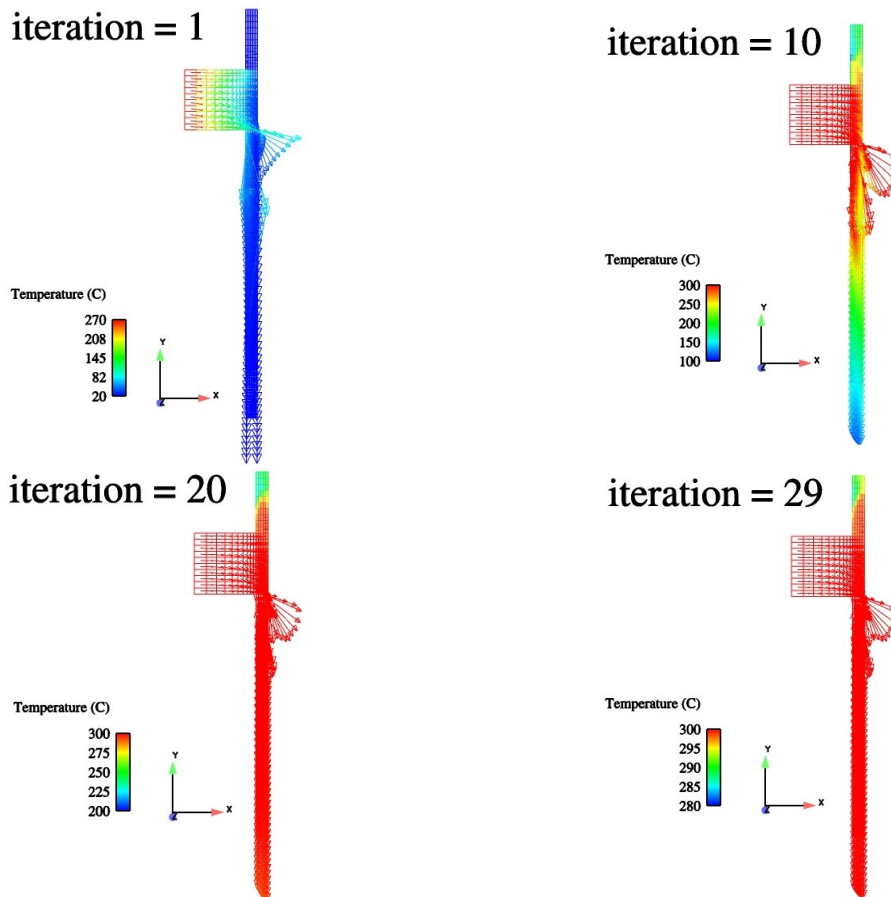


Figure II.4: Water velocity field colored by temperature at different time steps

Part III

FULL DOMAIN

1 General description

1.1 Objective

This aim of this case is to tackle the merging of initially separate meshes into a single fluid domain. The questions of mesh joining and hanging nodes will be addressed. The test case will then be used to present more complex calculations, with time dependent variables and Fortran user routines.

1.2 Description of the configuration

The fluid domain is composed of three separate meshes, very roughly representing elements of a nuclear pressurized water reactor vessel:

- the downcomer
- the vessel's bottom
- the lower core plate and core

Figure III.1 represents the complete domain. The flow circulates from the top left horizontal junction to the right vertical outlet.

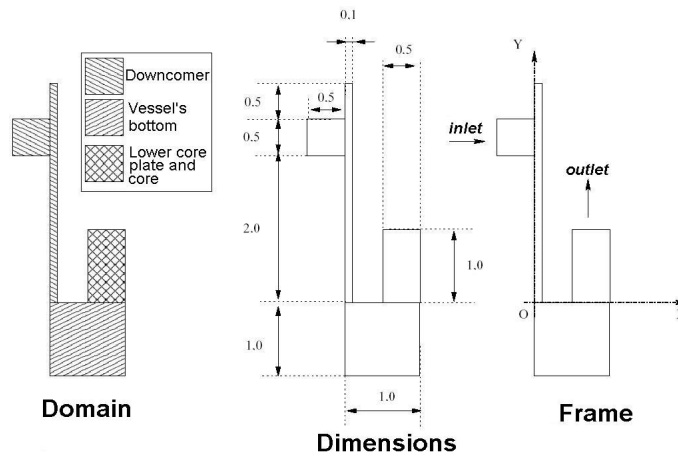


Figure III.1: Geometry of the complete domain

1.3 Characteristics

The characteristics of the geometry and the flow are:

Height of downcomer	$H = 3.00 \text{ m}$
Thickness of downcomer	$E_d = 0.10 \text{ m}$
Diameter of the inlet cold branch	$D_b = 0.50 \text{ m}$
Height of vessel's bottom	$H_{fc} = 1.00 \text{ m}$
Width of vessel's bottom	$l_{fc} = 1.00 \text{ m}$
Height of core above the lower core plate	$H_{pic} = 1.00 \text{ m}$
Width of core above the lower core plate	$l_{pic} = 0.50 \text{ m}$
Inlet velocity of fluid	$V = 1 \text{ m.s}^{-1}$

Physical characteristics of fluid:

The initial water temperature in the domain is equal to 20°C. The inlet temperature of water in the cold branch is 300°C. Water characteristics are considered constant¹ and their values taken at 300°C and 150×10^5 Pa, except density which is considered variable in cases 3 and 4:

- density: $\rho = 725.735 \text{ kg.m}^{-3}$
- dynamic viscosity: $\mu = 0.895 \times 10^{-4} \text{ kg.m}^{-1}.\text{s}^{-1}$
- heat capacity: $C_p = 5483 \text{ J.kg}^{-1}.\text{°C}^{-1}$
- Thermal Conductivity = $0.02495 \text{ W.m}^{-1}.\text{K}^{-1}$

1.4 Mesh characteristics

Figure III.2 shows a global view of the mesh and some details of the joining zones, to show that *Code_Saturne* can deal with hanging nodes. This mesh is composed of 1 650 cells, which is very small compared to those used in real studies. This is a deliberate choice so that tutorial calculations run fast.

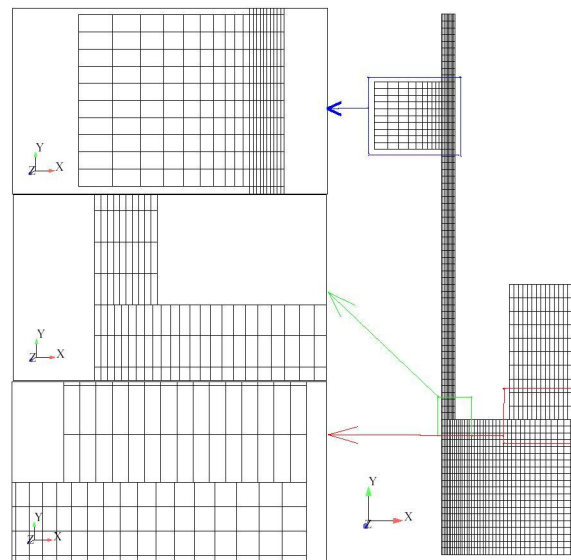


Figure III.2: View of the full domain mesh with zoom on the joining regions

Type: block structured mesh

Coordinates system: cartesian, origin on the edge of the main pipe at the outlet level, on the nozzle side (figure III.2)

Mesh generator used: SIMAIL and mesh joining with the Preprocessor of *Code_Saturne* (in order to deal with hanging nodes)

Color definition: see figure III.3

1.5 Summary of the different calculations

Three cases will be studied with this geometry. The following table gives a summary of their different characteristics.

¹which makes temperature a passive scalar ... but it is only for simplification purposes

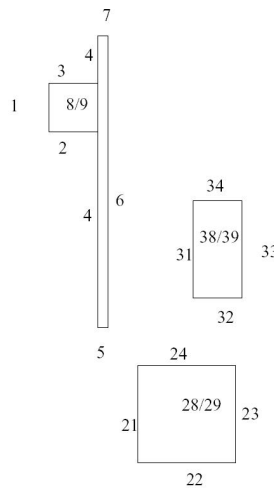


Figure III.3: Colors of the boundary faces

CASE	characteristics
CASE 2	unsteady flow, additionnal passive scalar, output management
CASE 3	same as case 2 with time dependent boundary conditions, fluid density depending on the temperature and calculation restart
CASE 4	same as case 3 with head loss, parallelism and spatial average

2 CASE 2: Passive scalar with various boundary conditions and output management

2.1 Calculation options

Some options are similar to case 1:

- Turbulence model: $k - \epsilon$
- Scalar(s): 1 - temperature
- Physical properties: uniform and constant

The new options are:

- Flow type: unsteady flow
- Time step: uniform and constant
- Scalar(s): 2 - passive scalar²
- Management of monitoring points

2.2 Initial and boundary conditions

- Initialization: 20°C for temperature (default value)
10 for the passive scalar

²could correspond to a tracer concentration for instance

The boundary conditions are defined in the user interface and depend on the boundary zone.

- **Flow inlet:** Dirichlet condition, an inlet velocity of 1 m.s^{-1} , an inlet temperature of 300°C and an inlet value of 200 for the passive scalar are imposed
- **Outlet:** default value
- **Walls:** velocity, pressure and thermal scalar: default value
passive scalar: different conditions depending on the color and geometric parameters

In order to test the ability to specify boundary condition regions in the Graphical Interface, various conditions will be imposed for the passive scalar, as specified in the following table:

Wall	Nature	Value
wall_1	Dirichlet	0
wall_2	Dirichlet	5
wall_3	Dirichlet	0
wall_4	Dirichlet	25
wall_5	Dirichlet	320
wall_6	Dirichlet	40

The “wall_1” to “wall_6” regions are defined as follows, through color references and geometric localization:

Label	Color and geometric parameters
wall_1	24 and $0.1 \leq X$ and $X \leq 0.5$
wall_2	2 or 3
wall_3	4 or 7 or 21 or 22 or 23
wall_4	6 and $Y > 1$
wall_5	6 and $Y \leq 1$
wall_6	31 or 33

Figure III.3 shows the colors used for boundary conditions and table III.1 defines the correspondance between the colors and the type of boundary condition to use.

Colors	Conditions
1	Inlet
34	Outlet
2 3 4 6 7 21 22 23 24 31 33	Wall
8 9 28 29 38 39	Symmetry

Table III.1: Boundary faces colors and associated references

2.3 Parameters and User routines

All parameters necessary to this study can be defined through the Graphical Interface without using any user Fortran files.

Calculation control parameters	
Number of iterations	300
Reference time step	0.05
Output period for post-processing files	2

In order to join the separate meshes into a single domain, colors 5, 24 and 32 will have to be joined through the Graphical Interface.

2.4 Output management

In this case, different aspects of output management will be addressed.

By default in the Graphical Interface, all variables are set to appear in the listing, the post-processing and the chronological records. This default choice can be modified by the user.

In this case, the *Pressure*, the *Tubulent energy* and the *Dissipation* will be removed from the listing file.

The *Courant number* (CFL) and *Fourier number* will be removed from the post-processing results³.

Eventually, probes will be defined for chronological records, following the data given in figure III.4. Then the *total pressure* will be deactivated for all probes and the *Velocity U* will only be activated on probes 1, 2, 6, 7 and 8.

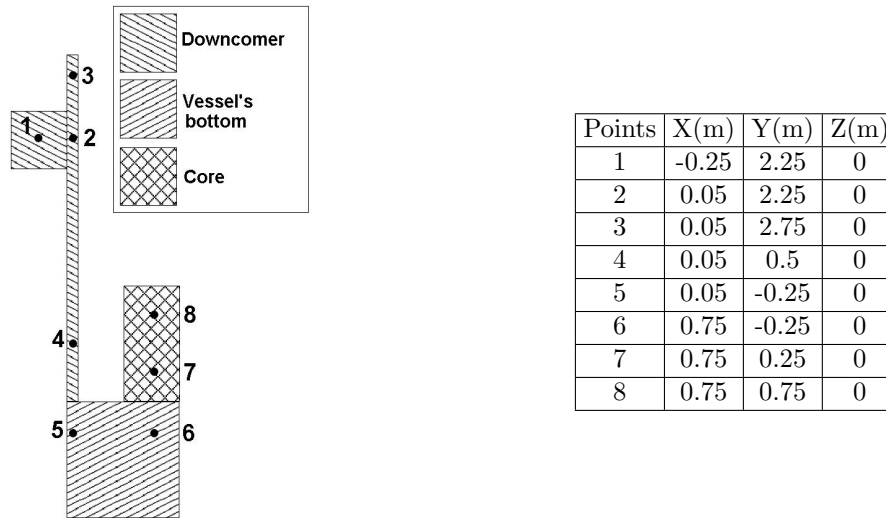


Figure III.4: Position and coordinates of probes in the full domain

In addition the domain boundary will be post-processed. This allows to check the boundary conditions, and especially that of the passive scalar.

2.5 Results

Figure III.5 shows the boundary domain colored by the passive scalar boundary conditions. The different regions of boundary conditions defined earlier can be checked.

Figure III.6 presents results obtained at different times of the calculation. They were plotted from the post-processing files, with EnSight.

³this can be very useful to save some disk space if some variables are of no interest, as post-processing files can be large

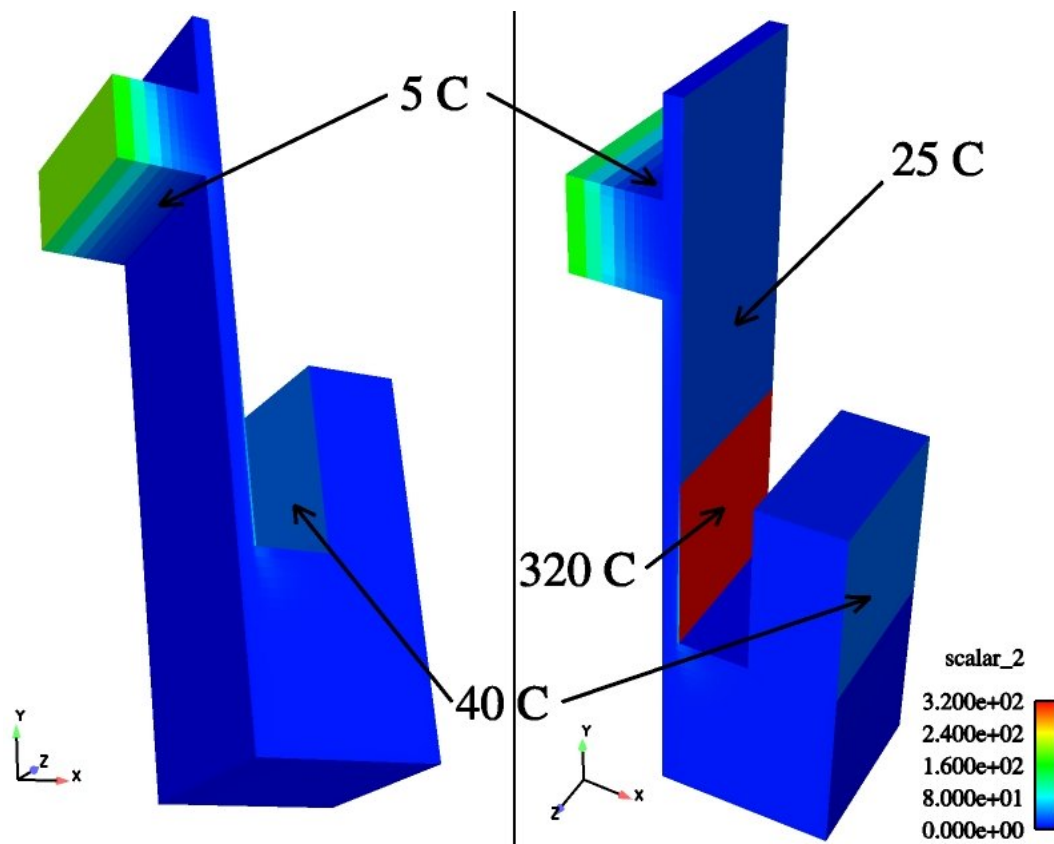


Figure III.5: View of the boundary domain colored by the scalar_2 variable - Case 2

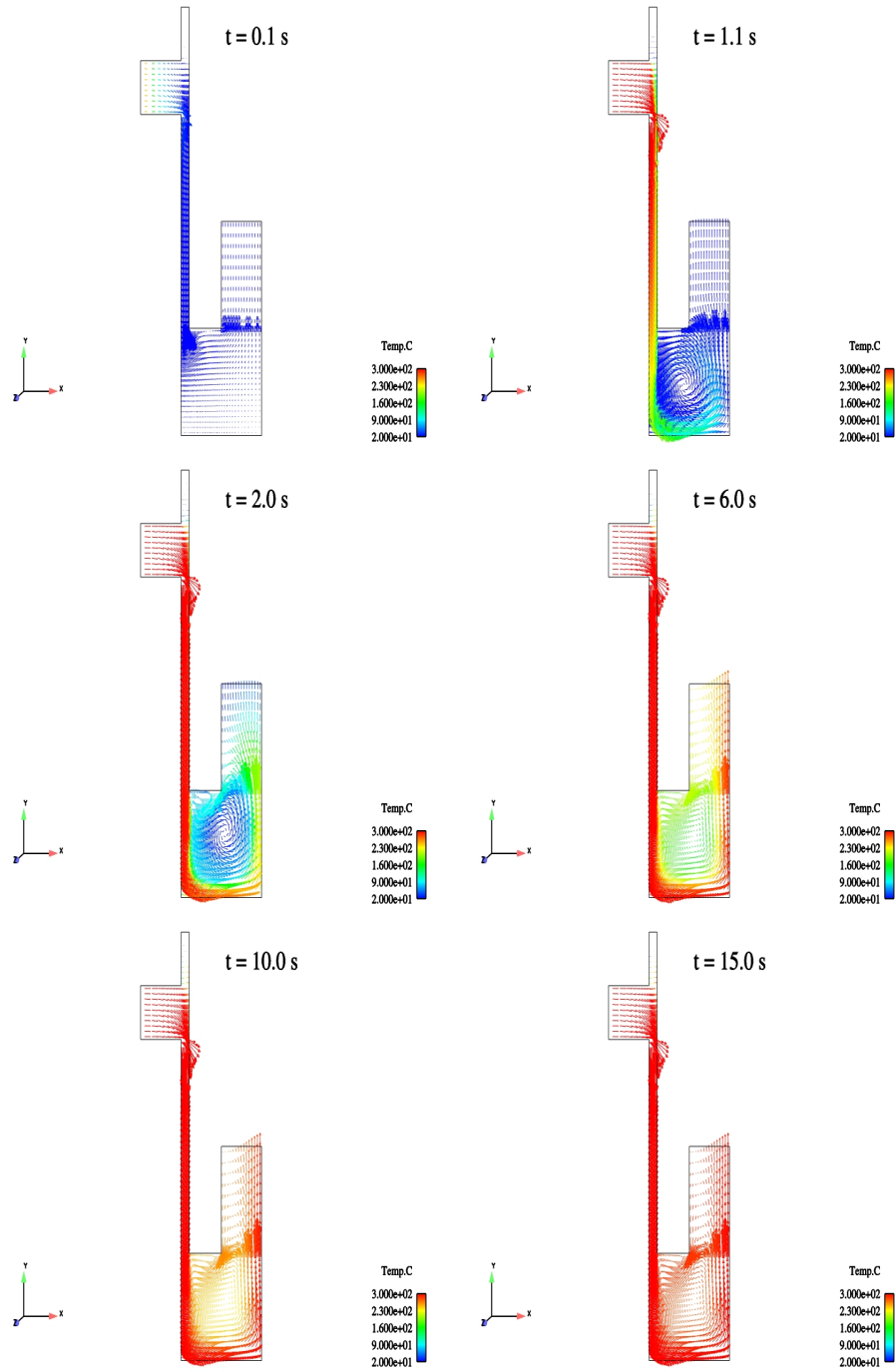


Figure III.6: Water velocity field colored by temperature at different time steps - Case 2

3 CASE 3: Time dependent boundary conditions and variable fluid density

In this case some boundary conditions will be time dependent and some physical characteristics of the fluid will be dependent on the temperature.

3.1 Calculation options

The options for this case are the same as in case 2, except for the variable fluid density:

- Flow type: unsteady flow
- Time step: uniform and constant
- Turbulence model: $k - \epsilon$
- Scalar(s): 1 - temperature
2 - passive scalar
- Physical properties: uniform and constant (except density)
- Management of monitoring points

3.2 Initial and boundary conditions

- Initialization: 20°C for temperature (default value)
10 for the passive scalar

The boundary conditions are defined in the user interface and depend on the boundary zone. The time dependence of the temperature boundary condition implies the use of a Fortran user routine (see below).

- **Flow inlet:** Dirichlet condition, an inlet velocity of 1 m.s^{-1} , a time dependent inlet temperature and a value of 200 for the passive scalar are imposed
- **Outlet:** default value
- **Walls:** velocity, pressure and thermal scalar: default value
passive scalar: different conditions depending on the color and geometric parameters

The boundary conditions for the passive scalar are identical as in case 2, as specified in the following table:

Wall	Nature	Value
wall_1	Dirichlet	0
wall_2	Dirichlet	5
wall_3	Dirichlet	0
wall_4	Dirichlet	25
wall_5	Dirichlet	320
wall_6	Dirichlet	40

The “wall_1” to “wall_6” regions are defined as follows, through color references and geometric localization:

Label	Color and geometric parameters
wall_1	24 and $0.1 \leq X$ and $X \leq 0.5$
wall_2	2 or 3
wall_3	4 or 7 or 21 or 22 or 23
wall_4	6 and $Y > 1$
wall_5	6 and $Y \leq 1$
wall_6	31 or 33

Figure III.3 shows the colors used for boundary conditions and table III.2 defines the correspondance between the colors and the type of boundary condition to use.

Colors	Conditions
1	Inlet
34	Outlet
2 3 4 6 7 21 22 23 31 33	Wall
24 for $0.1 \leq X \leq 0.5$	Wall
8 9 28 29 38 39	Symmetry

Table III.2: Boundary faces colors and associated references

3.3 Variable Density

In this case the density is a function of temperature, the variation law is defined in the Graphical User Interface although it can also be defined in a Fortran user routine. The expression is:

$$\rho = T.(A.T + B) + C \quad (\text{III.1})$$

where ρ is the density, T is the temperature, $A = -4.0668 \times 10^{-3}$, $B = -5.0754 \times 10^{-2}$ and $C = 1\,000.9$

In order for the variable density to have an effect on the flow, gravity must be set to a non-zero value. $\underline{g} = -9.81\mathbf{e}_y$ will be specified in the Graphical Interface.

3.4 Parameters

All the parameters necessary to this study can be defined through the Graphical Interface, except the time dependent boundary conditions that have to be specified in user routines.

Parameters of calculation control	
Number of iterations	300
Reference time step	0.05
Output period for post-processing files	2

In order to join the separate meshes into a single domain, colors 5, 24 and 32 will have to be joined through the Graphical Interface.

3.5 User routine

The following routine has to be copied from the folder SRC/REFERENCE/base into the folder SRC⁴: usclim.f90.

usclim.f90

This routine allows to define advanced boundary conditions on the boundary faces. Even if usclim.f90

⁴only when it appears in the SRC directory will it be taken into account by the code

is used, all boundary conditions have to be defined in the Graphical User Interface. Only the conditions that differ from this first definition need to appear in `usclim.f90`. The boundary conditions defined in `usclim.f90` will replace those specified in the Graphical Interface.

In this case, the temperature at entry is supposed variable in time, following the law:

$$\begin{cases} T = 20 + 100t & \text{for } 0 \leq t \leq 3.8 \\ T = 400 & \text{for } t > 3.8 \end{cases} \quad (\text{III.2})$$

where T is the temperature in $^{\circ}\text{C}$ and t is the time in s .

