FLUIDITY

Indoor-outdoor exchanges
Urban environment simulations

Version 1.0.a

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Chapter 1

Introduction

1.1 Purpose and aim of the document

The aim of this document is to show how **Fluidity** can be used to set up typical indoor simulations under a range of conditions. Further information can also be found in the **Fluidity** manual [1] and online http://fluidityproject.github.io/.
The purpose of this document is to allow a new **Fluidity** user to quickly become independent and start running simulations early on. Despite its length, it should be read carefully and followed step by step. Concrete examples will be used and developed along this document, all sections being equally important. In addition, the tricks and information given might be directly experience based and as such might not appear in the **Fluidity** manual [1].

1.2 Getting and installing Fluidity

The following is more or less copied from the **Fluidity** manual [1] and describes how to get and install **Fluidity**. The user is advised to refer to the manual [1] for a detailed description. The following described how to install **Fluidity** on an Ubuntu machine (**Fluidity** does not work under Windows). When this manual was written, all the following were working properly up to Ubuntu 16.04. Some troubles happen on Ubuntu 18.04: the package *fluidity* was not yet available, while *fluidity-dev* was.

1.2.1 Getting binary source of Fluidity: for user only

In that section, **Fluidity** will be installed on the computer but the installation will be transparent for the user, i.e. the code cannot be changed. Add the package archive to the system, update it and install **Fluidity** along with the required supporting software by typing:

```
user@mypc:~$ sudo apt-add-repository -y ppa:fluidity-core/ppa
user@mypc:~$ sudo apt-get update
user@mypc:~$ sudo apt-get -y install fluidity
```

Command 1.1: Getting and installing Fluidity from binary sources.

Fluidity is now installed on the computer. Ready to be used. Typing `fluidity` in a terminal to ensure that it works.

1.2.2 Getting source code of Fluidity: for developer

To develop or locally build **Fluidity**, the *fluidity-dev* package need to be install, which depends on all the other software required for building **Fluidity** (see Appendix C of the **Fluidity** manual [1] for more details about all the other required software and libraries). **To minimise the number of potential errors and libraries to install manually, it is recommended to firstly install the 'standard' Fluidity as explain in the section 1.2.1**: this will automatically install lot of libraries that **Fluidity** needs.
Add the package archive to the system, update it and install the developer version of **Fluidity** by typing:

```
user@mypc:~$ sudo apt-add-repository -y ppa:fluidity-core/ppa
user@mypc:~$ sudo apt-get update
user@mypc:~$ sudo apt-get -y install fluidity-dev
```

Command 1.2: Getting and installing Fluidity from sources.

If GitHub is not already install on your system, install it (first line of Command 1.3). Clone a copy of the latest correct and usable version of **Fluidity**, then change the right of the `fluidity` folder created by typing:

```
user@mypc:~$ sudo apt-get install github
user@mypc:~$ git clone https://github.com/FluidityProject/fluidity.git
user@mypc:~$ sudo chmod -R a+rwx fluidity/
```

Command 1.3: GitHub.

The build process for **Fluidity** then comprises a configuration stage and a compile stage. Go in the directory containing your local source code (the `fluidity` folder downloaded by the GitHub command above), denoted `<<FluiditySourcePath>>` here, and run:

```
user@mypc:~$ cd <<FluiditySourcePath>>
user@mypc:~$ sudo ./configure --enable-sam
user@mypc:~$ sudo make
user@mypc:~$ sudo make install
```

Command 1.4: Installing Fluidity by hand from source code.

The above was tested on a 'blank' computer and two libraries where missing: **PETSc** and **ParMetis**. If you don't yet have them on your system, following are how to install them. Once they are install re-do the whole commands in Command 1.4. If other libraries are missing, please refer to the Annex C of the **Fluidity** manual [1].

PETSc installation

To install **PETSc**, type:

```
user@mypc:~$ sudo apt-get install petsc-dev
```

Command 1.5: Installing PETSc.

ParMetis installation

Note that **Fluidity** will NOT work correctly with versions of **ParMetis** higher than 3.2. **ParMetis** can be downloaded from http://glaros.dtc.umn.edu/gkhome/fsroot/sw/parmetis/OLD. Once downloaded, **ParMetis** is built in the source directory typing:

```
user@mypc:~$ make
```

Command 1.6: Installing ParMetis.

It is then recommended to copy-paste the libraries generated not only in the `fluidity` folder as suggested in the **Fluidity** manual [1] but also in the `/usr/` folder, typing:

```
user@mypc:~$ sudo cp lib*.a /usr/lib
user@mypc:~$ sudo cp parmetis.h /usr/include
user@mypc:~$ sudo cp lib*.a <<FluiditySourcePath>>/lib
user@mypc:~$ sudo cp parmetis.h <<FluiditySourcePath>>/include
```

Command 1.7: Copying ParMetis libraries.

1.3 Quick start

Running a simulation with **Fluidity** consists of several systematic step described below:

- **Step 1:** Create the geometry (*Box.geo*) using **GMSH**. To visualise the geometry, run `gmsh Box.geo &`
- **Step 2:** Create the 3D mesh (*Box.msh*) running `gmsh -3 Box.geo`. To visualise the mesh, run `gmsh Box.msh &`
- **Step 3:** Check the mesh consistency using `gmsh -check Box.msh` and `checkmesh Box`. If none of the two commands return errors: the mesh is done.

- **Step 4:** Set up the **Fluidity** options in *Box.flml* using the graphical interface **Diamond** running `diamond Box.flml &`
- **Step 5:** Run **Fluidity** using `<<FluiditySourcePath>>/bin/fluidity -l -v3 Box.flml &`
- **Step 6:** Visualise the output (*Box.vtu*) using **ParaView**.
- **Step 7:** Post-process the output using python scripts.

Chapter 2

Geometry and mesh

2.1 Introduction

The software used to generate the geometry (**.geo*) and the mesh (**.msh*) is **GMSH** [2]. **GMSH** is a mesh generator freely available at `http://geuz.org/gmsh/`. Both the geometry and the mesh can be created by **GMSH** using the graphical interface and a number of tutorials can be found online. However, in this document, the choice was made to describe how to write a geometry file by hand and generate the mesh directly from this file. This approach gives more flexibility for the geometry and mesh generation. The file *Box.geo* is provided with this document and is used as a example in the following sections.

2.2 Quick start

- **Step 1:** Create the geometry (*Box.geo*). To visualise the geometry, run `gmsh Box.geo &`
- **Step 2:** Create the 3D mesh (*Box.msh*) running `gmsh -3 Box.geo`. To visualise the mesh, run `gmsh Box.msh &`
- **Step 3:** Check the mesh consistency using `gmsh -check Box.msh` and `checkmesh Box`. If none of the two commands return errors: the mesh is done.

The surface IDs needed in **Fluidity** to prescribe the boundary conditions are assigned in the **.geo* file.

2.3 Geometry

The extension of the geometry file is **.geo*. A **.geo* file is a text file that can be written and/or edited by hand using your favourite text editor. The file *Box.geo* is provided with this document and a number of comments (lines started with //) were added into

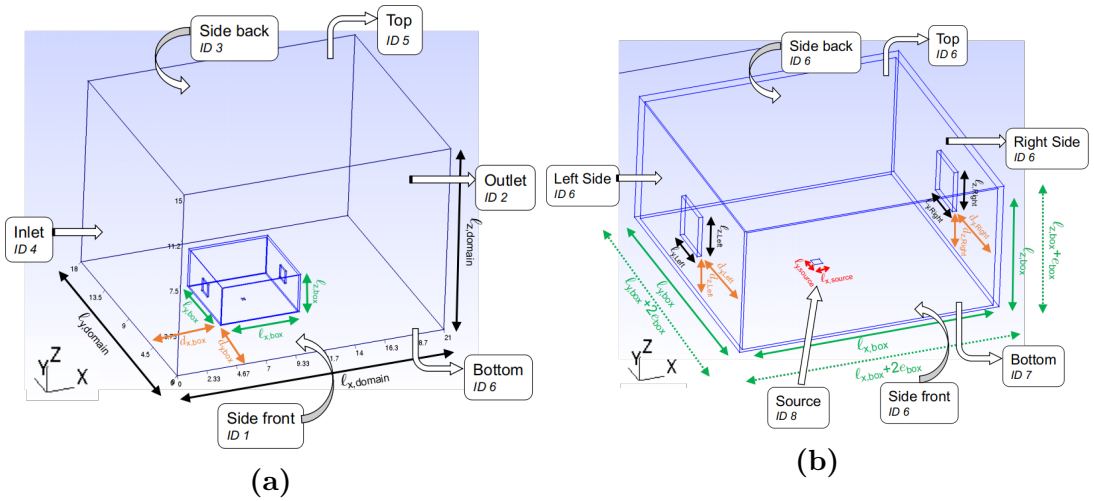


Figure 2.1: Geometry used in *Box.geo* example.

the file to help the user. In the following, the geometry file *Box.geo* is explained step by step and the geometry itself can be seen in Figure 2.1. The user should pay particular attention to section 2.3.5 as it is one of the most important when creating a geometry.