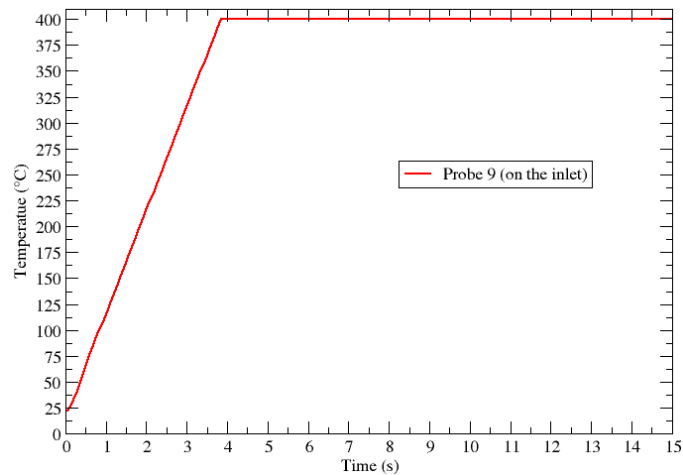


Figure III.7: Time evolution of the temperature at inlet

3.6 Output management

The output management is the same as in case 2, except that a ninth monitoring point will be added, just at the entry, to monitor the temperature evolution at inlet.

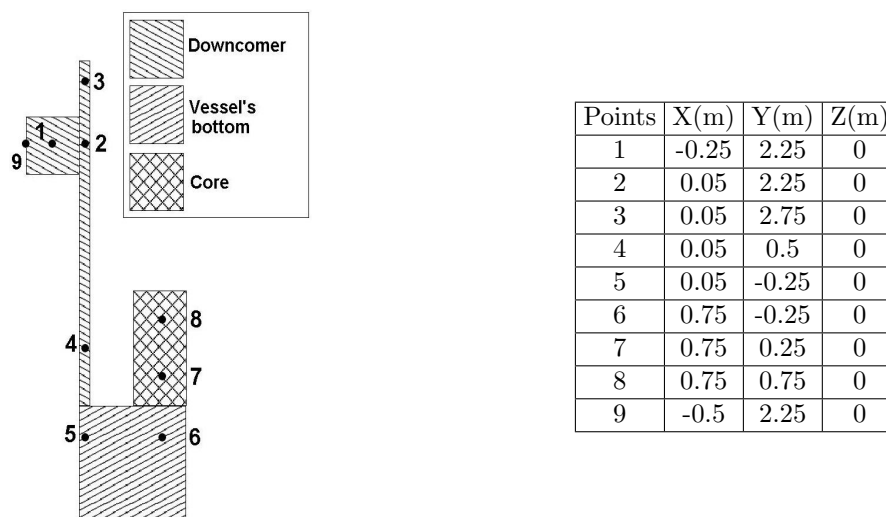


Figure III.8: Position and coordinates of probes in the full domain

In this case, the *Pressure*, the *Tubulent energy* and the *Dissipation* will be removed from the listing file.

The *Courant number* (CFL) and *Fourier number* will be removed from the post-processing results⁵.

Eventually, probes will be defined for chronological records, following the data given in figure III.4. Then the *total pressure* will be deactivated from all probes and the *Velocity U* will be only activated on probes 1, 2, 6, 7 and 8.

In addition the domain boundary will be post-processed. This allows to check the boundary conditions, and especially that of the temperature and passive scalar.

3.7 Calculation restart

After the first run, the calculation will be continued for another 400 time steps. The calculation restart is managed through the Graphical Interface.

3.8 Results

Figure III.9 shows the time evolution of temperature recorded on each monitoring probe.

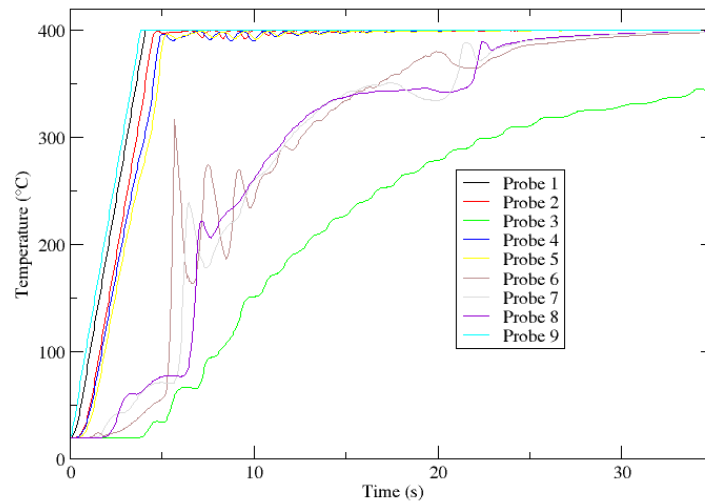


Figure III.9: Time evolution of temperature at monitoring probes for case 3

Figure III.10 shows the velocity fields colored by temperature in the first run of calculation. Figure III.11 shows the velocity fields in the second calculation (restart of the first one).

⁵this can be very useful to save some disk space if some variables are of no interest, as post-processing files can be large



Figure III.10: Water velocity field colored by temperature and inlet temperature value at different time steps (first calculation)

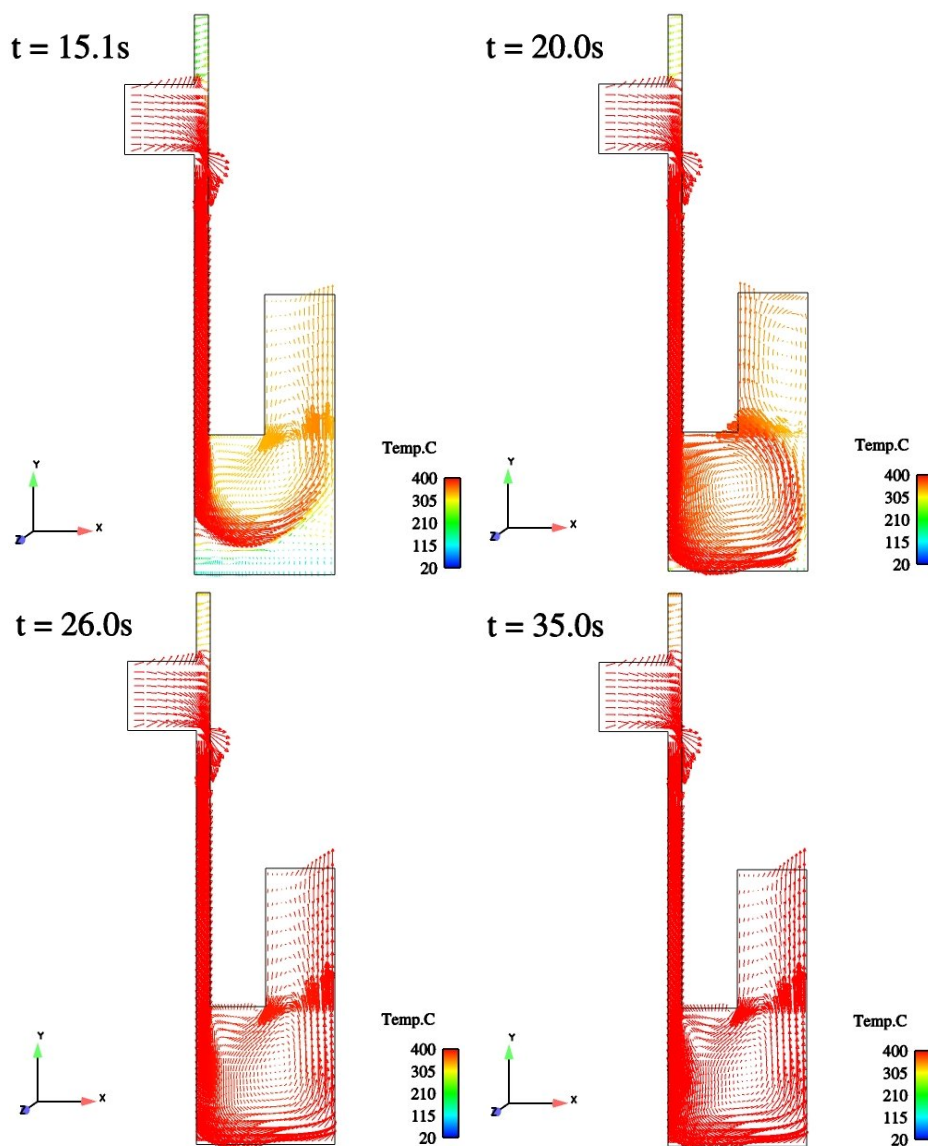


Figure III.11: Water velocity field colored by temperature and inlet temperature value at different time steps (second calculation)

4 CASE 4: Head loss, parallelism and spatial average

This case will be run in parallel on two processors. Head loss will be used to simulate the presence of an obstacle in the flow and the spatial average of the temperature will be calculated at each time step.

4.1 Calculation options

The options for this case are the same as in case 3:

- Flow type: unsteady flow
- Time step: uniform and constant
- Turbulence model: $k - \epsilon$
- Scalar(s): 1 - temperature
2 - passive scalar
- Physical properties: uniform and constant (except density)
- Management of monitoring points

4.2 Initial and boundary conditions

- Initialization: 20°C for temperature (default value)
10 for the passive scalar

The boundary conditions are defined in the user interface and depend on the boundary zone.

- **Flow inlet:** Dirichlet condition, an inlet velocity of 1 m.s^{-1} and a time dependent inlet temperature are imposed
- **Outlet:** default value
- **Walls:** velocity, pressure and thermal scalar: default value
passive scalar: different conditions depending on the color and geometric parameters

The boundary conditions for the passive scalar are identical as in case 2, as specified in the following table:

Wall	Nature	Value
wall_1	Dirichlet	0
wall_2	Dirichlet	5
wall_3	Dirichlet	0
wall_4	Dirichlet	25
wall_5	Dirichlet	320
wall_6	Dirichlet	40

The “wall_1” to “wall_6” regions are defined as follows, through color references and geometric localization:

Label	Color and geometric parameters
wall_1	24 and $0.1 \leq X$ and $X \leq 0.5$
wall_2	2 or 3
wall_3	4 or 7 or 21 or 22 or 23
wall_4	6 and $Y > 1$
wall_5	6 and $Y \leq 1$
wall_6	31 or 33

Figure III.3 shows the colors used for boundary conditions and table III.3 defines the correspondance between the colors and the type of boundary condition to use.

Colors	Conditions
1	Inlet
34	Outlet
2 3 4 6 7 21 22 23 31 33	Wall
24 for $0.1 \leq X \leq 0.5$	Wall
8 9 28 29 38 39	Symmetry

Table III.3: Boundary faces colors and associated references

4.3 Variable Density

In this case the density is a function of temperature, the variation law is defined in the Graphical User Interface although it can also be defined in a Fortran user routine. The expression is:

$$\rho = T.(A.T + B) + C \quad (\text{III.3})$$

where ρ is the density, T is the temperature, $A = -4.0668 \times 10^{-3}$, $B = -5.0754 \times 10^{-2}$ and $C = 1\,000.9$

In order for the variable density to have an effect on the flow, gravity must be set to a non-zero value. $\underline{g} = -9.81\mathbf{e}_y$ will be specified in the Graphical Interface.

4.4 Head loss

To simulate the presence of an obstacle 0.20 m large and 0.5 m high in the vessel, a zone of head loss will be created in the domain (fig III.12). The head loss zone is located between the coordinates $X = 0.2\text{ m}$ and $X = 0.4\text{ m}$, and $Y = -0.75\text{ m}$ and $Y = -0.25\text{ m}$. The head loss coefficient to apply is 10^4 and is isotropic.

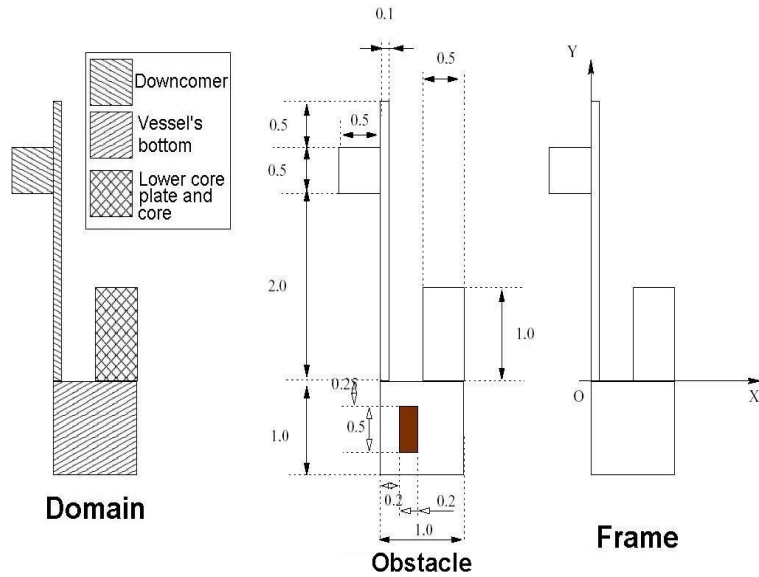


Figure III.12: Full domain geometry with the obstacle

4.5 Parameters

All the parameters necessary to this study can be defined through the Graphical Interface. However, the calculation of the spatial average is defined by a user routine.

Parameters of calculation control	
Number of iterations	300
Reference time step	0.05
Output period for post-processing files	2
The calculation will be run in parallel on 2 processors	

In order to join the separate meshes into a single domain, colors 5, 24 and 32 will have to be joined through the Graphical Interface.

4.6 User routines

The following routines have to be copied from the folder SRC/REFERENCE/base into the folder SRC⁶: `usclim.f90` and `usproj.f90`.

• `usclim.f90`

This routine allows to define advanced boundary conditions on the boundary faces. Even if `usclim.f90` is used, all boundary conditions have to be defined in the Graphical User Interface. Only the conditions that differ from this first definition need to appear in `usclim.f90`. The boundary conditions defined in `usclim.f90` will replace those specified in the Graphical Interface.

In this case, the temperature at entry is supposed variable in time, following the law:

$$\begin{cases} T = 20 + 100t & \text{for } 0 \leq t \leq 3.8 \\ T = 400 & \text{for } t > 3.8 \end{cases} \quad (\text{III.4})$$

where T is the temperature in °C and t is the time in s .

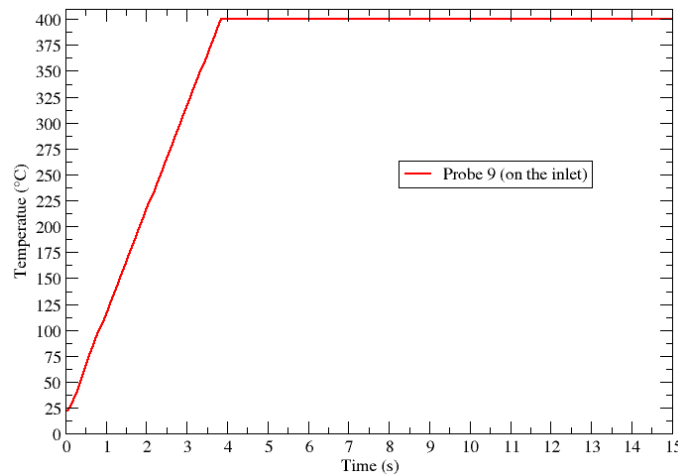


Figure III.13: Time evolution of the temperature at inlet

• `usproj.f90`

This routine is called at the end of each time step and has access to the whole set of variables of the code. It is therefore useful for many user-specific post-processing, including the calculation of a spatial

⁶only when they appear in the SRC directory will they be taken into account by the code

average in the present case.

The spatial average of the temperature will be calculated at each time step and the result wrote in a file named “moy.dat”. The values are saved in order to draw the time evolution of the average temperature.

Beware when calculating the average. Since the calculation is running in parallel, computing the sum of the temperatures on “all the cells” will only yield for each processor the sum on the cells managed by this processor. In order to obtain the full sum, the parallelism routine PARSOM must be used (see example).

Note: usproj.f90 contains many examples. They should be removed before running the case.

4.7 Output management

The output management is the same as in case 3.

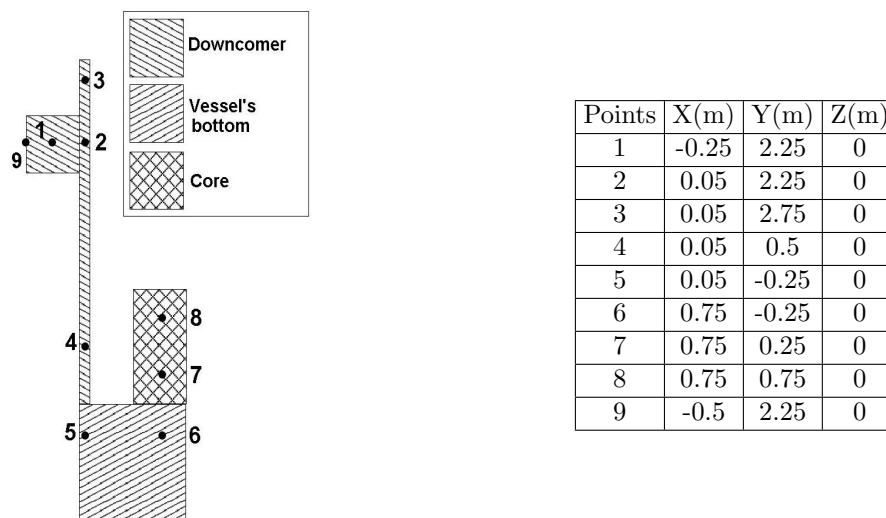


Figure III.14: Position and coordinates of probes in the full domain

In this case, the *Pressure*, the *Tubulent energy* and the *Dissipation* will be removed from the listing file.

The *Courant number* (CFL) and *Fourier number* will be removed from the post-processing results⁷.

Eventually, probes will be defined for chronological records, following the data given in figure III.4. Then the *total pressure* will be deactivated from all probes and the *Velocity U* will be only activated on probes 1, 2, 6, 7 and 8.

In addition the domain boundary will be post-processed. This allows to check the boundary conditions, and especially that of the temperature and passive scalar.

4.8 Results

Figure III.15 shows the evolution of the spatial average of the temperature.

Figure III.16 shows velocity fields colored by temperature. The effect of the head loss modeling the obstacle is clearly visible.

⁷this can be very useful to save some disk space if some variables are of no interest, as post-processing files can be large

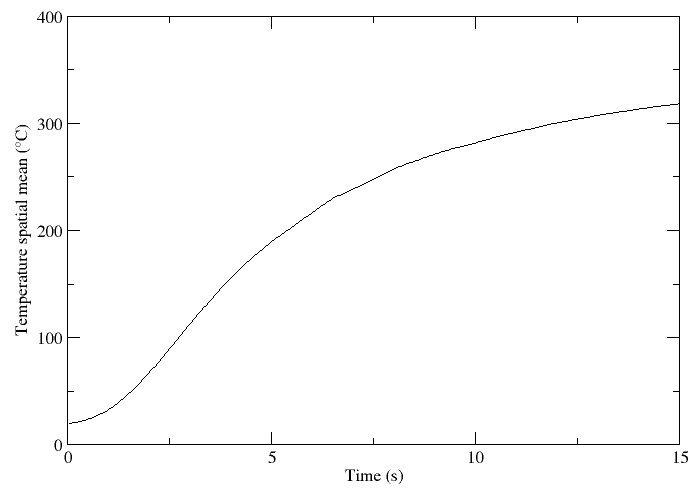


Figure III.15: Evolution of spatial average of the temperature as a function of time

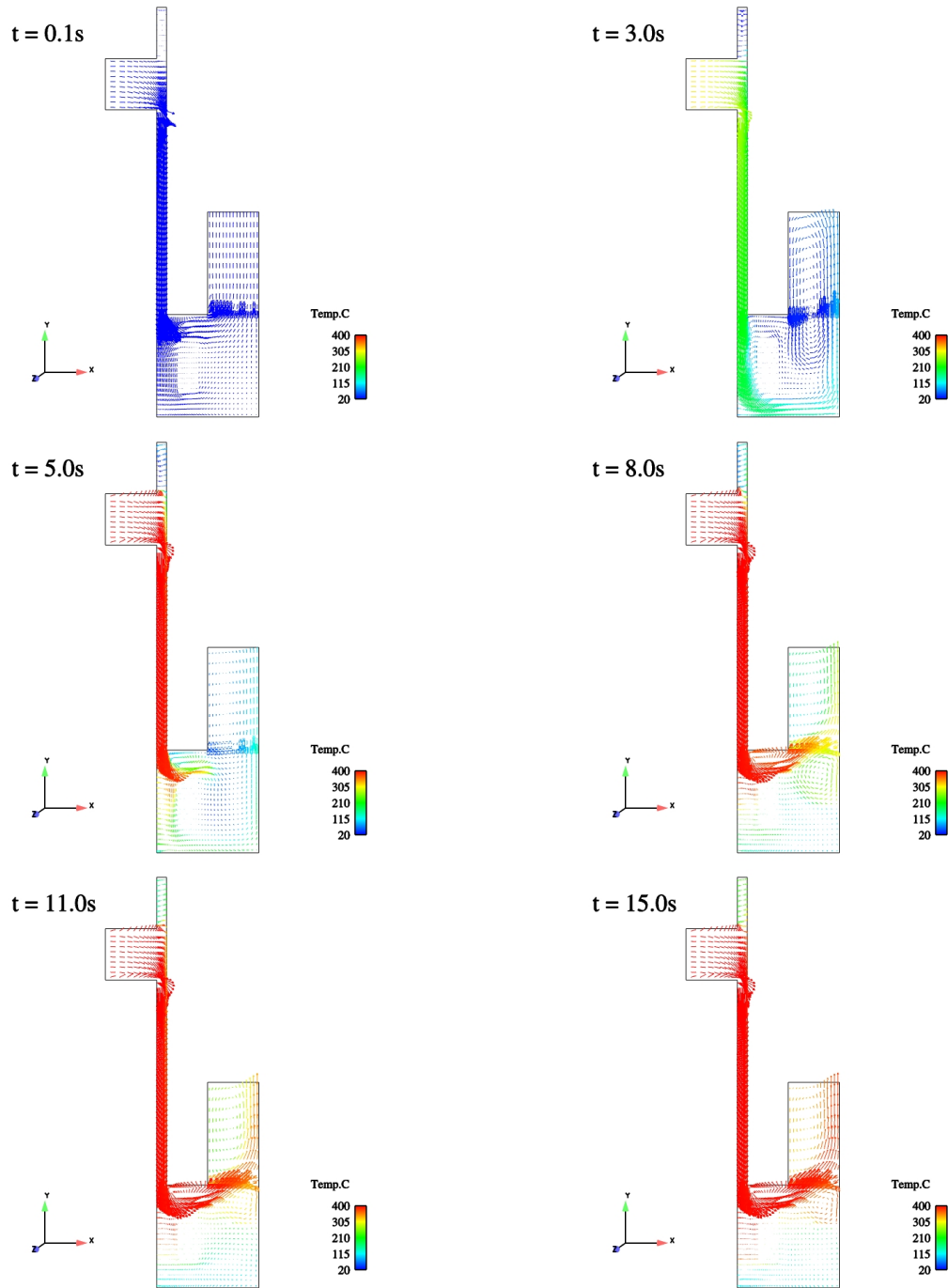


Figure III.16: Water velocity field colored by temperature

Part IV

STRATIFIED JUNCTION

1 General description

1.1 Objective

The aim of this case is to train the *Code_Saturne* user on a simplified but real 3D computation. It corresponds to a stratified flow in a T-junction. The test case will be used to present some advanced post-processing techniques.

1.2 Description of the configuration

The configuration is based on a real mock-up designed to characterize thermal stratification phenomena and associated fluctuations. The geometry is shown on figure IV.1.

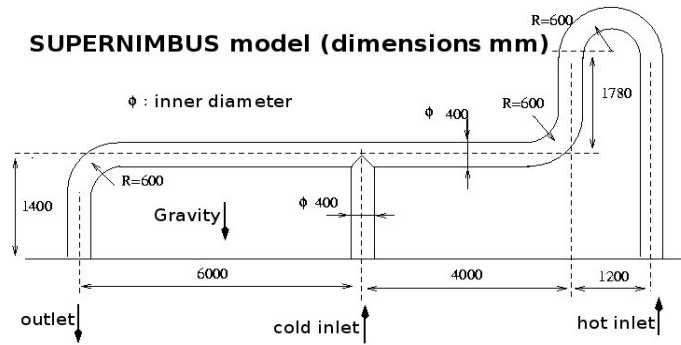


Figure IV.1: Geometry of the case

There are two inlets, a hot one in the main pipe and a cold one in the vertical nozzle. The volumic flow rate is identical in both inlets. It is chosen small enough so that gravity effects are important with respect to inertia forces. Therefore cold water creeps backwards from the nozzle towards the elbow until the flow reaches a stable stratified state.

1.3 Characteristics

Characteristics of the geometry:

Diameter of the pipe	$D_b = 0.40 \text{ m}$
----------------------	------------------------

Characteristics of flow:

Cold branch volume flow rate	$Dv_{cb} = 4 \text{ l.s}^{-1}$
Hot branch volume flow rate	$Dv_{hb} = 4 \text{ l.s}^{-1}$
Cold branch temperature	$T_{cb} = 18.26^\circ\text{C}$
Hot branch temperature	$T_{hb} = 38.5^\circ\text{C}$

The initial water temperature in the domain is equal to 38.5°C .

Water specific heat and thermal conductivity are considered constant and calculated at 18.26°C and 10^5 Pa :

- heat capacity: $C_p = 4,182.88 \text{ J.kg}^{-1}.\text{C}^{-1}$

- thermal conductivity: $\lambda = 0.601498 \text{ W.m}^{-1}.\text{°C}^{-1}$

The water density and dynamic viscosity are variable with the temperature. The functions are given below.

1.4 Mesh characteristics

The mesh used in the actual study had 125 000 elements. It has been coarsened for this example in order for calculations to run faster. The mesh used here contains 16 320 elements.

Type: unstructured mesh

Coordinates system: cartesian, origin on the middle of the horizontal pipe at the intersection with the nozzle.

Mesh generator used: SIMAIL

Color definition: see figure [IV.2](#).



Figure IV.2: Colors of the boundary faces

2 CASE 5: Stratified junction

In this case, advanced post-processing features will be used. A specific pos-processing sub-mesh will be created, containing all the cells with a temperature lower than 21°C, so that it can be visualized (with EnSight for instance). The variable “temperature” will be post-processed on this sub-mesh. A 2D clip plane will also be extracted along the symmetry plane of the domain and temperature will be written on it.

2.1 Calculation options

The following options are considered for the case:

- Flow type: unsteady flow
- Time step: variable in time and uniform in space
- Turbulence model: $k - \epsilon$
- Scalar(s): temperature
- Physical properties: uniform and constant for specific heat and thermal conductivity and variable for density and dynamic viscosity
- Pressure interpolation in stratified flows : improved

Colors	Conditions
2	Cold inlet
6	Hot inlet
7	Outlet
5	Wall

Table IV.1: Boundary faces colors and associated references

2.2 Initial and boundary conditions

→ Initialization: temperature initialization at 38.5°C

The boundary conditions are defined as follows:

- **Flow inlet:** Dirichlet condition
 - velocity of 0.03183 m.s^{-1} for both inlets
 - temperature of 38.5°C for the hot inlet
 - temperature of 18.6°C for the cold inlet
- **Outlet:** default value
- **Walls:** default value

Figure IV.2 shows the colors used for boundary conditions and table IV.1 defines the correspondance between the colors and the type of boundary condition to use.

2.3 Variable density and dynamic viscosity

In this case the density and the dynamic are functions of the temperature, the following variation laws are specified in the Graphical User Interface:

$$\rho = T.(A.T + B) + C \quad (\text{IV.1})$$

where ρ is the density, T is the temperature, $A = -4.0668 \times 10^{-3}$, $B = -5.0754 \times 10^{-2}$ and $C = 1\,000.9$

For the dynamic viscosity, the variation law is:

$$\mu = T.(T.(AM.T + BM) + CM) + DM \quad (\text{IV.2})$$

where μ is the dynamic viscosity, T is the temperature, $AM = -3.4016 \times 10^{-9}$, $BM = 6.2332 \times 10^{-7}$, $CM = -4.5577 \times 10^{-5}$ and $DM = 1.6935 \times 10^{-3}$

In order for the variable density to have an effect on the flow, gravity must be set to a non-zero value. $\underline{g} = -9.81\underline{e}_z$ will be specified in the Graphical Interface.

2.4 Parameters

All the parameters necessary to this study can be defined through the Graphical Interface, except the variable fluid characteristics and the advanced post-processing features that have to be specified in user routines.

Parameters of calculation control	
Reference time step	1 s
Number of iterations	100
Maximal CFL number	20
Maximal Fourier number	60
Minimal time step factor	0.01 s
Maximal time step factor	70 s
Time step maximal variation	0.1
Period of output chronological files	10

The time step limitation by gravity effects will also be activated.

2.5 Output management

The standard options for output management will be used. Four monitoring points will be created at the following coordinates:

Points	X(m)	Y(m)	Z(m)
1	0.010025	0.01534	-0.011765
2	1.625	0.01534	-0.031652
3	3.225	0.01534	-0.031652
4	3.8726	0.047481	7.25

Two vertical temperature profiles will be extracted, at the following locations:

profil16: $x = 1.6$ $y = 0$ $-0.2 \leq z \leq 0.2$ (m)
profil32: $x = 3.2$ $y = 0$ $-0.2 \leq z \leq 0.2$ (m)

2.6 User routines

The following routines have to be copied from the folder SRC/REFERENCE/base into the folder SRC¹: usdpst.f90, usvpst.f90 and usmpst.f90

In this test case, advanced post-processing features will be used. A clip plane will be created, along the symmetry plane of the domain, on which the temperature will be written. This plane will be added to the standard “writer” (*i.e.* it will be an extra part in the standard CHR.ENSIGHT case). The periodicity of output on the standard writer will be 10 iterations.

An additional writer will also be created, with a periodicity of 5 iterations. It will only contain one part (*i.e.* one sub-mesh): the set cells where the temperature is lower than 21°C. The temperature will be written on this part. The interest of this part is that it is time dependent as for the cells it contains.

Three Fortran routines will be used:

- **usdpst.f90**

This routine is called only once, at the beginning of the calculation. It allows to define the different writers and parts.

- **usmpst.f90**

This routine is called at each time step. It allows to redefine the content of certain parts using any variable, especially the temperature for this case.

- **usvpst.f90**

This routine is called at each time step. It allows to specify which variable will be written on which part.

¹only when they appear in the SRC directory will they be taken into account by the code

2.7 Results

Figure [IV.3](#) shows the evolution of the temperature in the domain at different time steps. The evolution of the stratification is clearly visible.

Figure [IV.4](#) shows the cells where the temperature is lower than 21°C. It is not an isosurface created from the full domain, but a visualization of the full sub-domain created through the post-processing routines.

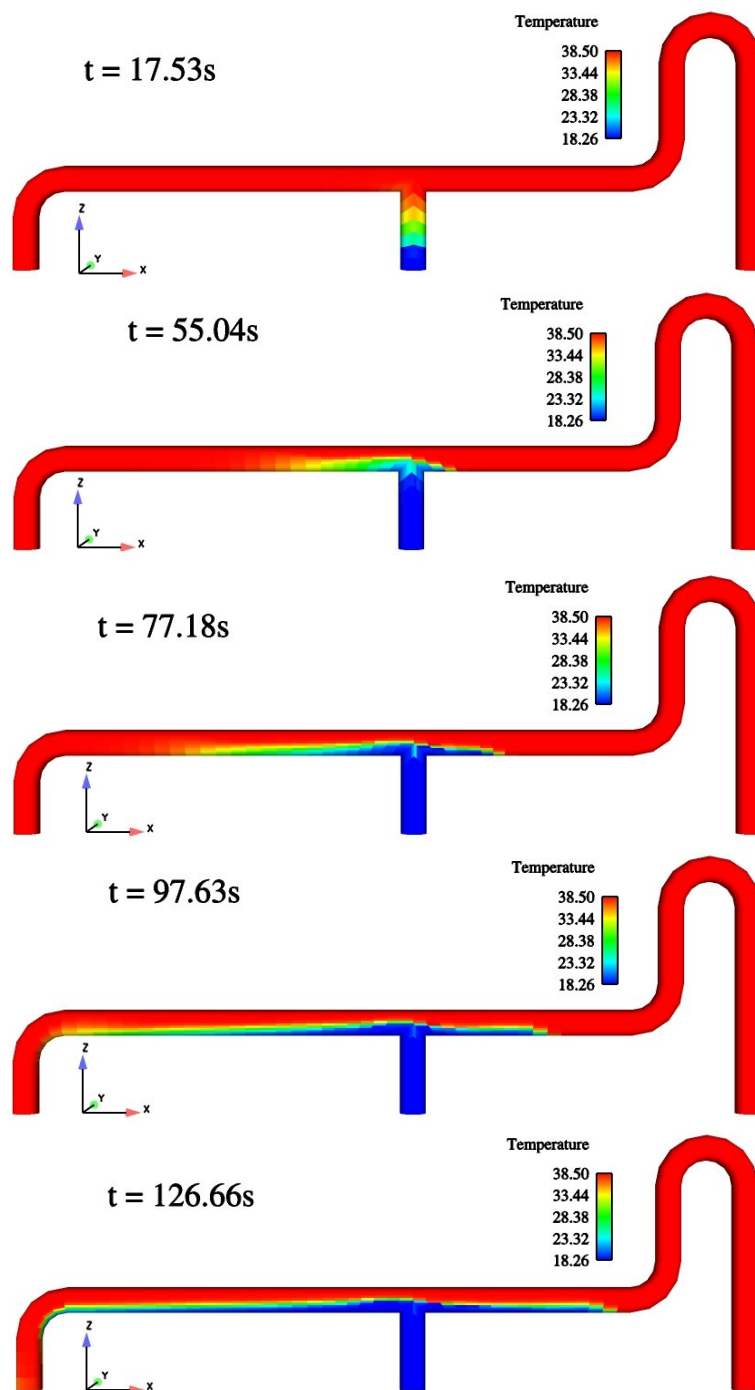


Figure IV.3: Evolution of temperature

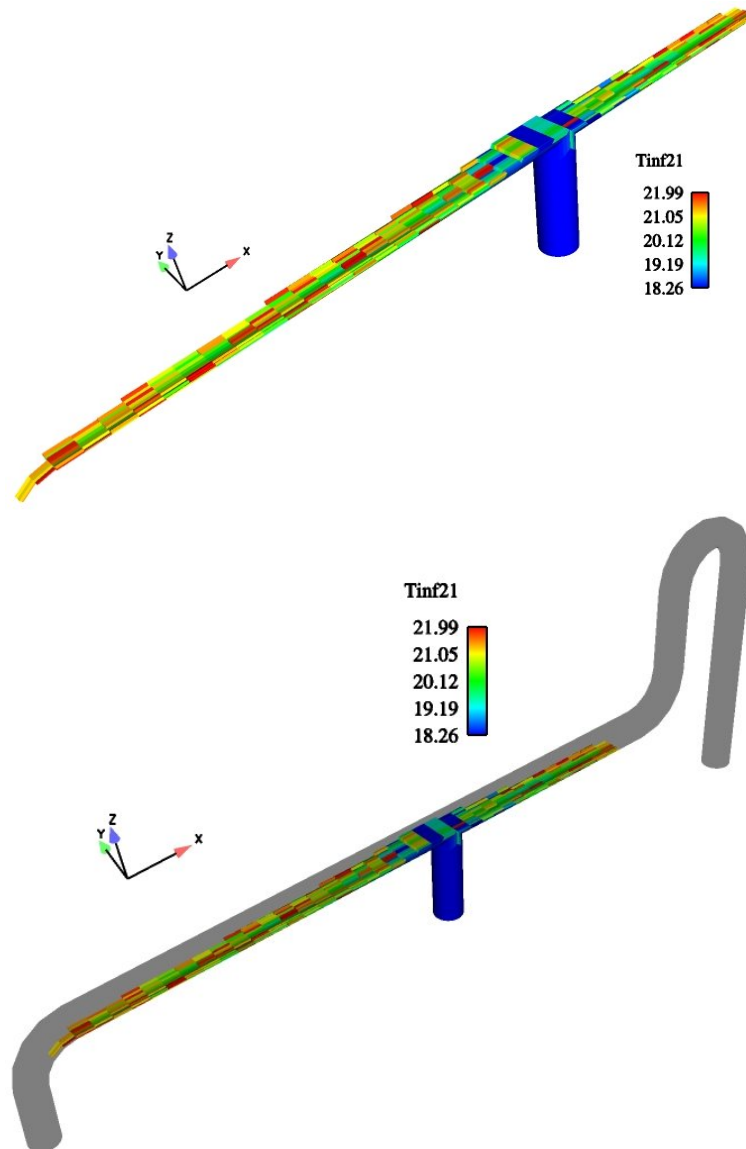


Figure IV.4: Sub-domain where the temperature is lower than 21°C (upper figure) and localization in the full domain (lower figure)

Part V

STEP BY STEP SOLUTION

1 SOLUTION FOR CASE 1

The first thing to do before running *Code_Saturne* is to prepare the computation directories. In this first example, the study directory “T_JUNCTION” will be created, containing a single calculation directory CAS1. This is done by typing the command:

```
code_saturne create -s T_JUNCTION -c CASE1
```

The mesh files should be copied in the directory MESH.

The *Code_Saturne* Graphical Interface is launched by typing the command `./SaturneGUI` in the DATA subdirectory of the CAS1 directory. The following graphic window opens (fig V.1).



Figure V.1: User interface

Go to the *File* menu and click on *New file* to open a new calculation data file, as shown in the figure [V.2](#).

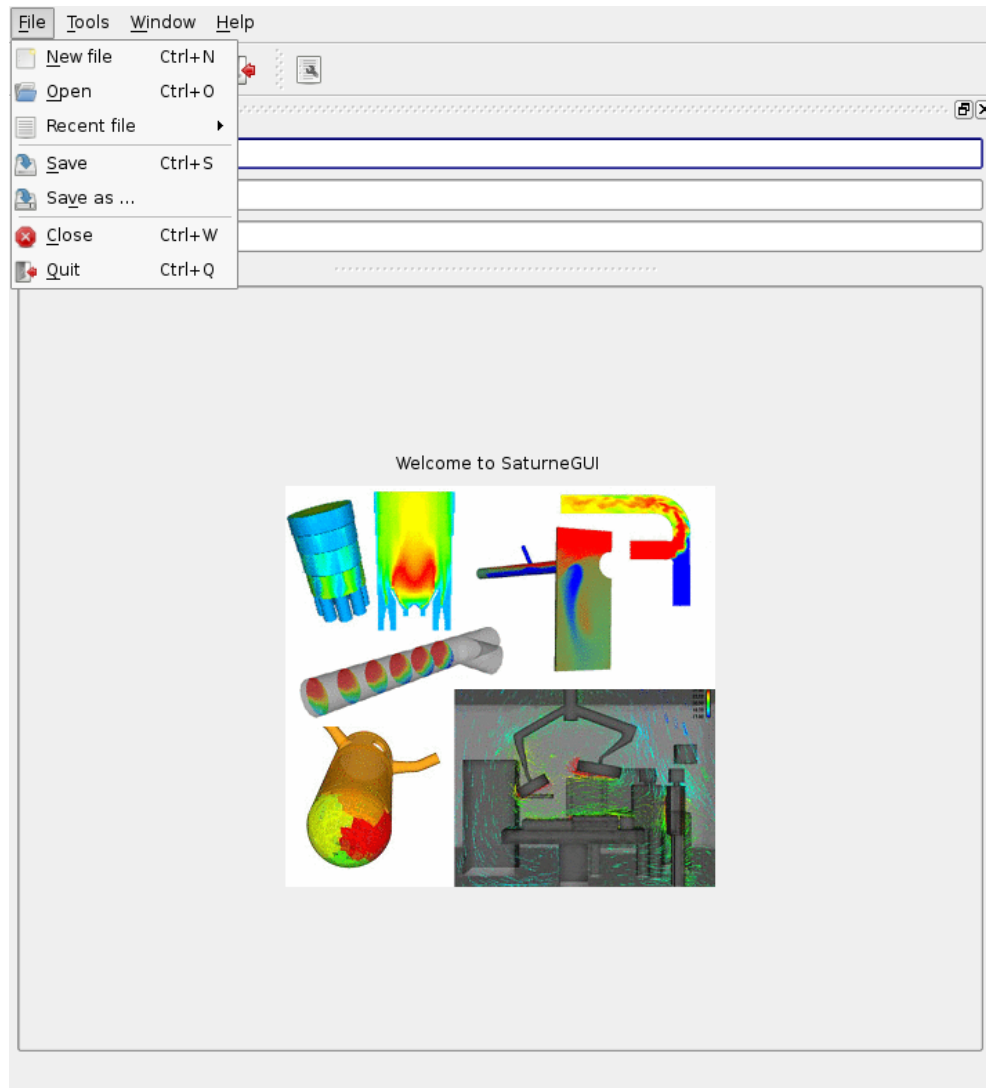


Figure V.2: Opening a new file

The interface automatically updates the following information:

- Study name
- Case name
- Directory of the case
- Associated sub-directories of the case

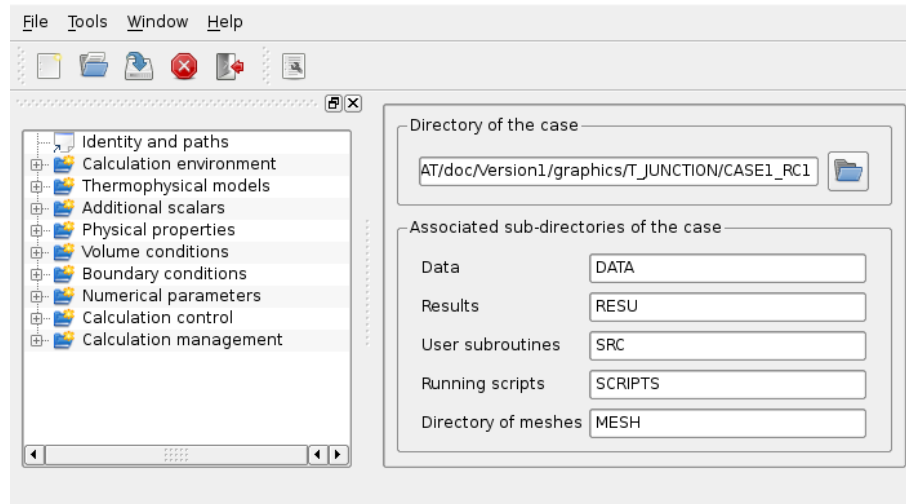


Figure V.3: Identity and paths

Save the case to give a name to the new *XML file* by opening the *File* menu and clicking on *Save as....*
A new window will appear, enter the name of the case in *File Name* then click on *Save*.

Remember to save the case regularly throughout the preparation of the calculation.



Figure V.4: Saving the *XML* file

The next step is to specify the mesh(es) to be used for the calculation. Click on the item *Solution Domain* under the heading *Analysis environment*. The list of all meshes available in the folder *MESH* appears in the window *List of meshes*. Delete the mesh(es) you will not use¹. In this case only the mesh *downcomer.des* is needed.

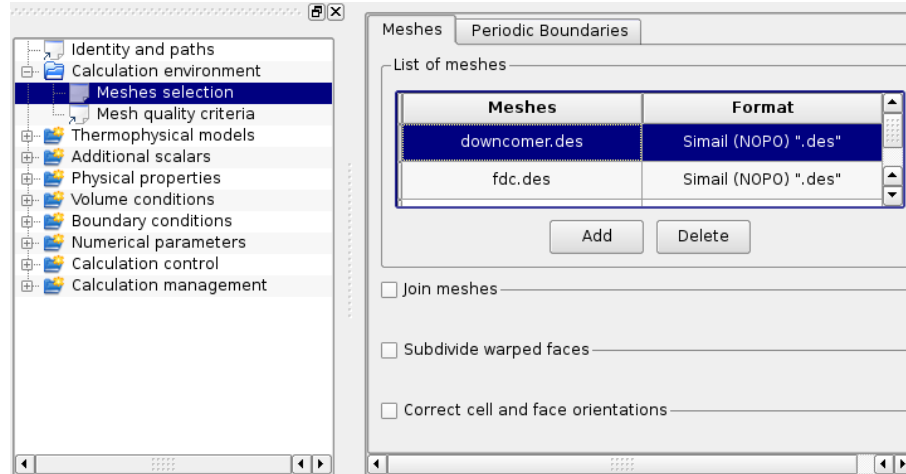


Figure V.5: Meshes: list of meshes

On this item (*Solution Domain*) there are three other tabs:

- PERIODIC BOUNDARIES
- SYRTHES COUPLING
- STAND-ALONES RUNNING

They are not used in this case. Keep the default values.

¹this operation only deletes the selected entries from the list, it does not delete the mesh file in the MESH directory

The item *Analysis features* under the heading *Thermophysical environment* allows to define the type of flow to be simulated. In this case, a steady flow will be chosen.

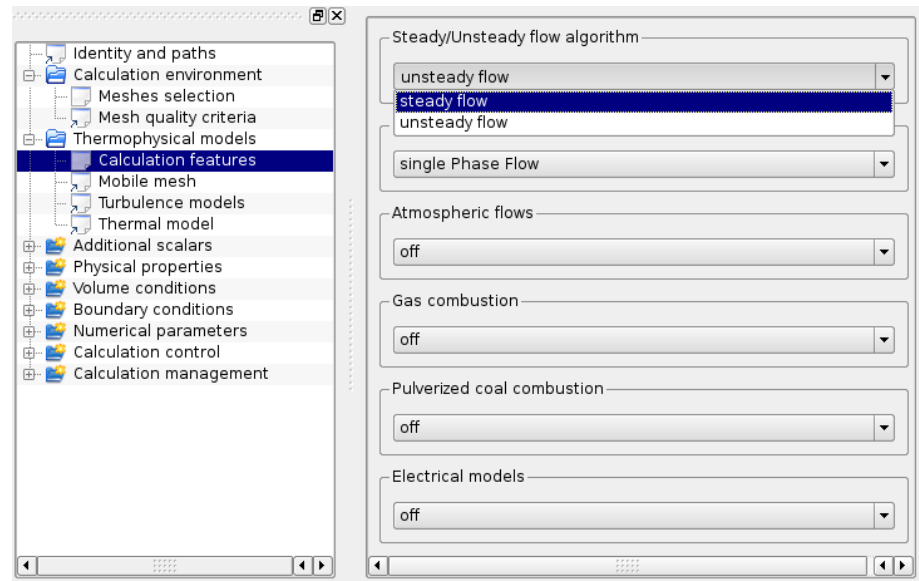


Figure V.6: Flow type

The turbulence model is selected in the following list:

- laminar flow (no model)
- mixing length
- $k-\varepsilon$
- $k-\varepsilon$ Linear Production
- Rij- ε LLR
- Rij- ε SSG
- $v2f$ (φ model)
- $k-\omega$ SST
- LES (Smagorinsky)
- LES (dynamic model)

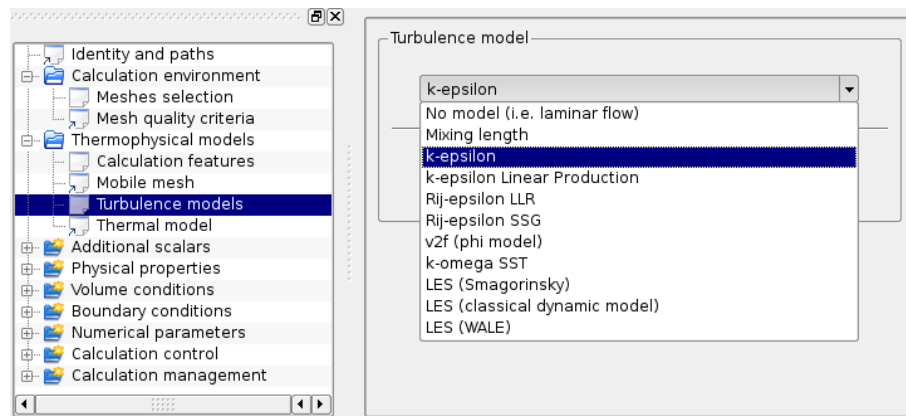


Figure V.7: Turbulence model: list of models

In this case, the $k-\varepsilon$ model is used.



Figure V.8: Turbulence model: choice of a model

For this study the equation for temperature must be solved. Click on the item *Thermal model* to choose between:

- No thermal scalar
- Temperature (Celsius degrees)
- Temperature (Kelvin)
- Enthalpy



Figure V.9: Thermal scalar conservation: list of models

In the present case, select *Temperature (Celsius degrees)*.