2.3.1 Checking the consistency of the geometry

At any time, the user can visualise the geometry using the graphical interface of **GMSH** (Command 2.1) and check its consistency by running Command 2.2 in a terminal.

```
user@mypc:~$ gmsh Box.geo
```

Command 2.1: Visualising the geometry in **GMSH**.

```
user@mypc:~$ gmsh -check Box.geo
```

Command 2.2: Checking the geometry in **GMSH**

2.3.2 Parameters of the geometry

At the beginning of the file (see Code 2.1), several parameters are defined to provide a certain flexibility in the creation of the geometry.

- If desired, the inner box can be rotated by an angle `theta` (in degree).
- `m_domain_top`, `m_domain_bottom`, `m_box`, `m_opening` and `m_source` define the size of the elements in the final mesh (units are in meters). It should be noted that different size can be assigned in different part of the domain. Decreasing these values will increase the number of elements in the final mesh.

- Finally, all the geometric parameters are defined, including the size and the position of the domain, the inner box and the openings. All units are in meters and the user can refer to Figure 2.1 to interpret each parameter.

```
//--------------------------------------//
// Parameters defining the geometry     //
//--------------------------------------//
// NB: All the following parameters are used to define the geometry.

//--> Rotation of the geometry
theta = 0.0; // in degree

//--> Elements size (edge length) of the mesh
m_domain_top     = 3.0;
m_domain_bottom  = 0.5;
m_box            = 0.5;
m_opening        = 0.2;
m_source         = 0.5;

//--> Position and size of the inner box. Unit in meters.
// The size is defined as the size of the inner volume of the box.
dx_box = 6.0; // x Position
dy_box = 6.0; // y Position

lx_box = 6.0; // Length in the x-direction
ly_box = 6.0; // Length in the y-direction
lz_box = 3.0; // Length in the z-direction

e_box  = 0.1; // Thickness of the walls 10cm
```

Code 2.1: Parameters defining the geometry - from **.geo* file

2.3.3 Defining the geometry

General idea

Defining a geometry can be broken down into the following 6 steps:

- **Point:** A point is defined as `Point(idP)={x,y,z,m};`, where `x`, `y` and `z` define the coordinates of the point having the ID `idP`. Each `idP` needs to be unique. `m` is the element size expected by the user near this point.

- **Line:** A line is defined as `Line(idL)={idP1,idP2};`, where `idL` is the ID of the line starting at point `idP1` and ending at point `idP2`. Each `idL` needs to be unique.

- **Line Loop:** A line loop is defined as `Line Loop(idLL)={idL1,idL2,idL3};`, where `idLL` is the ID of the line loop composed by the lines having the IDs `idL1`, `idL2` and `idL3`. Each `idLL` needs to be unique. Line loops are oriented and define

how each lines are connected to each other to create a surface (at least 3 lines need to be provided). As line loops are oriented, a minus sign '-' needs to be added in front of lines ID if needed (see line 101 in Code 2.2 for example).

- **Plane Surface:** A plane surface is defined as `Plane Surface(idS)={idLL};`, where `idS` is the ID of the plane surface defined by the line loop having the ID `idLL`. Each `idS` needs to be unique. Note that surfaces need to be plane. The plane surfaces define the 2D surfaces that need to be meshed.
- **Surface Loop:** A surface loop is defined as `Surface Loop(idSL)={idS1,idS2, ...};`, where `idSL` is the ID of the surface loop created with the surfaces `idS1`, `idS2`, ... Each `idSL` needs to be unique. The surface loop groups all the surfaces defining a closed geometry (i.e a volume).
- **Volume:** A volume is defined as `Volume(idV)={idSL};`, where `idV` is the ID of the volume defined by the surface loop having the ID `idSL`. Each `idV` needs to be unique. The volumes define the 3D space that needs to be meshed.