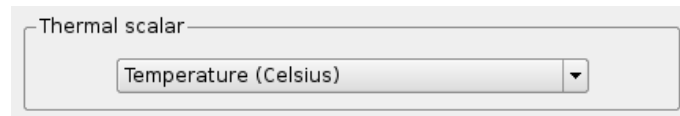


Figure V.10: Thermal scalar conservation: choice of a model

Once the thermal scalar selected, additional items appear. There are no radiative transfers in our case, so this item can be ignored.

To initialize the thermal scalar, go to the item *Definition and Initialization* under the heading *Additional scalars*, where more options concerning the scalars can be specified. The value of the initial value can be modified in any of the two pages. But in case there are additional scalars (*i.e.* other than the thermal scalar), their initialization is only possible in the *Additional scalars* page.

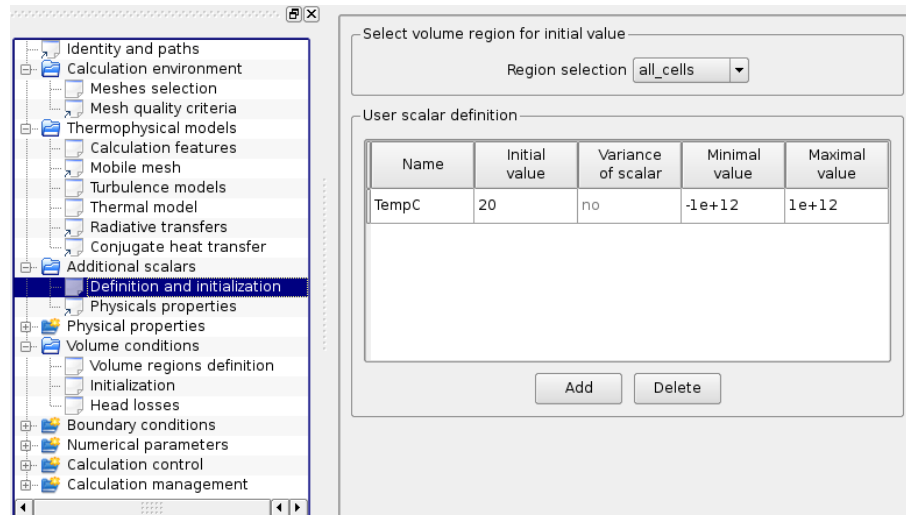


Figure V.11: Initialization of the scalar

Click on the thermal scalar in the list, to change:

- its name
- its initial value
- its minimal value
- its maximal value

In this case the temperature can vary between 0°C and 400°C.

Select volume region for initial value

Region selection all_cells

User scalar definition

Name	Initial value	Variance of scalar	Minimal value	Maximal value
Temp.C	20	no	0	400

Add Delete

Figure V.12: Initialization of the scalar

The item *Physicals properties* under the heading *Additional scalars*² is used to specify the physical properties of the additional scalars, *i.e.* those that are not the thermal scalar. In this case there are no additional scalars, the item is therefore unused.

²not to be confused with the heading *Physical properties* in the main list

Under the heading *Physical properties* in the main list, the item *Reference values* allows to set the reference pressure. Use the default value of 101 300 *Pa*.

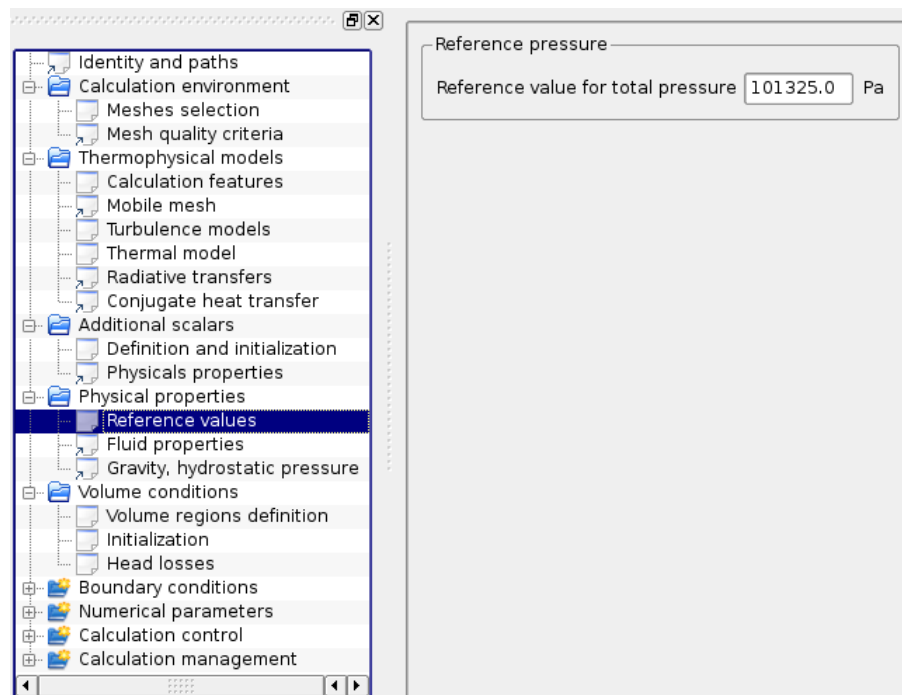


Figure V.13: Physical properties: reference pressure

Specify the fluid physical characteristics in the item *Fluid properties*:

- Density
- Viscosity
- Specific Heat
- Thermal Conductivity

In this case they are all constant.

- Density = $725.735 \text{ kg.m}^{-3}$
- Viscosity = $0.895 \times 10^{-4} \text{ kg.m}^{-1}.s^{-1}$
- Specific Heat = $5483 \text{ J.kg}^{-1}.\text{°C}^{-1}$
- Thermal Conductivity = $0.02495 \text{ W.m}^{-1}.K^{-1}$

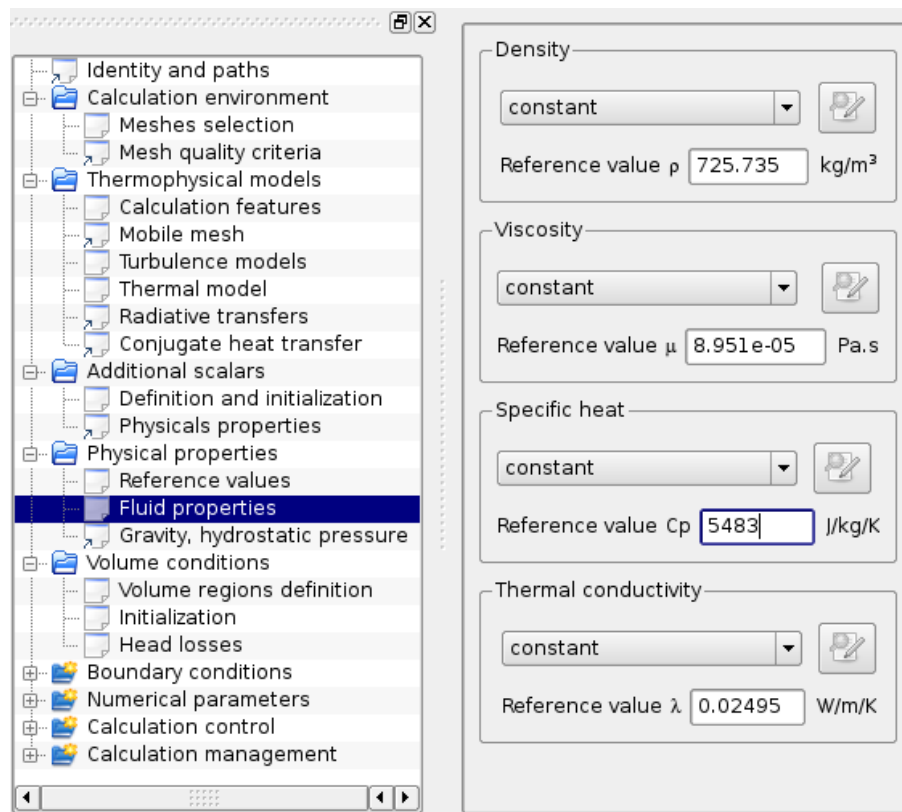


Figure V.14: Physical properties: fluid properties

Set the three components of gravity in the *Gravity, hydrostatic pressure* item. In this case, since the gravity doesn't have any influence on the flow, gravity can be set to 0. As for the pressure interpolation method, keep the standard default value.

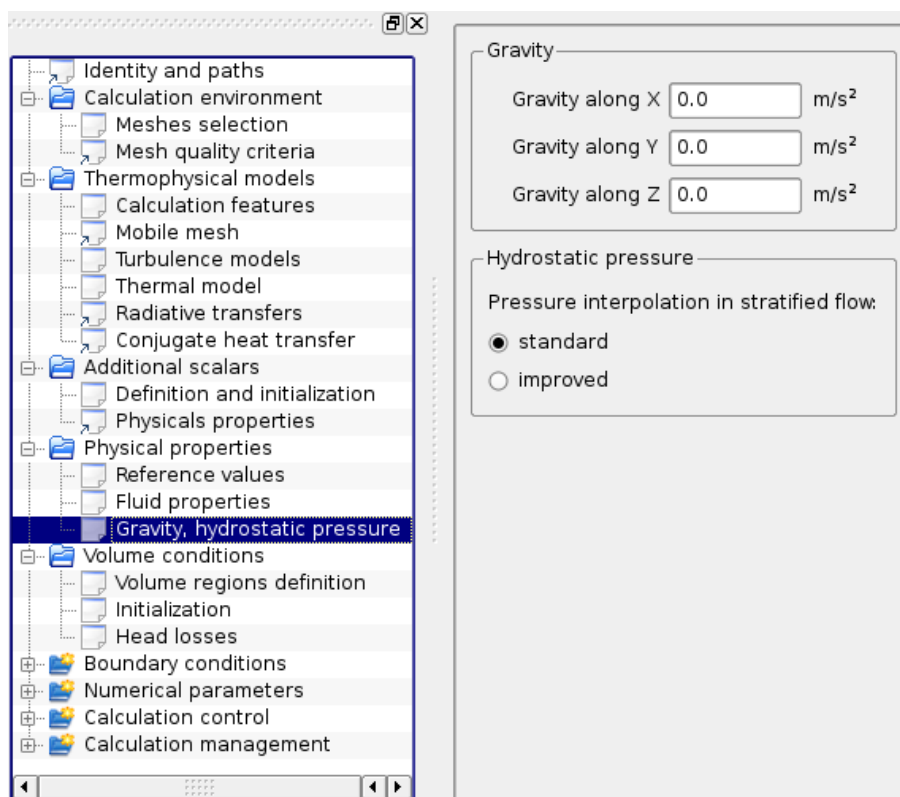


Figure V.15: Physical properties: gravity, hydrostatic pressure

To initialize variables at the instant $t = 0$ s, go to the item *Initialization* under the heading *Volume conditions*. Here the velocity, the thermal scalar and the turbulence can be initialized. In this case, the default values can be kept: zero velocity, an initial temperature of 20°C (consistent with previous initialization) and a turbulence level based on a reference velocity of 1 $m.s^{-1}$. Specific zones can be defined with different initializations. In this case, only the default “all cells” is used.



Figure V.16: Initialization of dynamic variables

Boundary conditions now need to be defined. Go to the item *Define boundary regions* under the heading *Boundary conditions*. The following window opens (fig [V.19](#)).

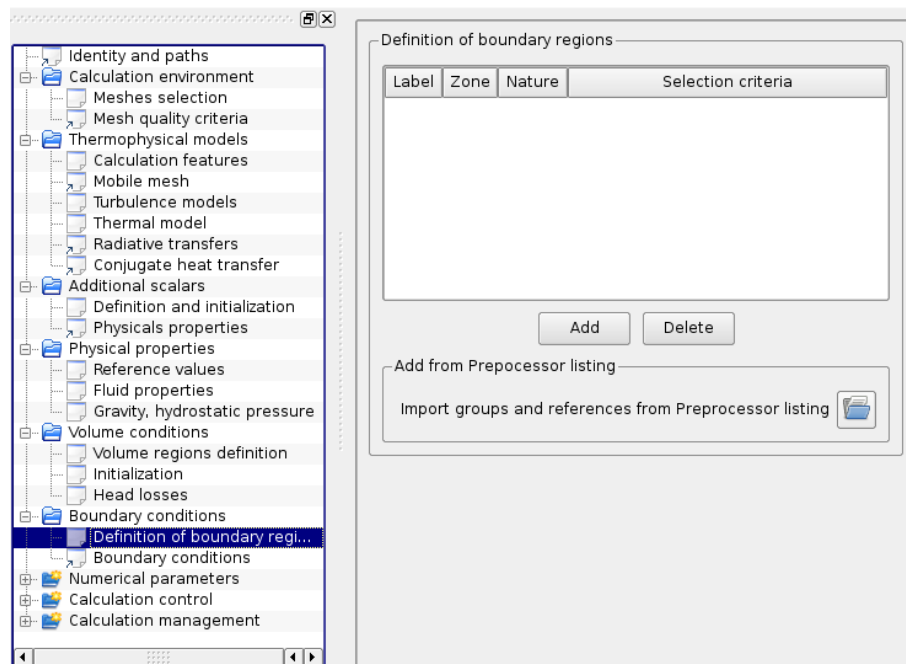


Figure V.17: Creation of a boundary region

Each boundary must be defined. Click on *Add* to edit a new boundary. The boundary faces will be grouped in user-defined zones, based on their color or on geometrical conditions. For each zone, a reference number, a label, a nature and a selection criteria must be assigned. The different natures that can be assigned are:

- wall
- inlet
- symmetry
- outlet

The *Label* can be any character string. It is used to identify the zone more easily. It usually corresponds to the nature of the zone.

The *Zone* number can be any integer. It will be used by the code to identify the zone. No specific order or continuity in the numbering is needed.

The *Selection criteria* is used to define the faces that belong to the zone. It can be a color number, a group reference, geometrical conditions, on a combination of them, related by “or” or “and” keywords.

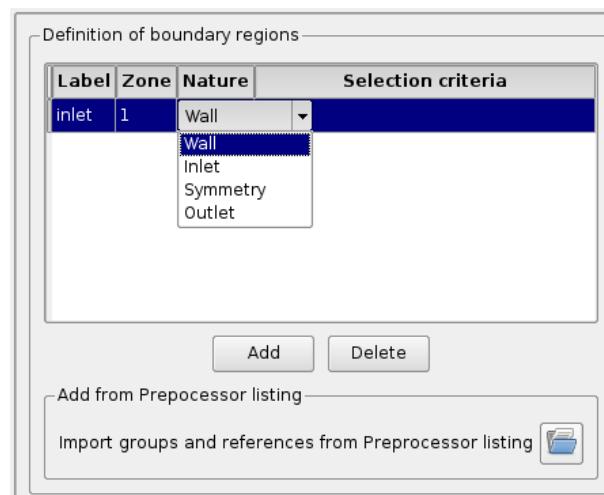


Figure V.18: Creation of a boundary region

The specification of the inlet condition is detailed in the following pages. The settings will be as follows:

- *Label*: inlet
- *Zone*: 1
- *Nature*: inlet
- *Selection criteria*: 1

Type all the information in the fields, the result displays as figure [V.19](#)

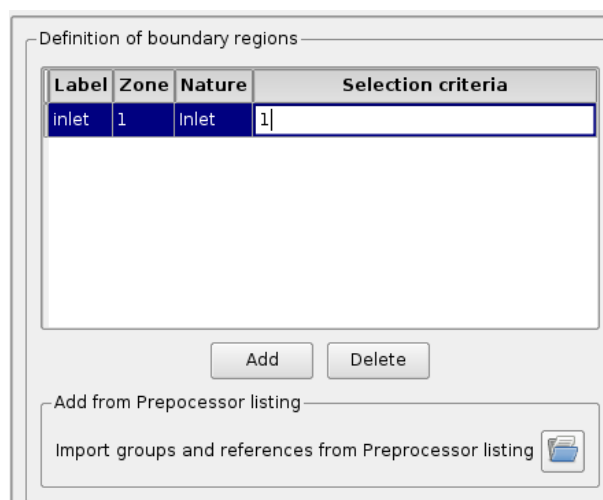


Figure V.19: Creation of a boundary region

Remember to save the Xml file regularly!

Do the same thing for the other boundaries.

In our case, colors 8 and 9 are symmetry boundaries. One option can be to define a separate zone for each color, as follows:

Label	symmetry_1	symmetry_2
Zone	3	4
Nature	symmetry	symmetry
Localization	8	9

But it is usually faster to regroup the different colors in one single zone, as shown on figure [V.20](#). In our case, the localization for this zone is the string “8 or 9”.



Figure V.20: Creation of boundary regions: symmetry region

The same treatment must be done for the wall conditions. All colors 2, 3, 4, 6 and 7 can be grouped in a single boundary zone.

After defining all the boundary zones, the Interface window will look as in figure [V.21](#).

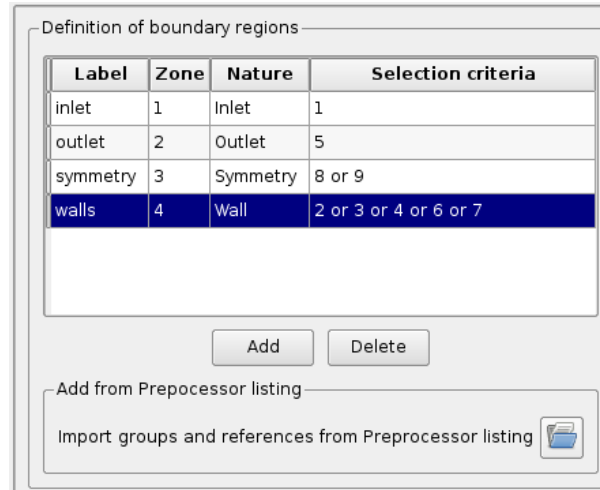


Figure V.21: Creation of boundary regions

Now that the boundary zones are defined, the boundary conditions assigned to them will be specified. Click on the item *Boundary conditions* to set the inlet boundary conditions for velocity and turbulence. As shown on figure V.22, outlet and wall boundary zones also appear in the window.

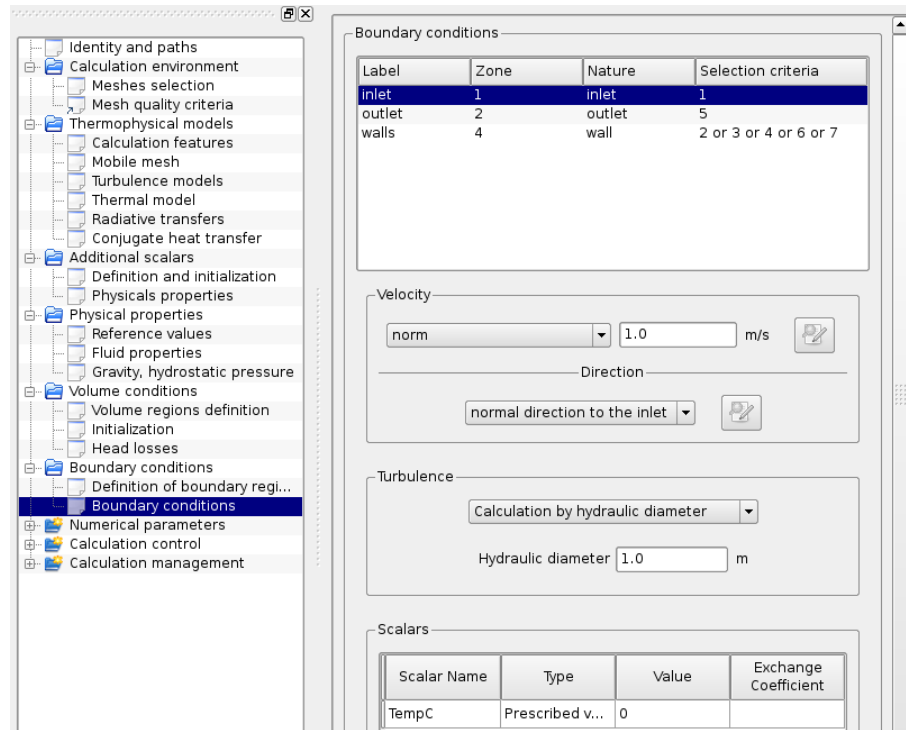


Figure V.22: Dynamic variables boundary conditions

Click on the label *inlet*. In the section *Velocity*, select *norm*, then in the sub-section *Direction* choose *specified coordinates* and enter the normal vector components of the inlet velocity. For the turbulence, chose the inlet condition based on a hydraulic diameter and specify it.

- $X = 1 \text{ m}$
- $Y = 0 \text{ m}$
- $Z = 0 \text{ m}$
- $D = 0.5 \text{ m}$

The screenshot shows the 'Boundary conditions' dialog box in Code_Saturne. It contains a table of boundary conditions and three sections for configuring the 'inlet' boundary.

Label	Zone	Nature	Selection criteria
inlet	1	inlet	1
outlet	2	outlet	5
walls	4	wall	2 or 3 or 4 or 6 or 7

Velocity

norm m/s

Direction

specified coordinates

X Y Z

Turbulence

Calculation by hydraulic diameter

Hydraulic diameter m

Figure V.23: Dynamic variables boundary: inlet

As for the wall boundary zone, the specifications the user might have to give is when the wall is sliding, and if the wall is "smooth" or "rough". In this case, the walls are fixed so the option is not selected, and the wall is considered as "smooth".

Note that if one of the walls had been sliding, it would have been necessary to isolate the corresponding boundary faces in a specific boundary region.

Boundary conditions

Label	Zone	Nature	Selection criteria
inlet	1	inlet	1
outlet	2	outlet	5
walls	4	wall	2 or 3 or 4 or 6 or 7

Smooth or rough wall

☒ smooth wall
☐ rough wall

☐ Sliding wall

Scalars

Scalar Name	Type	Value	Exchange Coefficient
Temp.C	Prescribed flux	0	

Figure V.24: Dynamic variables boundary: walls

The boundary conditions on the temperature are only applied on inlets, outlets and walls.

For the walls, three conditions are available:

- *Prescribed value*
- *Prescribed flux*
- *Exchange Coefficient*

For the outlet, only *Prescribed value* and *Prescribed flux* are available, but they are taken into account only when the flow re-enters from the outlet. Otherwise, homogeneous *Prescribed flux* is considered by *Code_Saturne*.

For the inlets, only *Prescribed value* is available.

In this case all walls are adiabatic. So the boundary condition for the temperature will be a *Prescribed flux* set to 0.

Boundary conditions

Label	Zone	Nature	Selection criteria
inlet	1	inlet	1
outlet	2	outlet	5
walls	4	wall	2 or 3 or 4 or 6 or 7

Smooth or rough wall

☒ smooth wall ☐ rough wall

☐ Sliding wall

Scalars

Scalar Name	Type	Value	Exchange Coefficient
TempC	Prescribed value	0	

Prescribed value
Prescribed flux
Exchange Coefficient

Figure V.25: Scalars boundaries: walls

Click on *inlet* to choose the temperature inlet value. Here this value is 300°C. The default value is left for the outlet.

Scalars

Scalar Name	Type	Value	Exchange Coefficient
Temp.C	Prescribed value	300	

Figure V.26: Scalars boundaries: inlet

The calculation parameters need then to be specified, under the header *Numerical parameters*.

Go to the item *Steady flow management* to specify the number of iterations, 30 in this case. The default value of the relaxation coefficient will be kept and the *Zero iteration option* will not be activated.