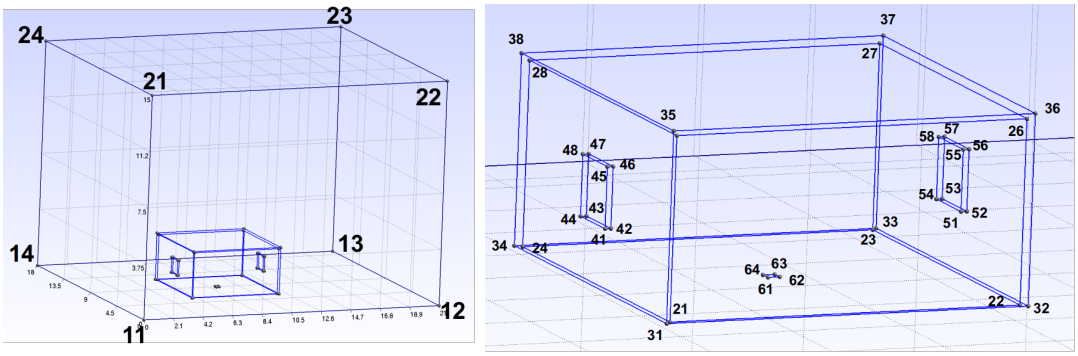
Useful trick

Even for simple geometries, it is easy to get confused with the IDs of points, lines, surfaces... These IDs can be seen on the graphical interface of **GMSH** for convenience. In a terminal, run `gmsh Box.geo &` to open the geometry. In **GMSH**, under `Tools/Options/Geometry/Visibility/`, the `Point labels`, `Line labels` and `Surface labels` can be easily displayed.

Example

In the example provided (*Box.geo*), the geometry of the domain is defined as in Code 2.2. The final `Surface Loop` and `Volume` are defined as shown in Code 2.4. The user can check, using any text editor, that the inner box, the opening and the source are defined like the domain. To help the user, the IDs of the points are given in Figure 2.2.

```
58 //+------------------------------------------+//
59 //    ----    OUTER BOX - Domain      ----     //
60 //+------------------------------------------+//
61 //--------------//
62 //    POINTS    //
63 //--------------//
64 // - Bottom points
65 Point(11) =  {0.0,       0.0,       0.0, m_domain_bottom};
66 Point(12) =  {lx_domain, 0.0,       0.0, m_domain_bottom};
67 Point(13) =  {lx_domain, ly_domain, 0.0, m_domain_bottom};
68 Point(14) =  {0.0,       ly_domain, 0.0, m_domain_bottom};
69
70 // - Top points
71 Point(15) =  {0.0,       0.0,       lz_domain,  m_domain_top};
72 Point(16) =  {lx_domain, 0.0,       lz_domain,  m_domain_top};
```



(a) **(b)**

Figure 2.2: IDs of points used in example *Box.geo*.

```
Point(17) =  {lx_domain, ly_domain, lz_domain,  m_domain_top};
Point(18) =  {0.0,       ly_domain, lz_domain,  m_domain_top};


//---------------//
//    LINES      //
//---------------//
// - Horizontal lines
Line(101) = {11,12};
Line(102) = {12,13};
Line(103) = {13,14};
Line(104) = {14,11};

Line(105) = {15,16};
Line(106) = {16,17};
Line(107) = {17,18};
Line(108) = {18,15};

// - Vertical lines
Line(109) = {11,15};
Line(110) = {12,16};
Line(111) = {13,17};
Line(112) = {14,18};

//-------------------//
//    LINE LOOP      //
//-------------------//
// NB: Line loop are oriented that is why you can see a sign "-" in
    front of some lines ID.
Line Loop(1001) = {109,  105, -110, -101}; // Side front
Line Loop(1002) = {110,  106, -111, -102}; // Outlet
Line Loop(1003) = {111,  107, -112, -103}; // Side back
Line Loop(1004) = {112,  108, -109, -104}; // Inlet

Line Loop(1005) = {105,  106,  107,  108}; // Top
```

```
107 Line Loop(1006) = {101,  102,  103,  104}; // Bottom
108
109 //------------------//
110 //    SURFACES      //
111 //------------------//
112 // NB: Only the inlet, outlet, top and sides surfaces are defined. The
        bottom surface will be defined later because we need to subtract
       the surface of the inner box.
113 Plane Surface(10001) = {1001}; // Side front
114 Plane Surface(10002) = {1002}; // Outlet
115 Plane Surface(10003) = {1003}; // Side back
116 Plane Surface(10004) = {1004}; // Inlet
117 Plane Surface(10005) = {1005}; // Top
```

Code 2.2: Defining the geometry of the domain - from **.geo* file.