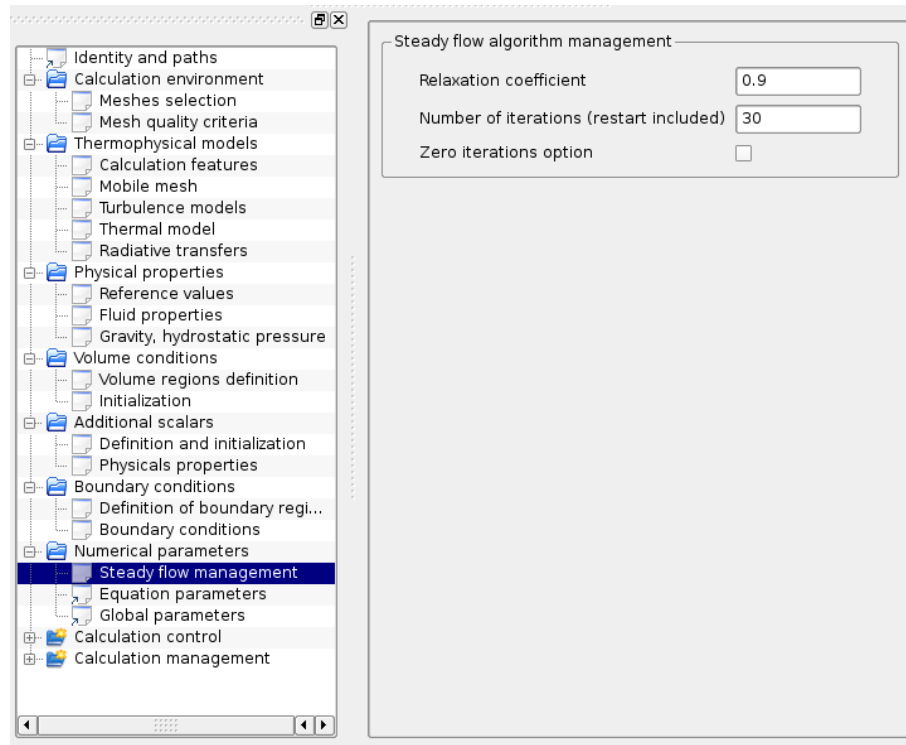


Figure V.27: Steady flow management

After selecting the item *Equation parameters*, the tab *Scheme* allows to change different more advanced numerical parameters. In this case none of them should be changed from their default value.



Figure V.28: Numerical parameters



Figure V.29: Numerical parameters

Under the heading *Calculation control*, click on the item *Output control* to change the frequency for the printing of information in the output listing. The options are:

- *No output*
- *Output listing at each time step*
- *Output at each 'n' time step* (the value of 'n' must then be specified)

Here and in most cases, the second option should be chosen.

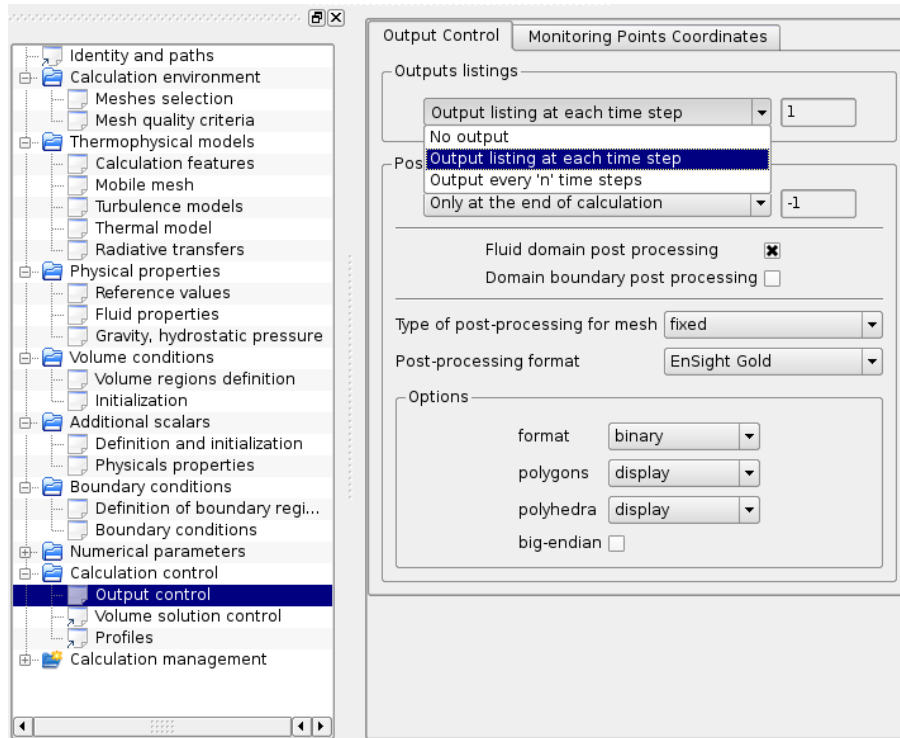


Figure V.30: Output control: output listing

For the post-processing (by default EnSight format files), there are three options:

- *Only at the end of calculation*
- *At each time step*
- *Post-processing every 'n' time steps*

In this case, we are interested in the evolution of the variables during the calculation, so the second option is chosen.

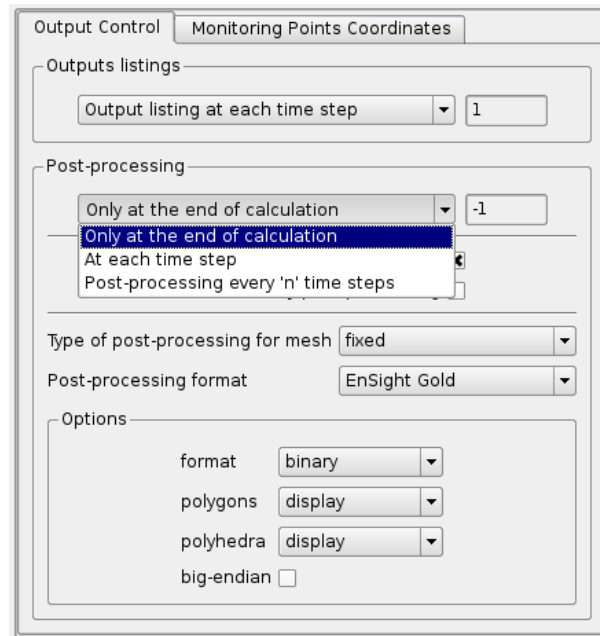


Figure V.31: Output control: post-processing

The other options are kept to their default value.

The screenshot shows the 'Output Control' dialog box with the 'Monitoring Points Coordinates' tab selected. The dialog is organized into several sections:

- Outputs listings:** Contains a dropdown menu set to 'Output listing at each time step' and a text box containing the value '1'.
- Post-processing:** Contains a dropdown menu set to 'At each time step' and a text box containing the value '1'. Below this, there are two checkboxes: 'Fluid domain post processing' (checked with an 'x') and 'Domain boundary post processing' (unchecked).
- Type of post-processing for mesh:** A dropdown menu set to 'fixed'.
- Post-processing format:** A dropdown menu set to 'EnSight Gold'.
- Options:** A section containing four settings:
 - 'format' set to 'binary' (dropdown)
 - 'polygons' set to 'display' (dropdown)
 - 'polyhedra' set to 'display' (dropdown)
 - 'big-endian' (unchecked checkbox)

Figure V.32: Output control

The *Monitoring Points Coordinates* tab allows to define specific points in the domain (monitoring probes) where the time evolution of the different variables will be stored in historic files. In this case no monitoring points are defined.

The item *Volume solution control* allows to specify which variable will appear in the output listing, in the post-processing files or on the monitoring probes. In this case, the default value is kept, where every variable is activated.



Figure V.33: Solution control

When using Fortran routines, it is sometimes useful to allocate pre-defined user arrays, that are present in every sub-routine. This allocation can be specified in the *User arrays* item, under the *Calculation management* heading. It is not the case in the present calculation.

The item *Memory management* allows to set the memory size for the calculation. It is the size of the integer and real arrays that will be used to store most of the variables in the Fortran parts of *Code_Saturne*. It is dependent on the number of cells in the mesh. In parallel mode, it depends on the number of cells treated by each processor, and not the total number of cells. For this simple case, the default values are appropriate.



Figure V.34: User arrays

The item *Start/Restart* allows to start a new calculation from the results of a former one. It is not the case in the present calculation so nothing has to be modified.

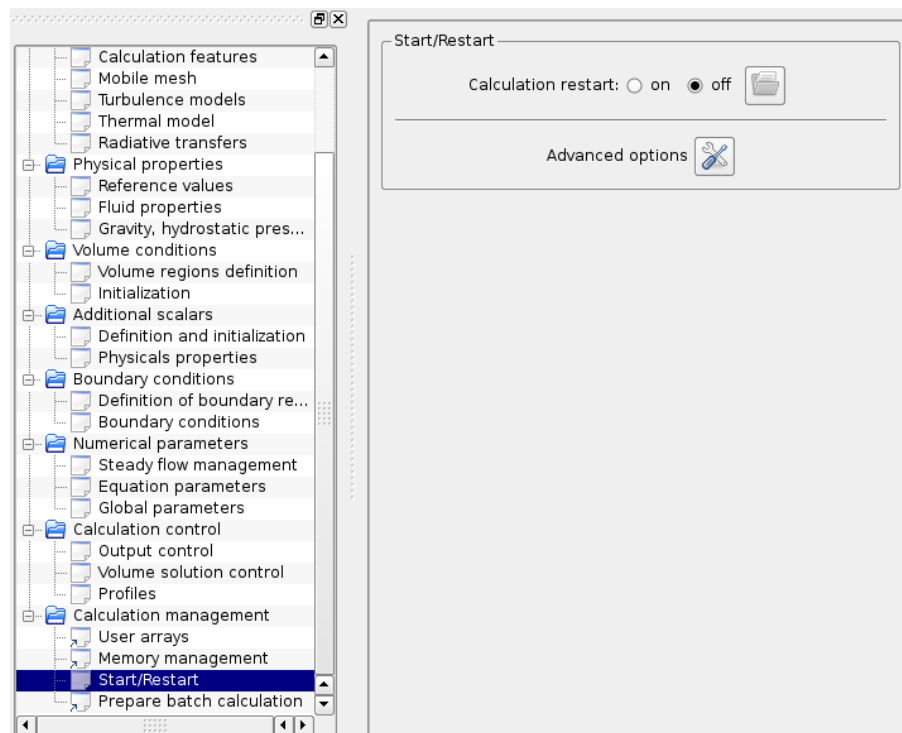


Figure V.35: Start/Restart

The final item, *Prepare batch calculation*, is used to prepare the launch script and, on certain architectures, launch the calculation.

Calculations can be launched from the Graphical Interface in interactive mode (*Workstation*) or in a PBS batch queue (*Management of batch PBS*). In this simple case, choose the Workstation.



Figure V.36: Prepare batch analysis: Computer selection

Click on the icon to *Select the batch script file* to select the launch script. The default launch script is named *runcase* and is located in the SCRIPTS directory. Select it and click on *Open*.

Remember to save the Xml file before opening the launch script.

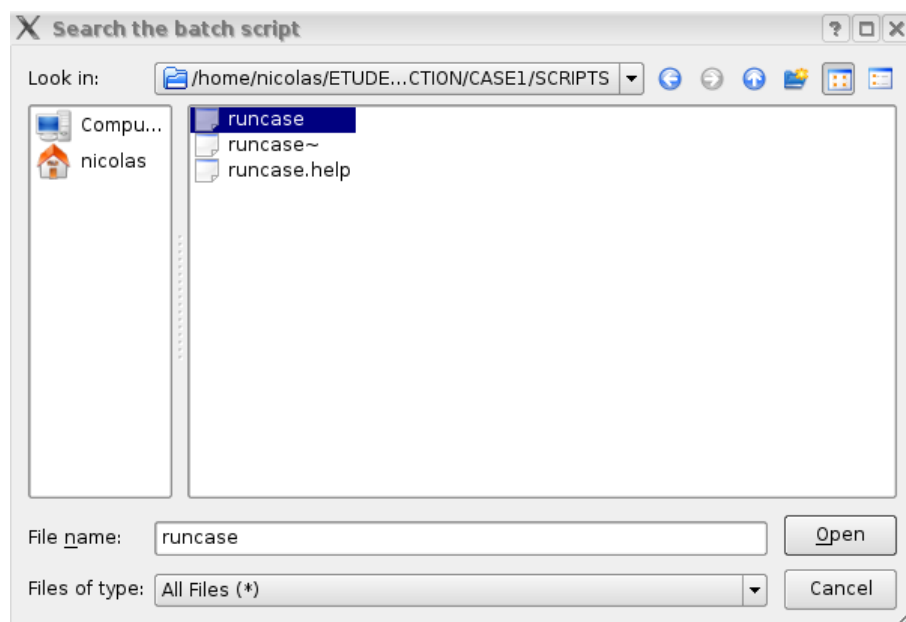


Figure V.37: Prepare batch analysis: Batch script file selection

When the script is selected, new options will appear. On this calculation, the number of processors used will be left to 1.

When launching a calculation, a temporary directory is created on the machine, where the script copies and creates temporary files and from where the *Code_Saturne* executable is launched. Should some user routines read or write case-specific files, they must be copied in the temporary directory, or from the temporary directory into the RESU directory. The *User files* icon allows the user to specify user data files (in the DATA directory) or user result files, that will then be copied automatically to or from the temporary directory. In this example, no user file is needed.

Finally, the *Advanced options* icon allows to change some more advanced parameters that will not be needed in this simple case.

Eventually, save the Xml file and execute it by clicking on *Code_Saturnebatch running*. The results will be copied in the RESU directory.

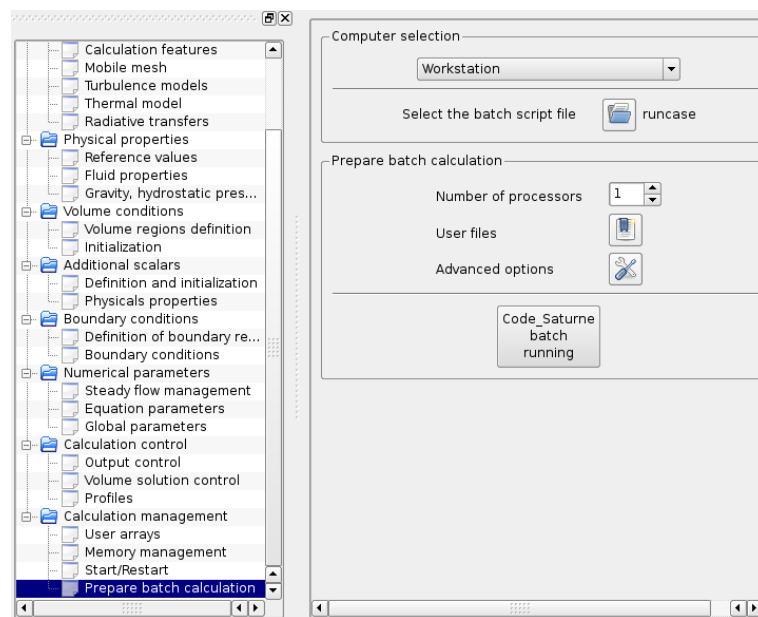


Figure V.38: Prepare batch analysis: Execution

2 SOLUTION FOR CASE 2

This case corresponds to a new study, in which there will be three calculation cases (cases 2, 3 and 4). All of them can be created in a single *code_saturne create* command, or additional cases can be added later. To test both possibilities, first create the study directory, with cases directories CAS2 and CAS4:

```
code_saturne create -s FULL_DOMAIN CAS2 CAS4
```

then go in the study directory and add the CAS3 directory:

```
cd FULL_DOMAIN
```

```
code_saturne create -c CAS3
```

Go to the DATA directory in CAS2, open a new case and select the meshes to use. Click on the heading *Calculation environment* then on the item *Meshes selection*. In this case the three meshes have to be joined. So don't delete any mesh and activate the *Join meshes* option by clicking in the box. Additional information appears on the page. If it is left untouched, the *Code_Saturne* Preprocessor will test all the boundary faces for potential joining (based on geometrical criteria). To make mesh joining more efficient, this analysis can be restricted to a sub-set of boundary faces. This is the case in the present calculation, since only faces of colors 5, 24 and 32 are liable to be joined.

Click on the *New* icon to enter the list of colors to be joined.

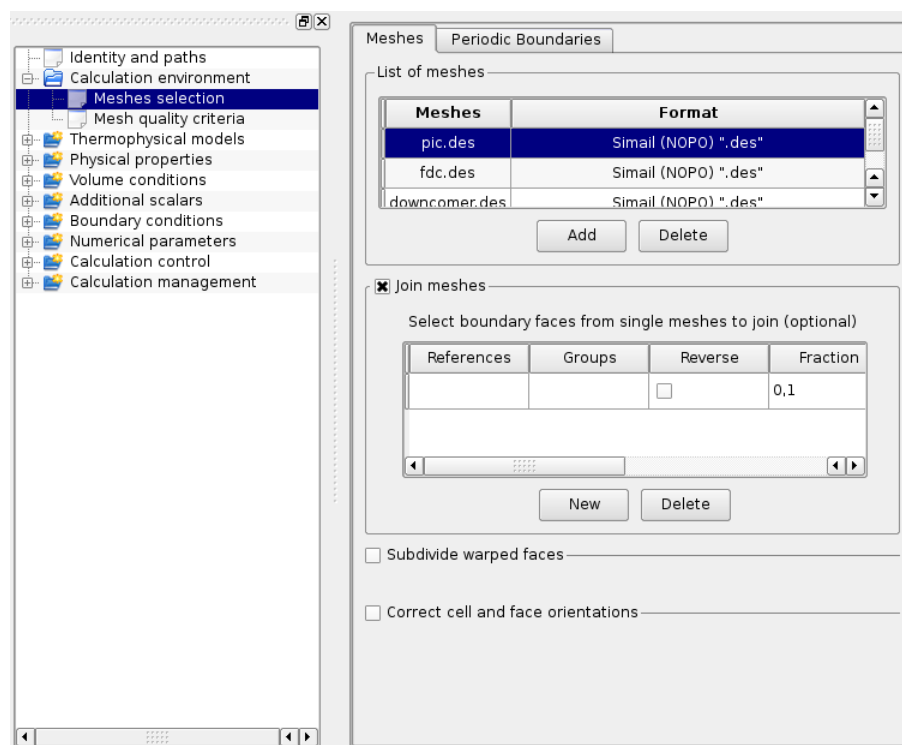


Figure V.39: Meshes: list of meshes

Fill the array *References* for the color reference to be joined: 5, 24 and 32. (different colors can be entered on a single line, separated by blanks).

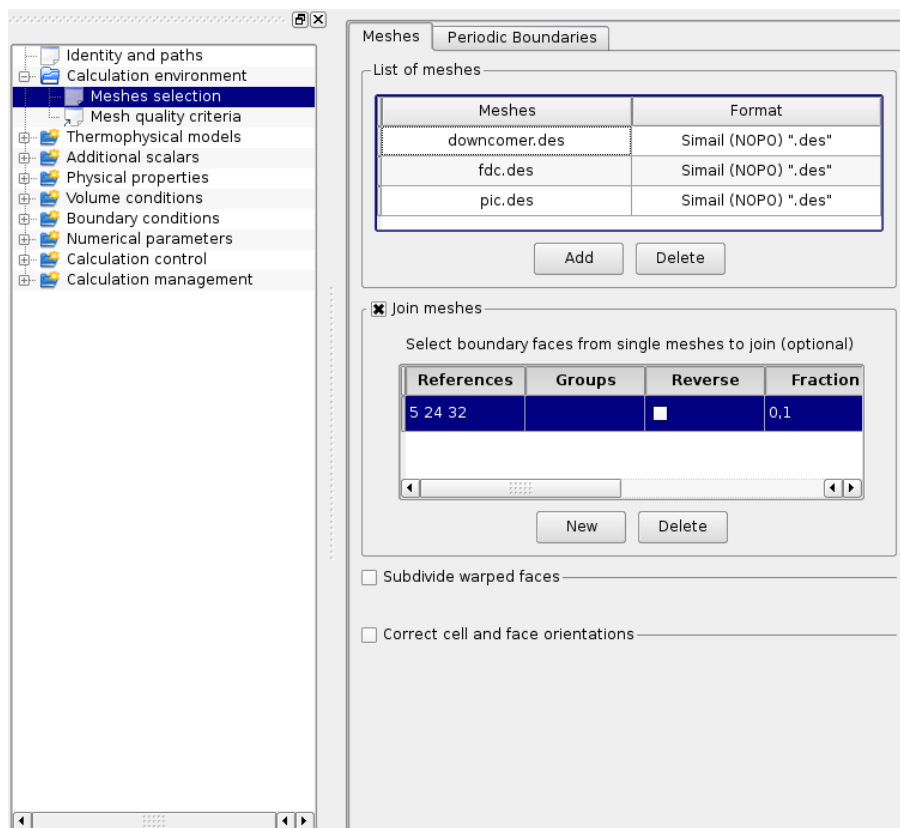


Figure V.40: Join a Mesh

In this case “Unsteady flow” must be selected in the *Analysis features* item.

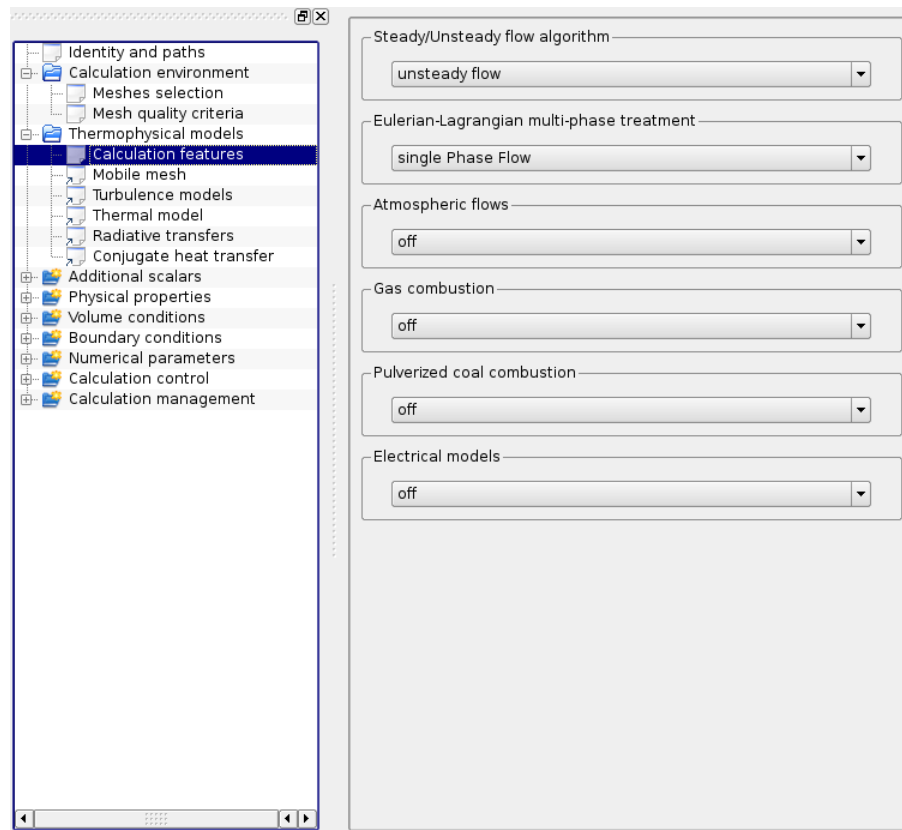


Figure V.41: Thermophysical models - Analysis features - Unsteady flow

The rest of the heading *Thermophysical models* is identical to case 1.

To add an additional scalar, click on the *Definition and Initialization* item under the *Additional scalars* heading. The characteristics of the thermal scalar are still the same. Its initial value is 20°C and it can vary between 0°C and 400°C.

To create an additional scalar, click on *Add*, then enter:

- its *Name*: scalar_2
- its *Initial value*: 10
- its *Minimal value*: 0
- its *Maximal value*: 400

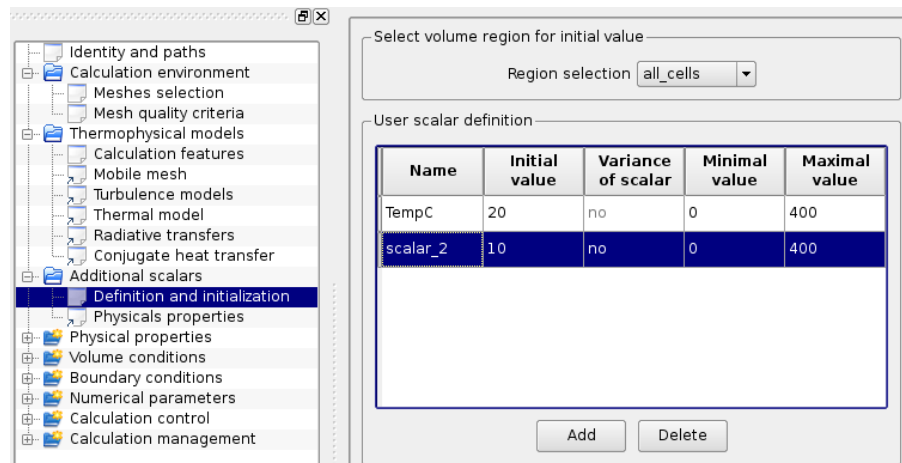


Figure V.42: Additional scalar - User scalar definition

In the item *Physical properties*, still under the heading *Additional scalars*, specify the diffusion coefficient of this new scalar. Click on the scalar name to highlight it, then enter the value in the box. In this case, the value is $0.895 \times 10^{-4} \text{ m}^2.\text{s}^{-1}$

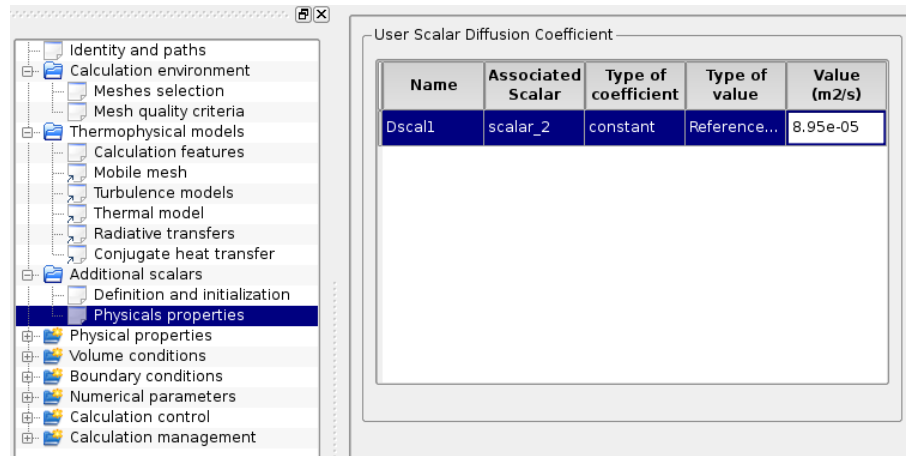


Figure V.43: Additional scalar - User scalar physical properties

Create the boundary zones. The procedure is the same as in case 1, but the colors are different. Note that colors 5 and 32 have completely disappeared in the joining process (they are now internal faces and are not considered as boundaries), while some boundary faces of color 24 remain.

Create the inlet, outlet and symmetry boundary zones with the following colors:

- inlet: color 1
- outlet: color 34
- symmetry: colors 8 9 28 29 38 39

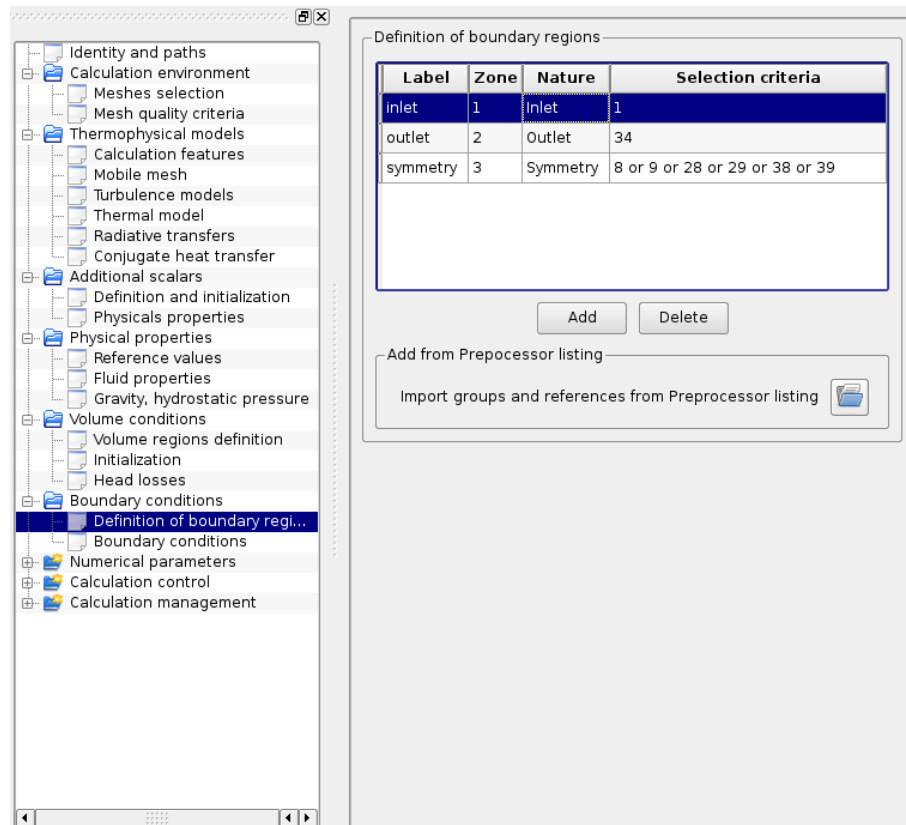


Figure V.44: Creation of the boundary zones

In this case, different conditions are applied for the walls. Separate corresponding wall boundary regions must therefore be created, following the data in the following table.

Label	Zone	Nature	Localization
wall_2	5	wall	2 or 3
wall_3	6	wall	4 or 7 or 21 or 22 or 23
wall_4	7	wall	6 and $Y > 1$
wall_5	8	wall	6 and $Y \leq 1$
wall_6	9	wall	31 or 33

The “wall_1” region combines color and geometrical criteria. The associated character string to enter in the “Selection criteria” box is as follows:

“24 and $0.1 \leq X$ and $0.5 \geq X$ ”³.

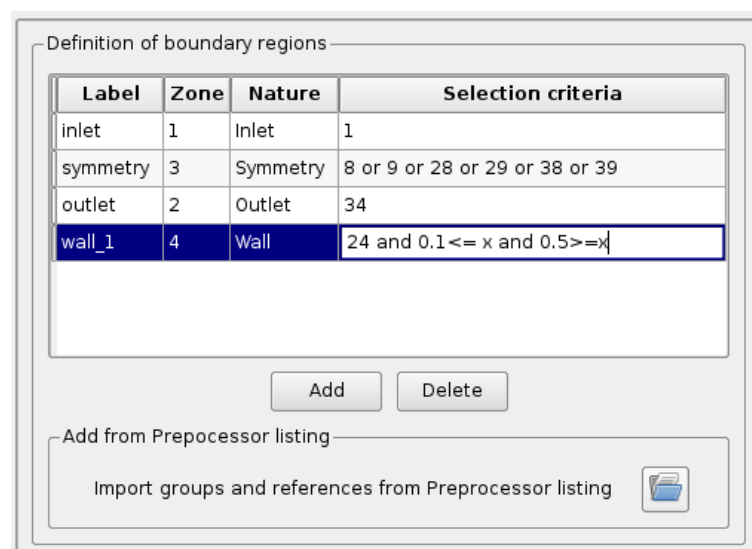


Figure V.45: Creation of a wall boundary region

³Note that, due to the joining process, there are in fact no boundary faces of color 24 with X coordinate outside the $[0.1; 0.5]$ interval. The geometrical criterium is therefore not necessary. It is presented here to show the capacity of the face selection module

Define the other wall boundary zones. The faces of color 6 have to be divided in two separate zones, based on a geometrical criterium on Y .

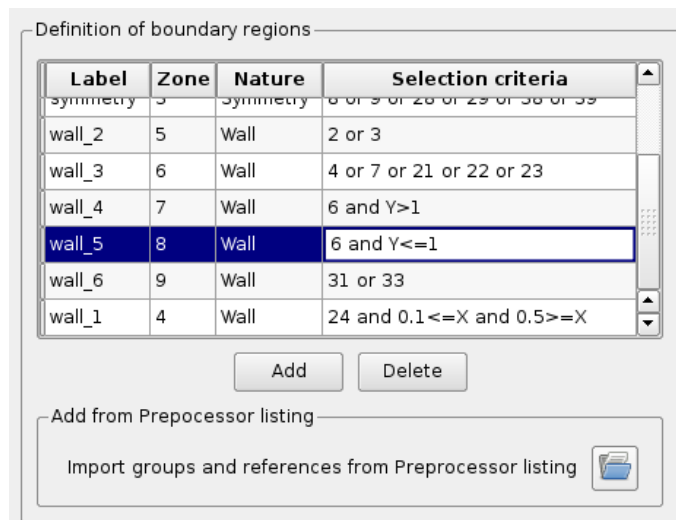


Figure V.46: Creation of wall boundary regions

The dynamic boundary conditions are the same as in case 1 for the inlet, and there are still no sliding walls.

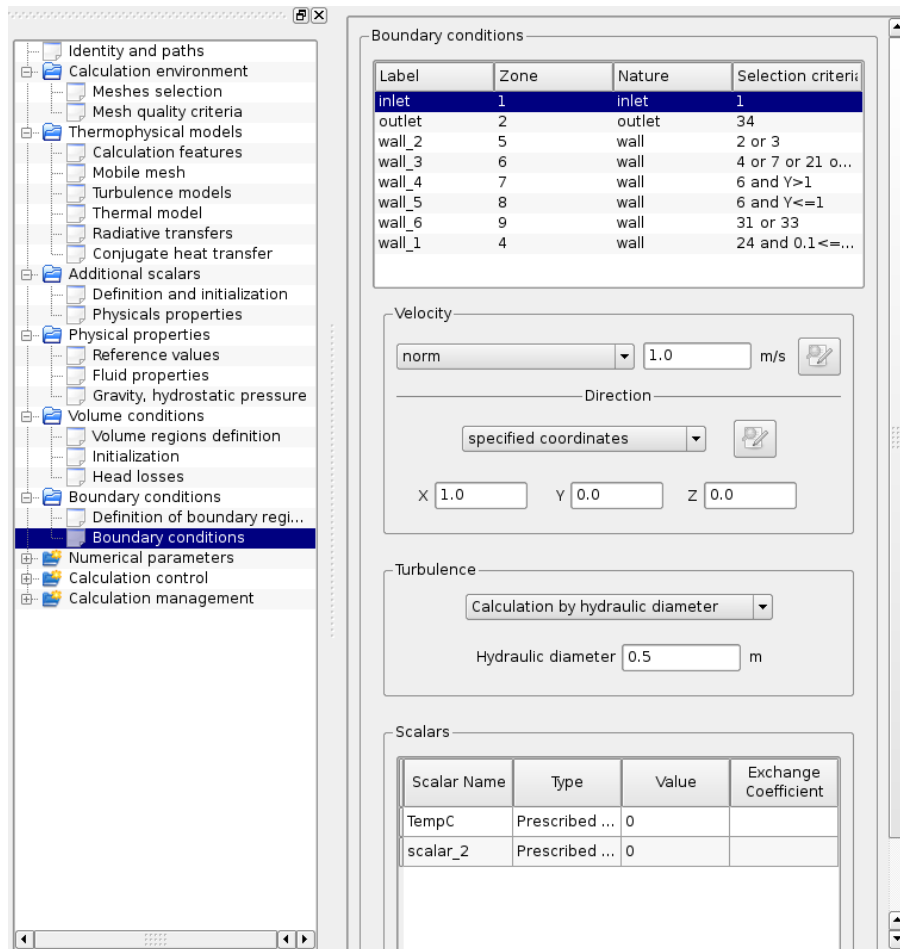


Figure V.47: Dynamic variables boundary: inlet

To configure the scalar boundary conditions on the walls, select individually each wall in the item *Boundary conditions*. On all the walls, a default homogeneous prescribed flux is set for temperature, and prescribed values are specified for the passive scalar, according to the following table:

Wall	Nature	Value
wall_1	Prescribed value	0
wall_2	Prescribed value	5
wall_3	Prescribed value	0
wall_4	Prescribed value	25
wall_5	Prescribed value	320
wall_6	Prescribed value	40

Boundary conditions

Label	Zone	Nature	Selection criteria
inlet	1	inlet	1
outlet	2	outlet	34
wall_2	5	wall	2 or 3
wall_3	6	wall	4 or 7 or 21 or 2...
wall_4	7	wall	6 and $Y > 1$
wall_5	8	wall	6 and $Y \leq 1$
wall_6	9	wall	31 or 33
wall_1	4	wall	24 and $0.1 \leq X \dots$

Smooth or rough wall

☒ smooth wall
☐ rough wall

☐ Sliding wall

Scalars

Scalar Name	Type	Value	Exchange Coefficient
TempC	Prescribed f...	0	
scalar_2	Prescribed ...	320	

Figure V.48: Scalars boundaries: wall_5

Click on *inlet*, to set the inlet values for the scalars: 300°C for temperature and 200 for the passive scalar.

Scalars			
Scalar Name	Type	Value	Exchange Coefficient
TempC	Prescribed ...	300	
scalar_2	Prescribed ...	200	

Figure V.49: Scalars boundaries: inlet

Some calculation parameters now need to be defined. Go to the item *Time step* under the heading *Numerical parameters*. In our case the time step is *Uniform and constant*. Set the number of iterations to 300 and the reference time step to 0.05 s.



Figure V.50: Time step setting

No change is needed in the *Equation parameters* and *Global parameters* items.

Go to the item *Output control* under the heading *Calculation control* to set the output parameters.

Keep the default value for the output listing frequency.

For the Post-processing, select the third option (output every 'n' time steps) and set the value of 'n' to 2.

Activate the post-processing on the boundary faces by ticking the *Domain boundary post processing* box. The EnSight format file will contain an additional part, composed of the boundary faces, on which boundary conditions and some other variables can be visualized. This allows to check if the boundary conditions for the passive scalar have been properly set.

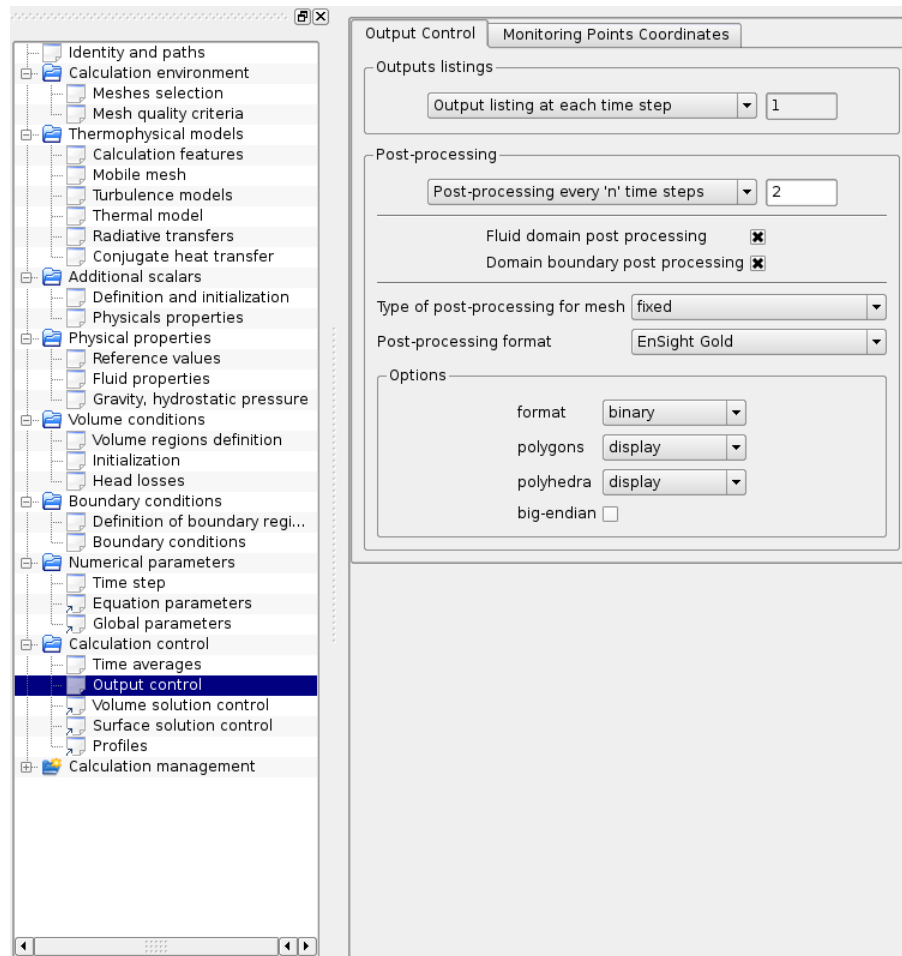


Figure V.51: Output control: post-processing

In this case, chronological records on specified monitoring probes are needed. To define the probes, click on the *Monitoring points Coordinates* tab.

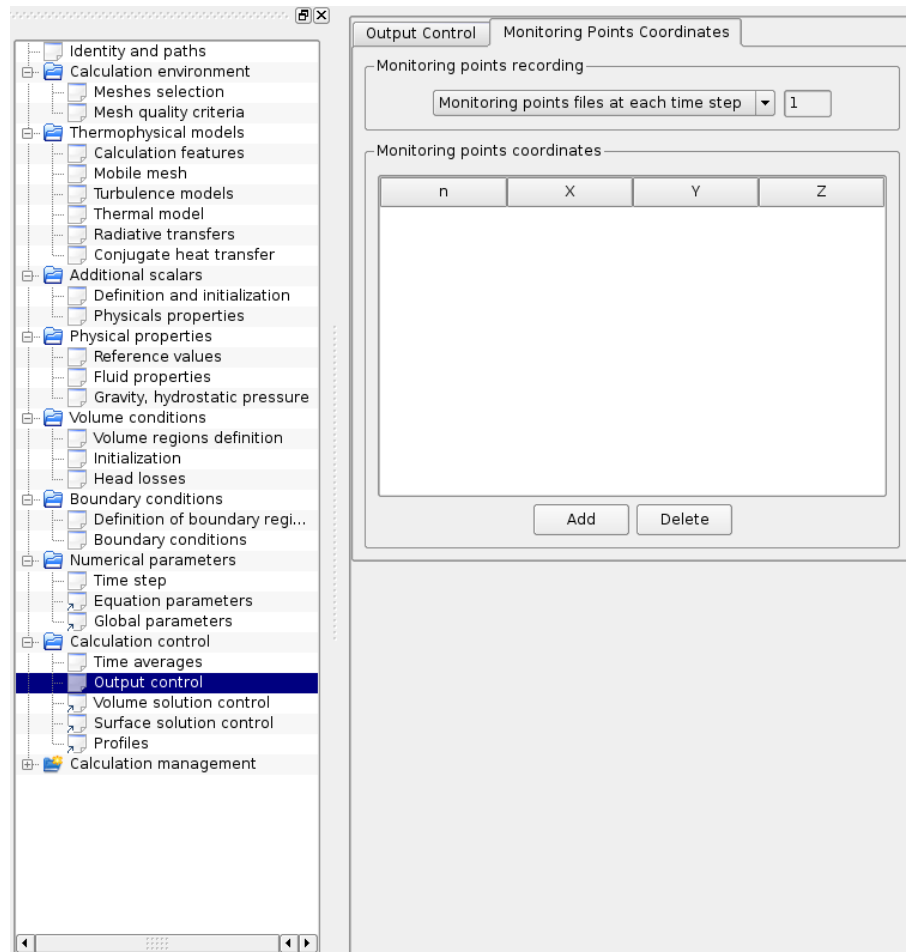
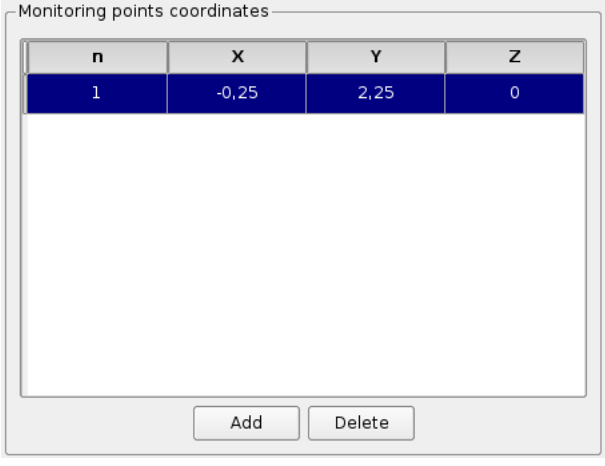


Figure V.52: Output control: monitoring points

Click on “Add” and enter the coordinates of the monitoring points you want to define. For the first point:

- $X = -0.25\ m$
- $Y = 2.25\ m$
- $Z = 0\ m$



A dialog box titled "Monitoring points coordinates" containing a table with 4 columns: n, X, Y, and Z. The first row of the table has values 1, -0.25, 2.25, and 0. Below the table are two buttons: "Add" and "Delete".

n	X	Y	Z
1	-0.25	2.25	0

Add Delete

Figure V.53: Output controls: monitoring points - 1st point

Repeat the procedure for the other probes. Their coordinates are indicated in the following table (the Z coordinate is always 0).

Points	X(m)	Y(m)
2	0.05	2.25
3	0.05	2.75
4	0.05	0.5
5	0.05	-0.25
6	0.75	-0.25
7	0.75	0.25
8	0.75	0.75

Monitoring points coordinates

n	X	Y	Z
1	-0,25	2,25	0
2	0,05	2,75	0
3	0,05	2,75	0
4	0,05	0,5	0
5	0,05	-0,25	0
6	0,75	-0,25	0
7	0,75	0,25	0
8	0,75	0,75	0

Add
Delete

Figure V.54: Output control: monitoring points

Remember to save the Xml file regularly.

Go to the item *Volume solution control* to define which variables will appear in the listing, the post-processing and the chronological records.

Uncheck the boxes in front of the *Pressure*, *Tubulent energy* and *Dissipation* variables, in the *Print in listing* column. Information on these three variables will not appear in the output listing anymore.

Uncheck the boxes in front of the *Courant number* and *Fourier number* variables in the *Post-processing* column. These variables will be removed from the post-processing results.

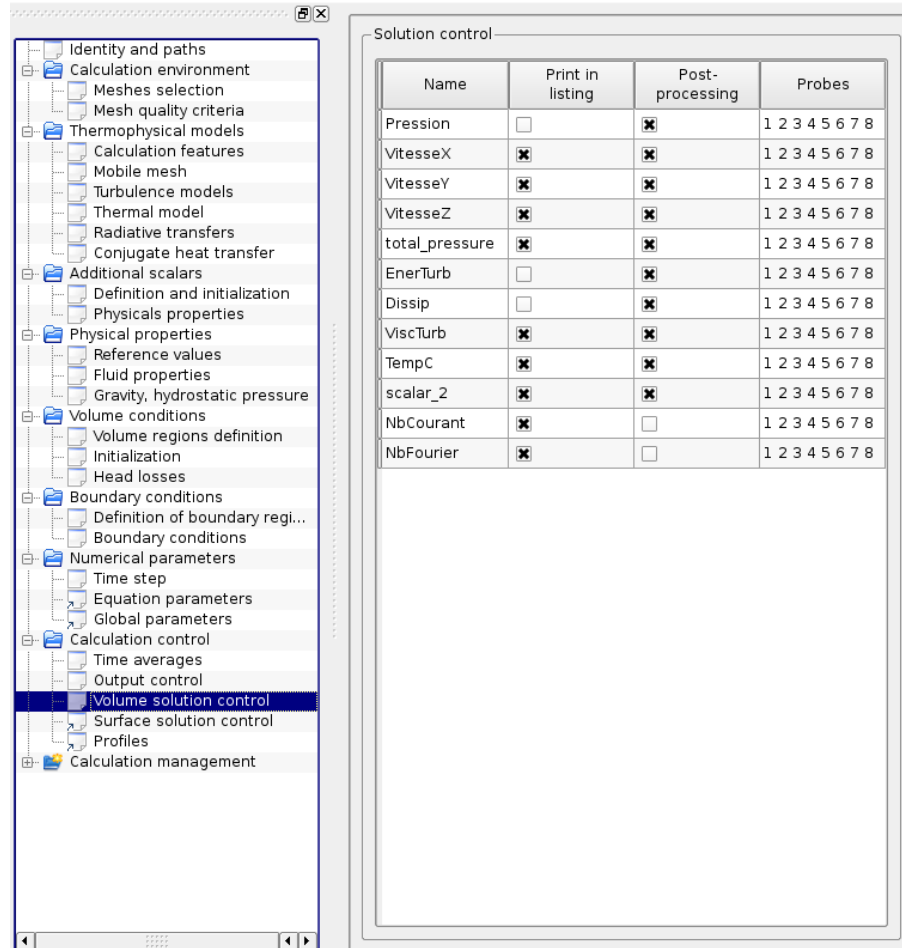


Figure V.55: Solution control - Output configuration

Delete all the probe numbers for the *total_pressure* variable. No chronological record will be created for this variable. As for the *VelocitX* variable, only select probes 1, 2, 6, 7 and 8. Time evolution on the other probes will not be recorded.