As shown in Code 2.3, if desired the inner box can be rotated, while keeping the external domain fixed.

```
203 Rotate{{0,0,1}, {x_center, y_center, z_center}, theta * Pi/180.}{Point
       {31, 32, 33, 34, 35, 36, 37, 38};}
```

Code 2.3: Rotation of points based on the centre of the box - from **.geo* file.

2.3.4 Surfaces with holes

General idea

A `Plane Surface` with holes is defined as:

- `Plane Surface(idS)={idLL1,idLL2,idLL3 ...};`, where the surface with the ID `idS` is a plane surface defined by the line loop `idLL1` minus the surfaces defined by the line loops `idLL2`, `idLL3`, ...

This is particularly useful in two cases:

- if a surface has actually a real hole (like the openings on the walls)
- if different boundary conditions have to be assigned to different regions (in this example, we would like to assign a different boundary condition for the domain's bottom and the box's bottom, see section 2.3.5 for further details).

Example

Examining *Box.geo* file, one can see that some surfaces are not directly defined as `Plane Surface` if they contains holes: it is the case of the walls with openings and the bottom of the ground for example. As shown in Code 2.4 (line 410), the bottom of the domain is the surface defined by the line loop with ID 1006, minus the surface defined by the line loop with ID 3006 (corresponding to the bottom line loop defined by the external walls).

```
//-------------------------------------------------------//
//----> Bottom and wall surfaces with openings    ---     //
//-------------------------------------------------------//
Plane Surface(10006) = {1006, 3006}; // Bottom of the domain
Plane Surface(20006) = {2006, 6001}; // Bottom of the box without the
   source

Plane Surface(20002) = {2002,5004}; // Box, Inner wall: Opening right
Plane Surface(30002) = {3002,5002}; // Box, Outer wall: Opening right

Plane Surface(20004) = {2004,4002}; // Box, Inner wall: Opening left
Plane Surface(30004) = {3004,4004}; // Box, Outer wall: Opening left

//----------------------//
//    DEFINE VOLUME     //
//----------------------//
Surface Loop(100001) = {10001, 10002, 10003, 10004, 10005, 10006,
   20001, 20002, 20003, 20004, 20005, 20006, 30001, 30002, 30003,
   30004, 30005, 40001, 40003, 40005, 40006, 50001, 50003, 50005,
   50006, 60001};
Volume(1000001) = {100001};
```

Code 2.4: Defining the surfaces with holes, the surface loop and the volume - from **.geo* file.

2.3.5 Defining the physical IDs

Surface IDs are used in **Fluidity** to mark different parts of the boundary of the computational domain so that different boundary conditions can be associated with them. In three dimensions, surface IDs are defined by assigning `Physical Surface` IDs in **GMSH**. The IDs are defined at the end of *Box.geo* as shown in Code 2.5. They are also summarised in the Figure 2.1.

```
//----------------------//
//    Physical ID       //
//----------------------//
// NB: These IDs are the one used in Fluidity
Physical Surface(1) = {10001};    // Side front
Physical Surface(2) = {10002};    // Outlet
Physical Surface(3) = {10003};    // Side back
Physical Surface(4) = {10004};    // Inlet
Physical Surface(5) = {10005};    // Top
Physical Surface(6) = {10006, 20001, 20002, 20003, 20004, 20005,
   30001, 30002, 30003, 30004, 30005, 40001, 40003, 40005, 40006,
   50001, 50003, 50005, 50006}; // Bottom and Walls excepted the
   ground of the box and the source
Physical Surface(7) = {20006}; // Ground of the box
Physical Surface(8) = {60001}; // Source
Physical Volume(1000002) = {1000001}; // Volume to be meshed
```

Code 2.5: Defining the IDs of surfaces and volumes - from **.geo* file.

2.3.6 Advice

It is recommended to add the line in Code 2.6 at the end of any **.geo* file. This function removes all duplicate elementary geometrical entities (e.g., points having identical coordinates).

```
439 Coherence;
```

Code 2.6: Coherence - from **.geo* file

2.4 Mesh

2.4.1 Generating the mesh

Method

The extension of the mesh file is **.msh*. To generate the mesh *Box.msh* associated with the geometry *Box.geo*, run the Command 2.3 in a terminal. The option `-3` in Command 2.3 means that the geometry is in 3 dimensions (2 should be used instead if the geometry is 2D).

```
user@mypc:~$ gmsh -3 Box.geo
```

Command 2.3: Generating the geometry using **GMSH**.

A file named *Box.msh* will be created. To visualise the mesh in **GMSH**, run the Command 2.4 in a terminal. In **GMSH**, under `Tools/Options/Mesh/Visibility`, the `Surface faces` or the `Volume edges` can be displayed as shown in Figure 2.3. By default, **GMSH** displays the `Surface edges` only. For convenience, the user can also choose to only display some part of the mesh. In **GMSH**, every surface and volume with respectively a `Physical Surface` or `Physical Volume` ID is listed under `Tools/Visibility/ List browser`. The user can select one or several surfaces at the same time to display in **GMSH** as done in Figure 2.3.

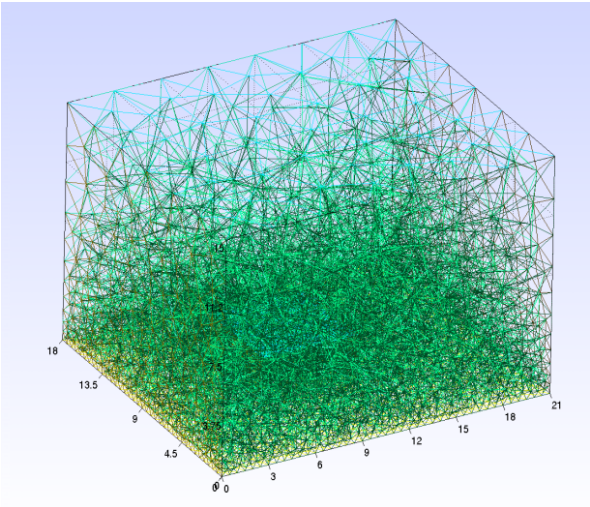
```
user@mypc:~$ gmsh Box.msh
```

Command 2.4: Visualising the geometry in **GMSH**.

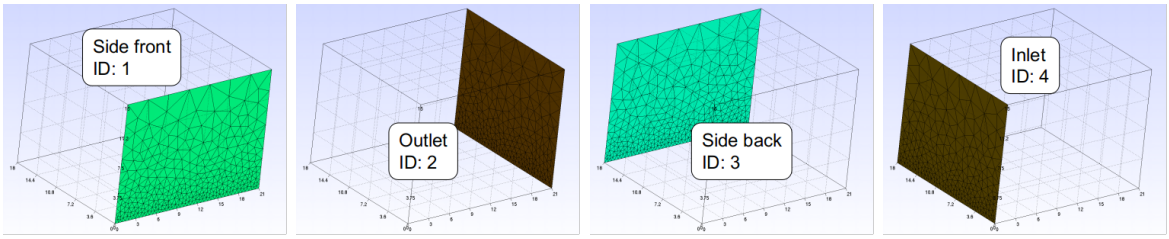
Common errors

The main common errors that occur when trying to generate the mesh are:

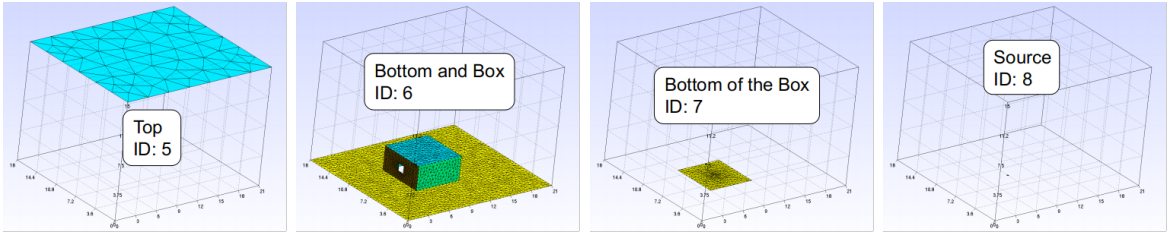
- *No tetrahedra in region idV*: this happens mainly if the `Surface Loop` is not closed.
- *Found two facets intersect each other*: two surfaces in `Surface Loop` are overlapping.
- *Found two duplicated facets*: a surface in `Surface Loop` is defined twice.