Solution control			
Name	Print in listing	Post-processing	Probes
Pression	<input type="checkbox"/>	<input checked="" type="checkbox"/>	1 2 3 4 5 6 7 8
VitesseX	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	1 2 6 7 8
VitesseY	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	1 2 3 4 5 6 7 8
VitesseZ	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	1 2 3 4 5 6 7 8
total_pressure	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	
EnerTurb	<input type="checkbox"/>	<input checked="" type="checkbox"/>	1 2 3 4 5 6 7 8
Dissip	<input type="checkbox"/>	<input checked="" type="checkbox"/>	1 2 3 4 5 6 7 8
ViscTurb	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	1 2 3 4 5 6 7 8
TempC	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	1 2 3 4 5 6 7 8
scalar_2	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	1 2 3 4 5 6 7 8
NbCourant	<input checked="" type="checkbox"/>	<input type="checkbox"/>	1 2 3 4 5 6 7 8
NbFourier	<input checked="" type="checkbox"/>	<input type="checkbox"/>	1 2 3 4 5 6 7 8

Figure V.56: Solution control - Probes

Switch to the *Calculation management* heading to prepare the launch script and run the calculation.

3 SOLUTION FOR CASE 3

Only a few elements are different from case 2.

In this case the density becomes variable. Go to the item *Fluid properties* under the heading *Physical properties* and change the nature of the density from *constant* to *user law*. Click on the highlighted icon and define the user law in the window that pops up. Follow the format used in the tab “Examples”.

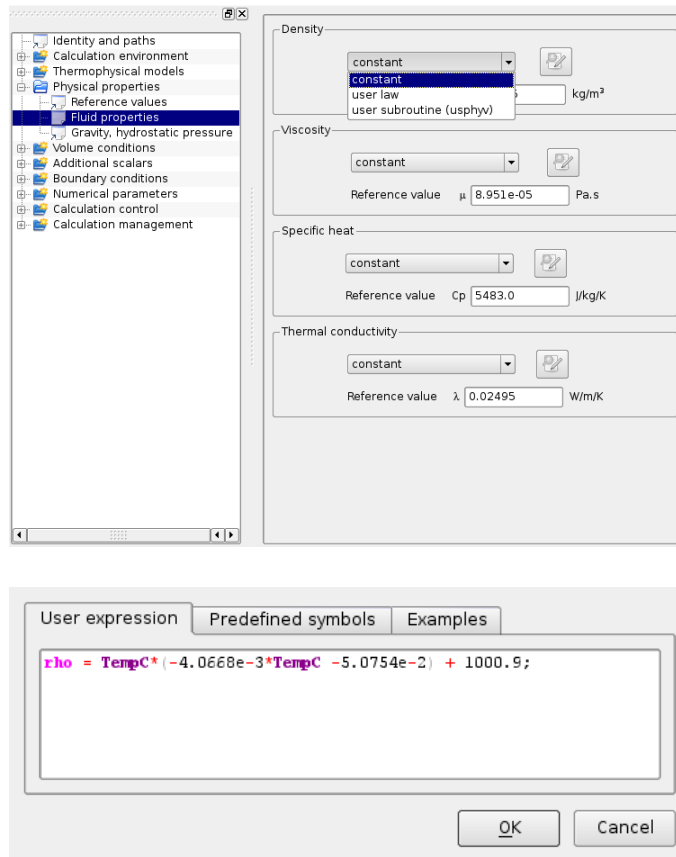


Figure V.57: Fluid properties - Variable density

As the density is variable, the influence of gravity has to be considered. In the heading *Physical properties* go to *Gravity, hydrostatic pressure* and set the value of each component of the gravity vector.

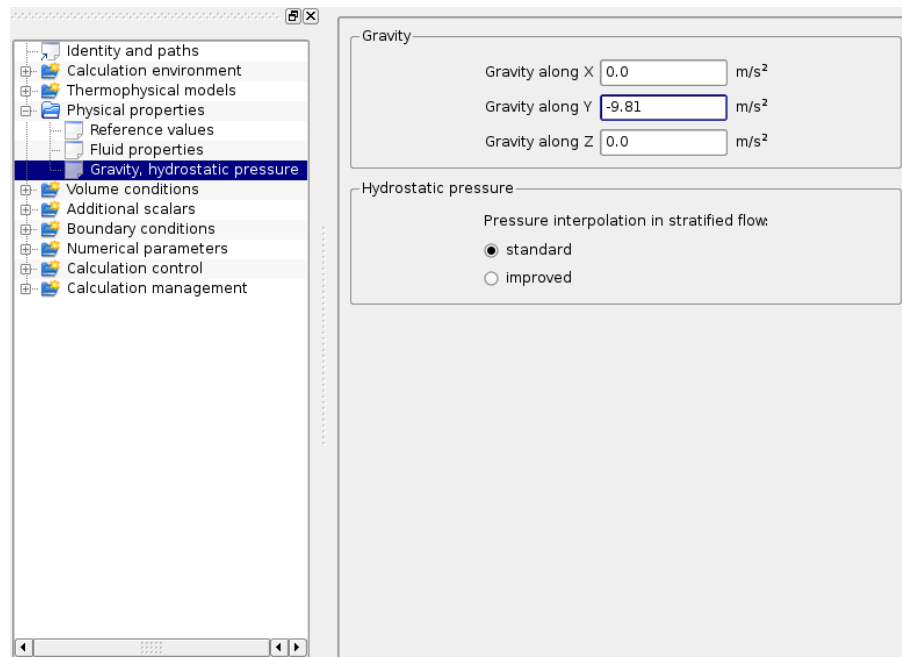


Figure V.58: Fluid properties - Gravity

Add a monitoring point close to the entry boundary condition in the *Output control* item.

Points	X(m)	Y(m)	Z(m)
9	-0.5	2.25	0

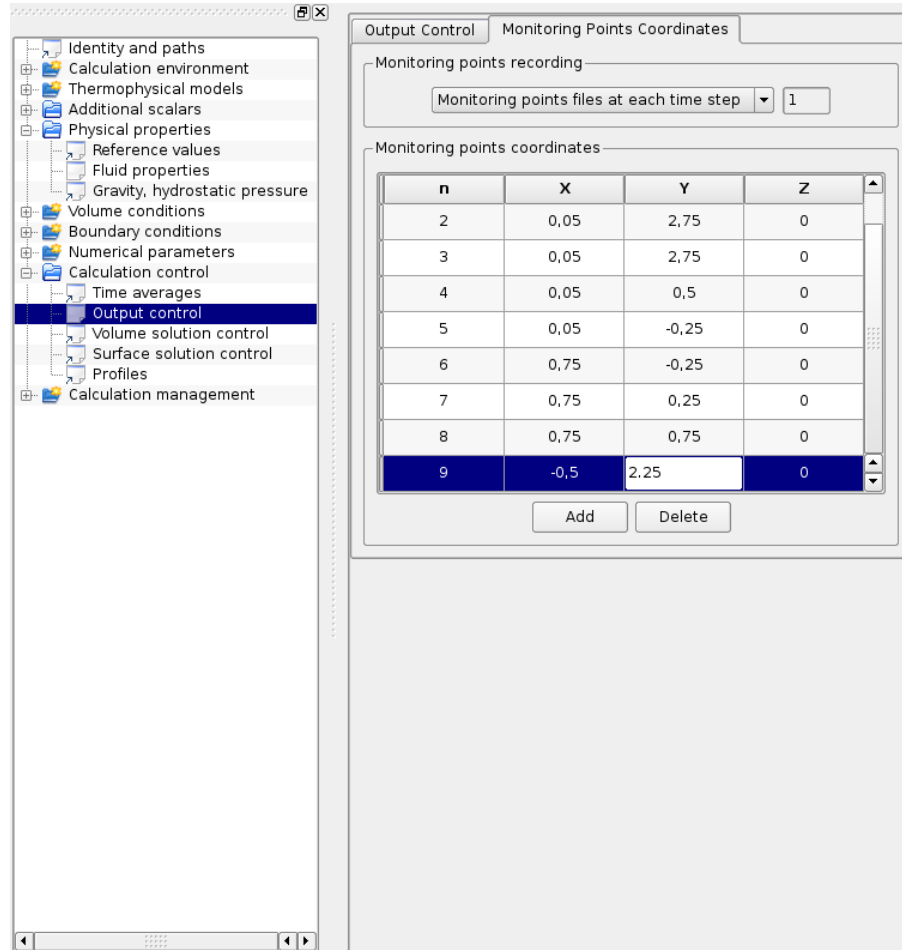


Figure V.59: New monitoring probe

After completing the interface, before running the calculation, some Fortran user routines need to be modified.

Go to the folder SRC/REFERENCE/base and copy *usclim.f90* in the SRC directory.

usclim.f90

In this case, *usclim.f90* is used to specify the time dependent boundary condition for the temperature. Refer to the comments in the routine or to the *Code_Saturne* user manual for more information on this routine.

In our case, you need to identify the boundary faces of color 1. The command `call getfbr('1',nlelt,lstelt)` will return an integer `nlelt`, corresponding to the number of boundary faces of color 1, and an integer array `lstelt` containing the list of the `nlelt` boundary faces of color 1. Note that the string '1' can be more complex and combine different colors, group references or geometrical criteria, with the same syntax as in the Graphical Interface.

For each boundary face `ifac` in the list, the Dirichlet value is given in the multi-dimension array `rcodcl` as follows:

```

if (ttcabs.lt.3.8d0) then
  do ielt = 1, nlelt
    ifac = lstelt(ielt)
    rcodcl(ifac,isca(1),1) = 20.d0 + 100.d0*ttcabs
  enddo
else
  do ielt = 1, nlelt
    ifac = lstelt(ielt)
    rcodcl(ifac,isca(1),1) = 400.d0
  enddo
endif

```

`isca(1)` refers to the first scalar and `ttcabs` is the current physical time.

See the example file in the directory **examples** for the complete *usclim.f90* file.

Note that, although the inlet boundary conditions for temperature are specified in the *usclim.f90* file, it is necessary to specify them also in the Graphical Interface. The value given in the Interface can be anything, it will be overwritten by the Fortran routine.

After updating the Fortran file, run the calculation as explained in case 2.

When a calculation is finished, *Code_Saturne* stores all the necessary elements to continue the computation in another execution, with total continuity. These elements are stored in several files, grouped in a RESTART.xxxxxxxx directory, in the RESU directory.

In this case, after the first calculation is finished, a second calculation will be run, starting from the results of the first one.

Go directly on the item *Start/Restart* under the heading *Calculation management*. Activate the *Calculation restart* by ticking the “on” box. Then click on the folder icon next to it to specify the restart files to use.

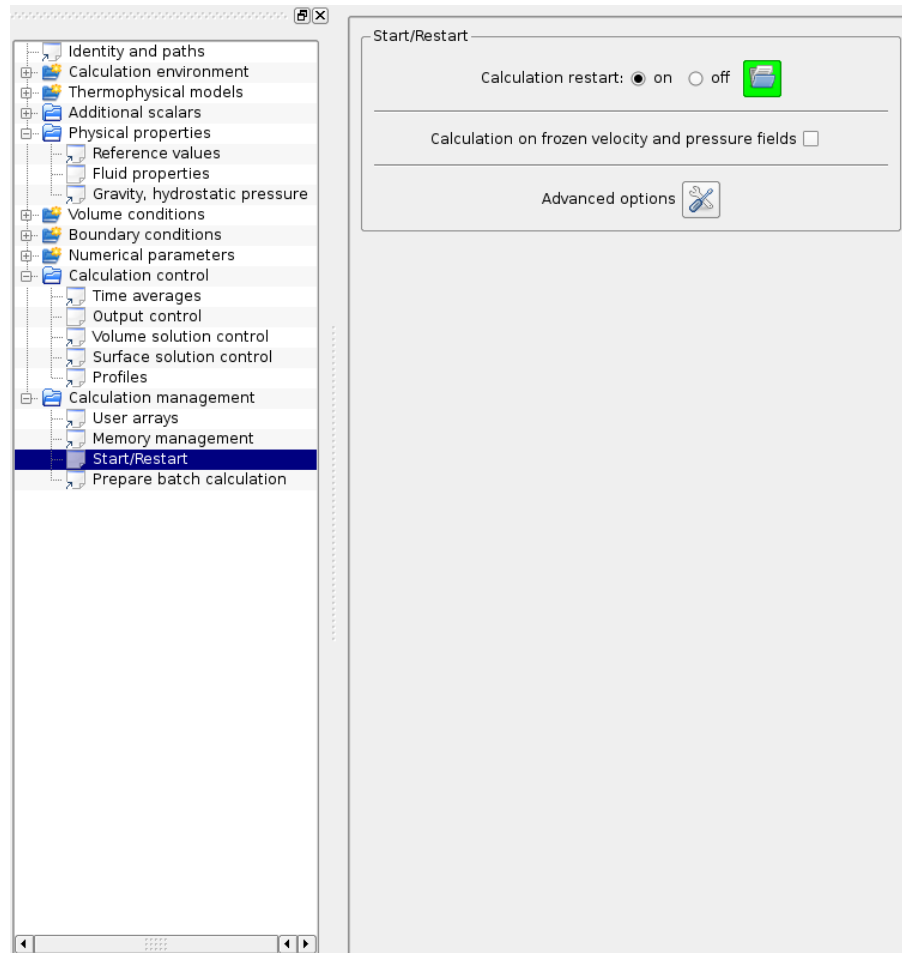


Figure V.60: Start / Restart

A window opens, with the architecture of the study sub-directories. Open the RESU folder and click on the folder RESTART.xxxxxxxx (where xxxxxxxx corresponds to the reference of the first calculation). Then click on *Validate*.

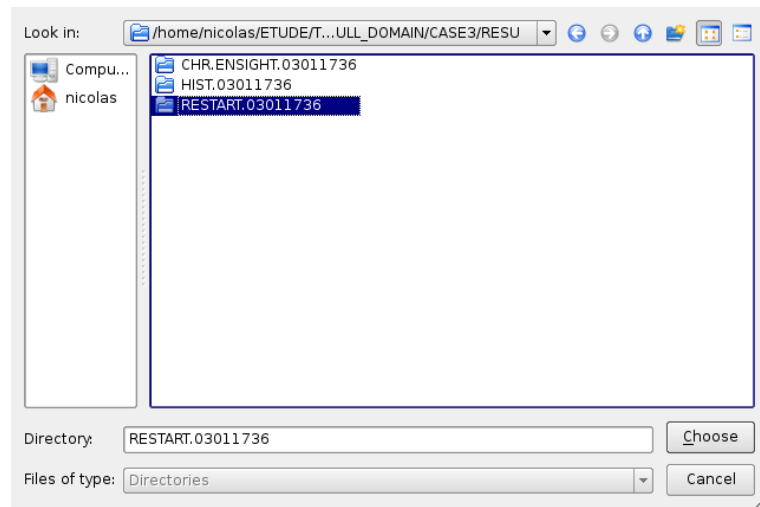


Figure V.61: Start / Restart - Selection of the restart directory

Go to the *Time step* item under the heading *Numerical parameters* and change the number of iterations. It must be the total number of iterations, from the beginning of the first calculation.

The first calculation was done with 300 iterations and another 400 iterations are needed for the present case. Therefore the value 700 must be entered.

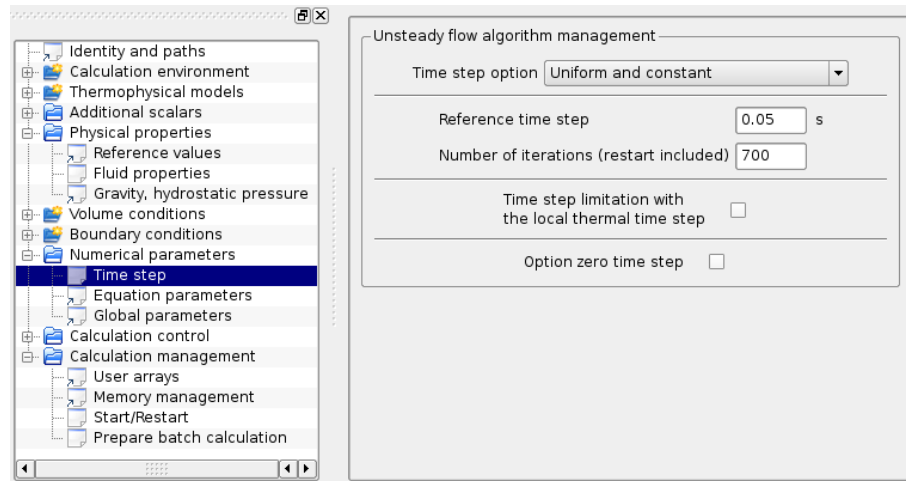


Figure V.62: Time step

Eventually, run the calculation.

4 SOLUTION FOR CASE 4

This case is similar to case 3, with the following differences:

- parallel computation on 2 processors
- head loss
- calculation of a spatial average
- dealing with a user results file

The head loss is defined in the Graphical User Interface. Go to *Volume regions definition* under the heading *Volume conditions*. Click on “Add”, unselect “Initialization” and select “Head losses” in the box named *Nature*. In the box named *Label*, name the head loss region. Define the limits of the head losses region in *Selection criteria*. The associated character string to enter is as follows: “ $0.2 \leq X$ and $0.4 \geq X$ and $-0.75 \leq Y$ and $-0.25 \geq Y$ ”



Figure V.63: Creation of head losses region

To specify the head losses coefficients go to the item *Head losses* and select the name of the head losses volume region. In this example, the coefficient is isotropic so that we use the same value for each α_{ii} . Please note that $\alpha_{ii} = 2 \times K_{ii}$, therefore if $K_{ii} = 10^4$, $\alpha_{ii} = 2 \times 10^4$.

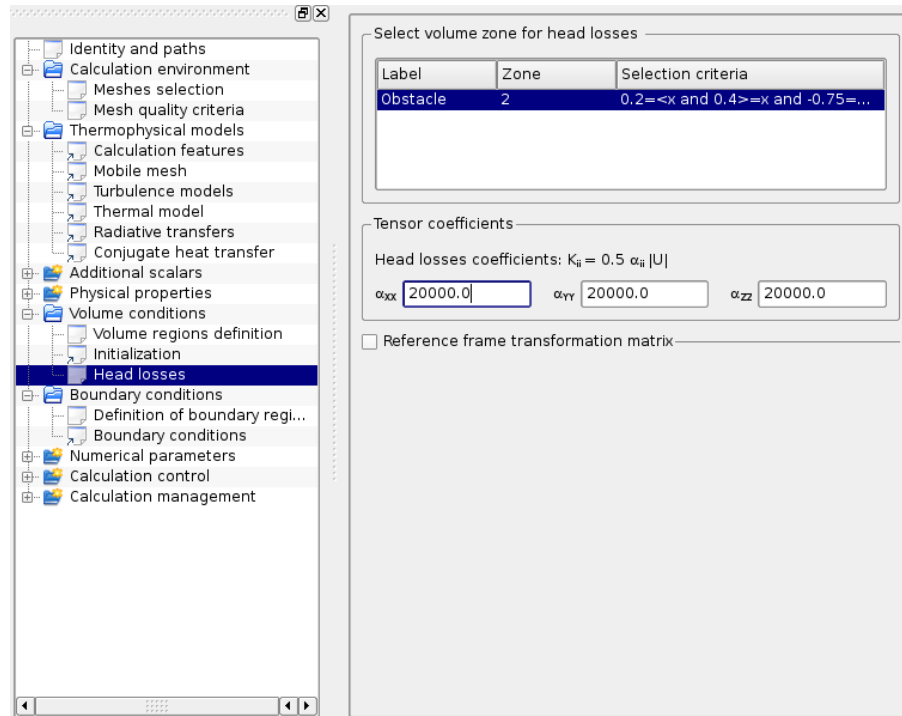


Figure V.64: Head losses coefficients

The calculation of the spatial average is done in the *usproj.f90* routine. Refer to the example file in the directory **examples** for the complete *usproj.f90* file.

The other two changes are controlled in the item *Prepare batch analysis*.

To run the calculation on two processors, simply change the number of processors indicator to 2. The launch script will automatically deal with the rest.



Figure V.65: Number of processors

As seen in paragraph 4, the file “moy.dat” created by *usproj.f90* will be written in the temporary execution directory. It must be identified in the launch script in order to be automatically copied in the RESU directory (More precisely, a RES_USERS.xxxxxxxx directory will be created in the RESU folder, in which the file will be copied).

Click on the icon *New user result file* to enter the associated dialog window. Enter the file name “moy.dat” in the field. Further file names can be added. When finished, click on *OK*.



Figure V.66: User results files

5 SOLUTION FOR CASE 5

The preparation of the calculation for case 5 is very similar to the other cases.

- Open the *Code_Saturne* interface
- Open a new case
- Check the name of the mesh
- Select a $k-\varepsilon$ model
- Use a thermal scalar in Celsius degrees

In the item *Initialization* under the heading *Volume conditions*, set the initial value of the temperature in the domain to 38.5°C . Initialize the turbulence with the reference velocity 0.03183 m.s^{-1} .

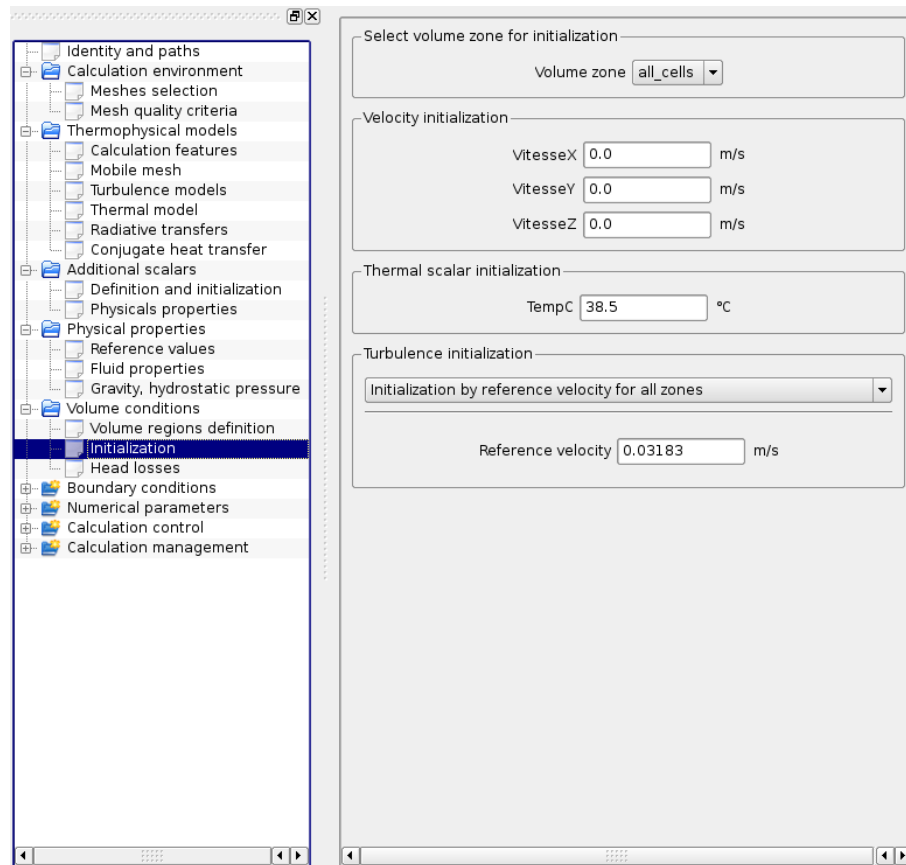


Figure V.67: Thermophysical models - Initialization

In the item *Fluid properties*, under the heading *Physical properties*, enter the following information:

Variable	Type	Value
Density	user law	$998.671 \text{ kg.m}^{-3}$
Viscosity	user law	$0.445 \times 10^{-4} \text{ kg.m}^{-1}.s^{-1}$
Specific Heat	Constant	$4182.88 \text{ J.kg}^{-1}.\text{°C}^{-1}$
Thermal Conductivity	Constant	$0.601498 \text{ W.m}^{-1}.K^{-1}$

For density and viscosity, the value given here will serve as a reference value (see user manual for details).

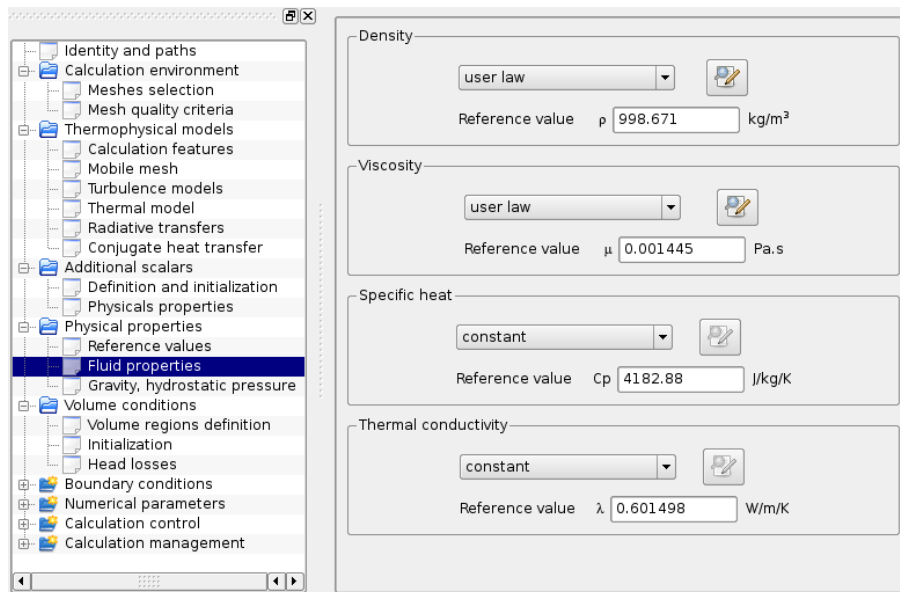


Figure V.68: Physical properties: fluid properties

For the density and viscosity, enter the expressions of the user laws as showed in figures V.69 and V.70, in the windows popping while clicking on the highlighted boxes.

User expression Predefined symbols Examples

```
rho = TempC*(-4.0668e-3*TempC -5.0754e-2) + 1000.9;
```

OK Cancel

Figure V.69: Variable density

User expression Predefined symbols Examples

```
mu = TempC*(TempC*(-3.4016e-9*TempC + 6.2332e-7) -4.5577e-5) + 1.6935e-9;
```

OK Cancel

Figure V.70: Variable viscosity

The aim of the calculation is to simulate a stratified flow. It is therefore necessary to have gravity. Set it to the right value in the item *Gravity, hydrostatic pressure*. In order to have a sharper stratification, the pressure interpolation method will be set to *improved*.

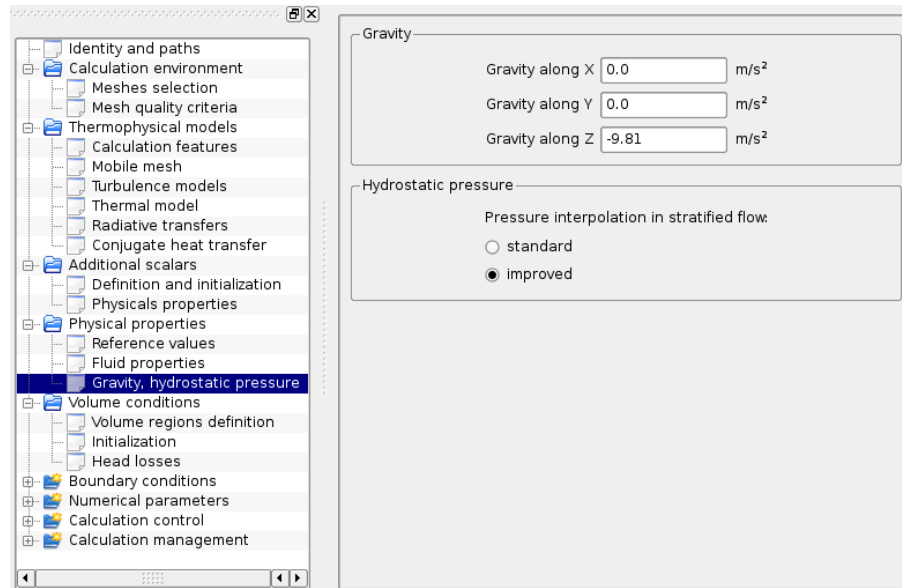


Figure V.71: Fluid properties - Gravity

Go to the item *Definition and initialization* under the heading *Additional scalars* to specify the minimal and maximal values for the temperature: 18.26°C and 38.5°C. Note that the initial value of 38.5°C set earlier is properly taken into account.

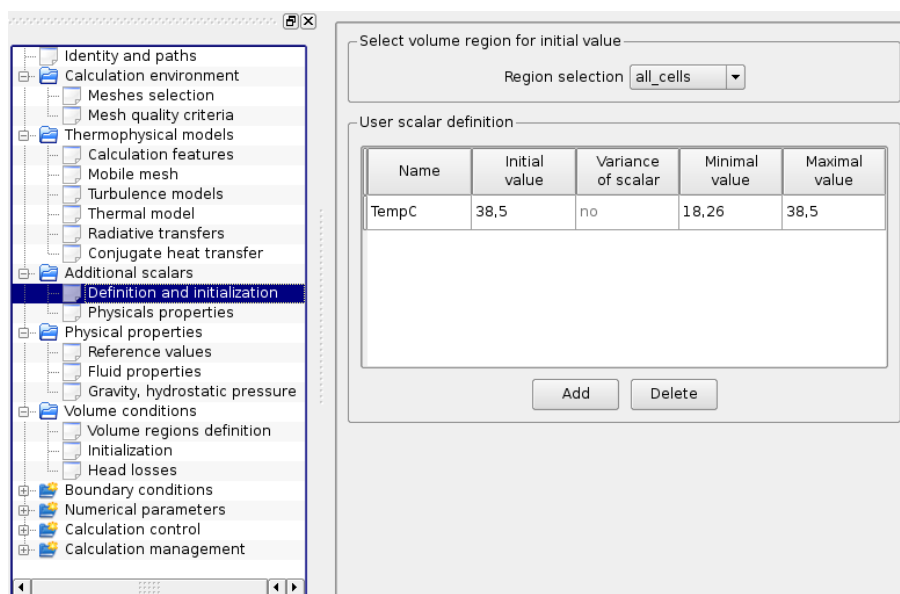


Figure V.72: Scalar initialization

Create the boundary regions.

Colors	Conditions
2	inlet
6	inlet
7	outlet
5	wall

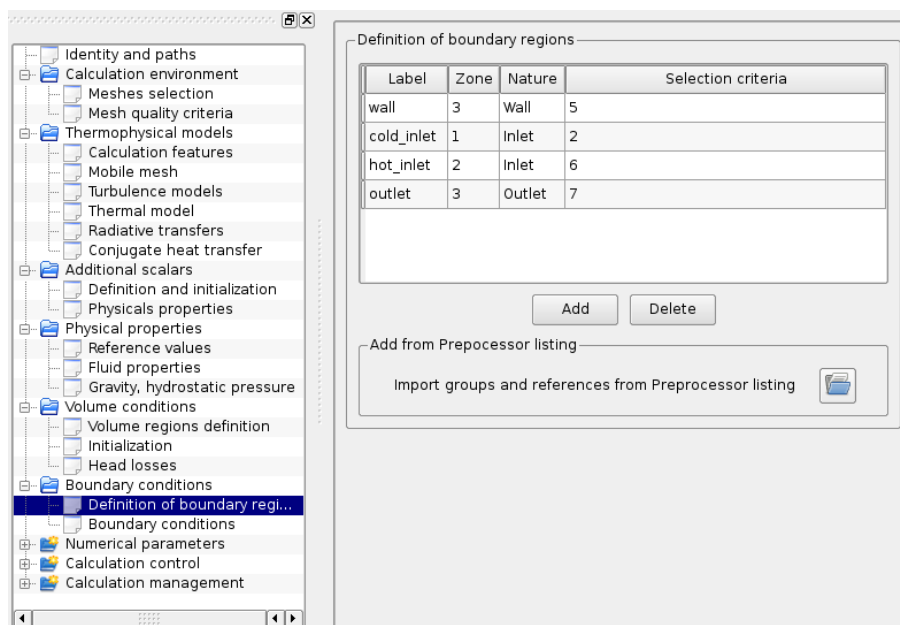


Figure V.73: Boundary regions

For the dynamic boundary conditions, the velocity is 0.03183 m.s^{-1} in the z direction and the hydraulic diameter 0.4 m for both inlets.

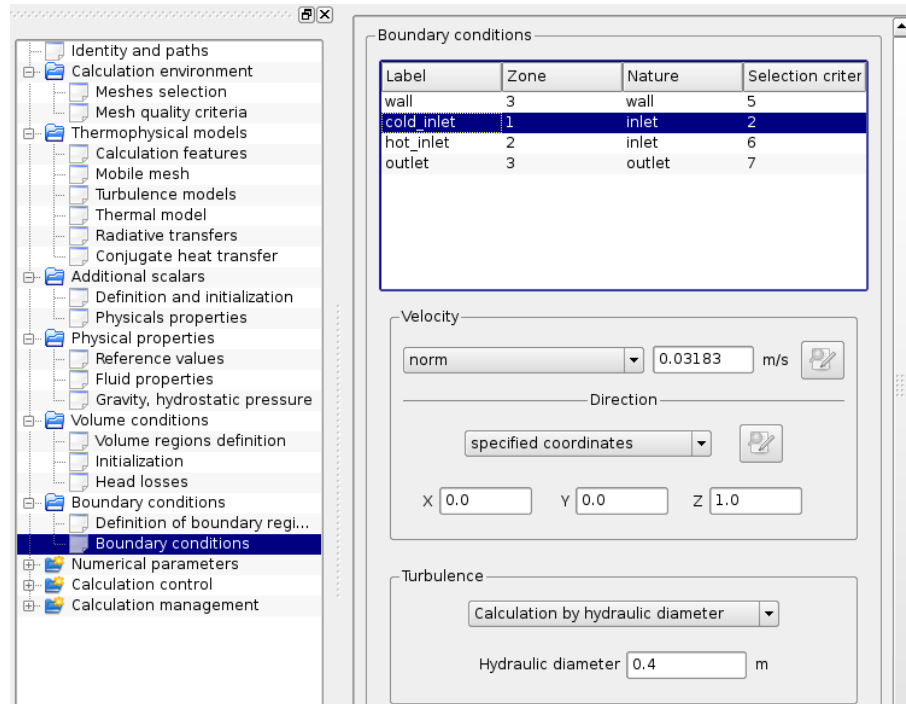


Figure V.74: Dynamic boundary conditions

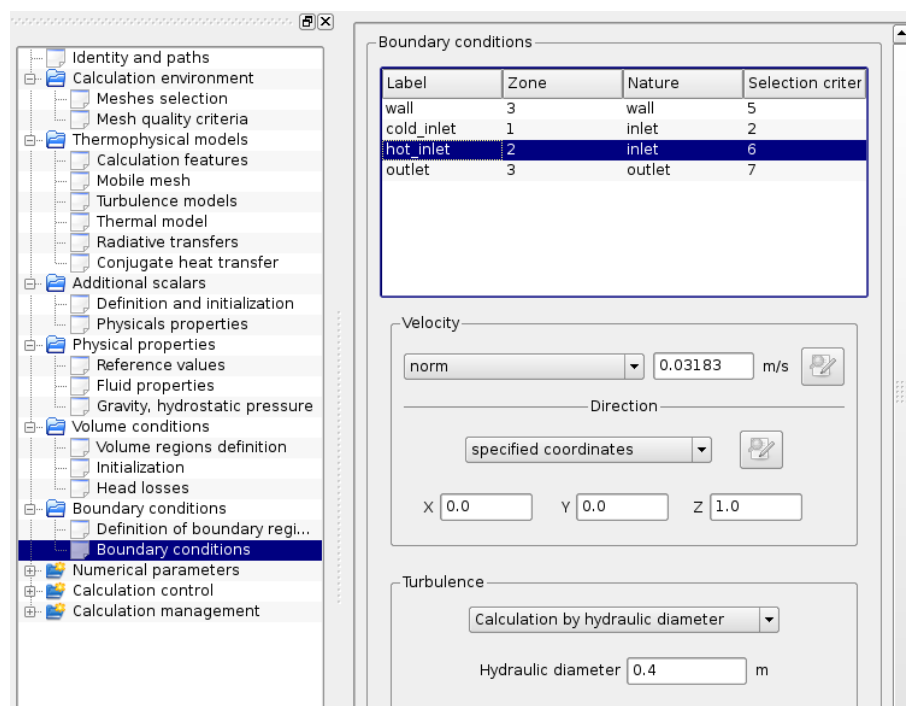


Figure V.75: Dynamic boundary conditions

For the scalar boundary conditions, the temperature of the cold inlet is 18.6°C and that of the hot inlet is 38.5°C.

Boundary conditions

Label	Zone	Nature	Selection criteria
wall	3	wall	5
cold_inlet	1	inlet	2
hot_inlet	2	inlet	6
outlet	3	outlet	7

Velocity

norm 0.03183 m/s

Direction

specified coordinates

X 0.0 Y 0.0 Z 1.0

Turbulence

Calculation by hydraulic diameter

Hydraulic diameter 0.4 m

Scalars

Scalar Name	Type	Value	Exchange Coefficient
TempC	Prescribed ...	18,6	

Figure V.76: Temperature boundary conditions

Boundary conditions

Label	Zone	Nature	Selection criteria
wall	3	wall	5
cold_inlet	1	inlet	2
hot_inlet	2	inlet	6
outlet	3	outlet	7

Velocity

norm 0.03183 m/s

Direction

specified coordinates

X 0.0 Y 0.0 Z 1.0

Turbulence

Calculation by hydraulic diameter

Hydraulic diameter 0.4 m

Scalars

Scalar Name	Type	Value	Exchange Coefficient
TempC	Prescribed ...	38,5	

Figure V.77: Temperature boundary conditions

Tick the appropriate box for the time step to be variable in time and uniform in space. In the boxes below, enter the following parameters:

Parameters of calculation control	
Number of iterations	100
Reference time step	1 s
Maximal CFL number	20
Maximal Fourier number	60
Minimal time step	0.01 s
Maximal time step	70 s
Time step maximal variation	0.1

And activate the option *Time step limitation with the local thermal time step*

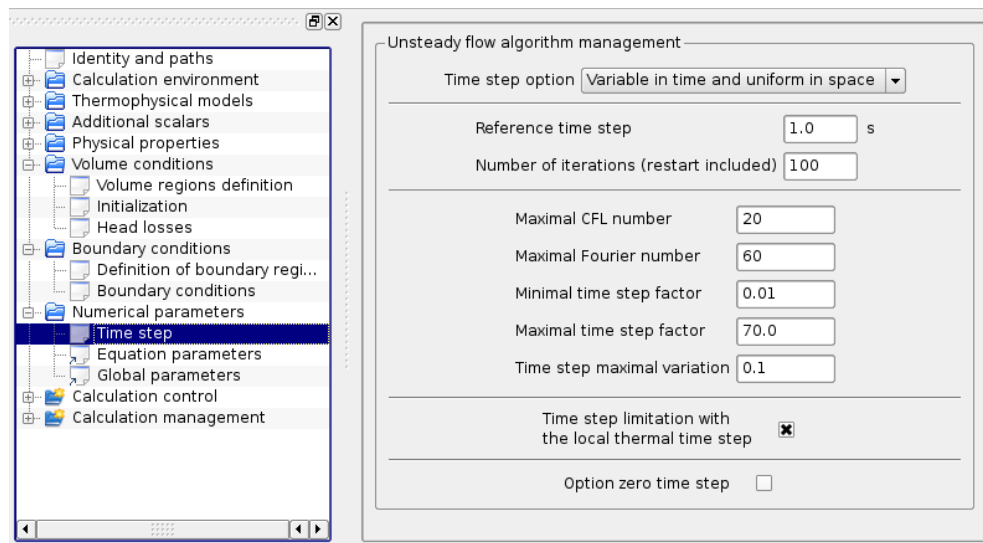


Figure V.78: Time step

Set the frequency of post-processing files to 10.

Create four monitoring probes at the following coordinates:

Points	X(m)	Y(m)	Z(m)
1	0.010025	0.01534	-0.011765
2	1.625	0.01534	-0.031652
3	3.225	0.01534	-0.031652
4	3.8726	0.047481	7.25

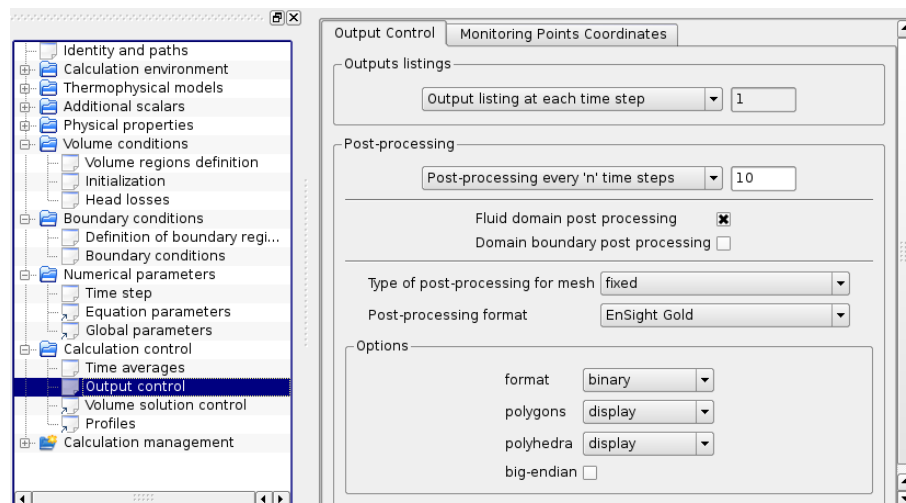


Figure V.79: Output management

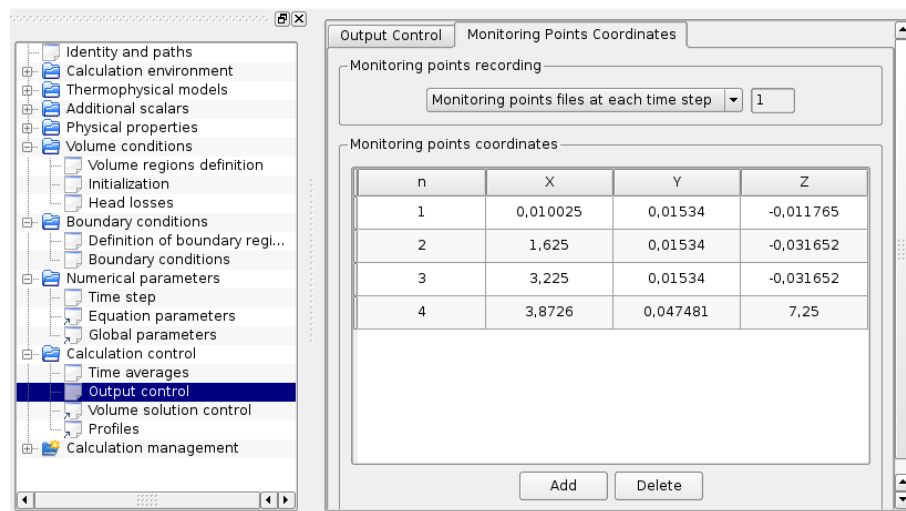


Figure V.80: Monitoring points

For the advanced post-processing features, copy the three routines *usdpst.f90*, *usmpst.f90* and *usvpst.f90* in the SRC directory. The general content of these routines is described in the user manual or in the examples available in the directory SRC/REFERENCE/base. The modified routines adapted to this test case are available in the **examples** directory. Only the main elements are mentioned here.

• **usdpst.f90**

This routine is called only once, at the beginning of the calculation. It allows to define the different writers and parts.

The first writer is the standard writer (which creates the directory CHR.ENSIGHT.xxxxxxxx). It is created by default and has the number -1.

Set the number of additional writers NBCAS to 1. For the first (and unique) additional writer, specify the following elements :

- NOMCAS = 'chr' prefix of the EnSight files
- NOMREP = 'Tinf21.ensight' name of the directory
- NOMFMT = 'EnSight Gold' format of the post-processing
- OPTFMT = 'binary' format options (here binary files) A
- INDMOD = 2 indicates that the parts in this writer will be time dependent in its content
- NTCHRL = 5 periodicity of output

directory TINF21.ENSIGHT.xxxxxxxx will be created with the post-processing results associated to this writer.

Set the number of additional parts NBPART to 2.

For each part, set the number of cells, internal faces and boundary faces (respectively NLCEL, NLFAC, NLFBR) and the lists LSTCEL, LSTFAC and LSTFBR of the elements in the part⁴.

The first part, the clip plane, will be created by detecting the internal faces which have a center of gravity (CDGFAC) between -0.01 and 0.01.

The second part, the cells where the temperature is lower than 21°C, will be specified in *usmpst.f90*. Yet it must be initialized in *usdpst.f90*. The easiest is to set NLCEL=NCEL, total number of cells (and when doing so, there is no need to specify the LSTCEL array).

Eventually, the different parts must be associated with the different writers, through the PSTASS routine. Part 1 is associated to the writer -1, and part 2 to the writer 1.

⁴parts can only contain similar elements, *i.e.* combinations of internal and boundary faces are allowed, but combinations of cells and faces are not

- **usmpst.f90**

This routine is called at each time step. It allows to redefine the content of certain parts using any variable, especially the temperature for this case.

Only part 2 is concerned. A DO/ENDDO loop on all the cells allows to identify those where the temperature is lower than 21°C and hence calculate the number of cells NCELPS in the part and the list of cells LSTCEL.

- **usvpst.f90**

This routine is called at each time step. It allows to specify which variable will be written on which part.

The writing in the post-processing files is triggered by the routine PSTEVA, that must be called for each part and each variable to write. The arguments for PSTEVA are:

- IPART part number
- NAMEVR character string of the name under which the variable will be written
- IDIMT dimension of the variable (1 or 3 for scalars or vectors)
- IENTLA for vectors, indicates if the components are interlaced (=1) or not (=0)
- IVARPR shortcut option for specific situations, set to 0 here
- NTCABS current time step (passed to *usvpst.f90* with the right value)
- TTCABS current physical time (passed to *usvpst.f90* with the right value)
- TRACEL array for variables on cells
- TRAFAC array for variables on internal faces
- TRAFBR array for boundary faces

Part 1 only contains internal faces, so only TRAFAC needs to be filled. Execute a loop on all the faces from the LSTFAC list. For each of them, the temperature will be stored in TRAFAC.

The temperature at each face will be calculated by interpolation from the value at the centers of the two neighboring cells. The numbers of the neighbors of face IFAC are IFACEL(IFAC,1) and IFACEL(IFAC,2). For a proper linear interpolation, see in the TEST_CASES directory for the use of the POND parameter, yielding the fractionnal position of the face on the line joining the two cell centers.

Note that in parallel computing, the cells on both side of the face can be managed by different processors. In order for the interpolation to be correct, a parallel synchronization must be done before the loop. A similar problem happens with periodic boundary conditions. Hence the calling of routines PARCOM and PERCOM shown in the example in the TEST_CASES directory.

As for part 2, it contains only cells so only TRACEL need be filled. For each cell in the LSTCEL list, just set TRACEL to the value of the temperature at the center of the cell.