(a) 3D mesh



(b) **(c)** **(d)** **(e)**



(f) **(g)** **(h)** **(i)**

Figure 2.3: Mesh generated from the geometry *Box.geo*.

2.4.2 Checking the consistency of the mesh

Method

At this stage, the mesh is created. Before running **Fluidity**, it is recommended to check if the generated mesh is consistent and suitable to run simulations. The check can be done in the following 3 steps:

- **Step 1:** The first check is visual: open the mesh into **GMSH** using the Command 2.4 and check the visualise aspect of the mesh using the tricks to display the mesh explained in section 2.4.1. Are the finer elements where expected? Do they seem fine enough?
- **Step 2:** The second step is to check if the mesh is consistent on a "**GMSH**" point of view. To this end, run the Command 2.5 in a terminal.

```
user@mypc:~$ gmsh -check Box.msh
```

Command 2.5: Check the consistency of the mesh using **GMSH** tool.

- **Step 3:** The third step consists of using a **Fluidity** tool to test if the mesh is consistent on a "**Fluidity**" point of view. This can be done with the Command 2.6.

```
user@mypc:~$ checkmesh Box
```

Command 2.6: Check the consistency of the mesh using **Fluidity** tool.

If all 3 steps suggested above are successful, then you are ready to run **Fluidity** simulations.

Common errors

Below are listed common errors that Command 2.5 and Command 2.6 can raise, as well as ideas on how to fix them:

- From **GMSH** tool (Command 2.5)
  - *duplicate vertex - duplicate elements*: A surface is defined twice and different `Physical Surface` ID were assigned to them.
- From **Fluidity** tool (Command 2.6):
  - *Degenerate surface element found*: if you have this error it is probably because you already had errors when generating the mesh. This is mainly due to the fact that the `Surface Loop` is not closed.
  - *Degenerate volume element found*: this error occurs if you have forgotten to define a `Volume` or to assign a `Physical Volume` ID to the volume.

– *Surface element does not exist in the mesh*: A surface defined by a `Physical Surface` ID is not present in the `Surface Loop`.

– *WARNING: an incomplete surface mesh has been provided. This will not work in parallel. All parts of the domain boundary need to be marked with a (physical) surface id*: The error is quite clear: each surface defining the `Surface Loop` has to have a `Physical Surface` ID and at least one surface does not.

Useful mesh statistics

Note that the tools using in Command 2.5 and Command 2.6 give also interesting information and statistics concerning the mesh:

- From **GMSH** tool (Command 2.5): Number of nodes and number of elements...
- From **Fluidity** tool (Command 2.6): Number of nodes, number of elements, minimum edge length and maximum edge length...

2.5 Playing around

It is recommended that the user plays around with the parameters defined at the beginning of the file, to change the position and/or size of the openings for example. The user can also rotate the box if desired. Interested exercises would consist of modifying the *Box.geo* file to have the openings as "doors" instead of "windows"; or having the box in the middle of the domain instead of clipped to the ground. To create these geometries, the *Box.geo* will need a number of changes (the bottom surface will be defined differently for example), but the *Box.geo* provided can easily be used as a starting point.
Other options to experiment with are the parameters defining the elements size. Hence, the user can see the impact of reducing or increasing these values on the mesh aspect.

Chapter 3

Equations and numerical methods

The aim of this chapter is not to give extended overview of the equations and their implementations but only a brief idea of them. The reader can refer to [1, 3, 4, 5, 6] for more details.

3.1 Equations

3.1.1 Navier-Stokes and Large Eddy Simulation (LES)

The Large Eddy Simulation (LES) formulation implemented in **Fluidity** describes turbulent flows based on the filtered (three dimensional) incompressible Navier-Stokes equations (continuity of mass and momentum equation, see equation 3.1 and equation 3.2):

$$\nabla.\overline{u} = 0 \tag{3.1}$$

$$\frac{\partial \overline{u}}{\partial t} + \overline{u}.\nabla\overline{u} = -\frac{1}{\rho}\nabla\overline{p} + \nabla.\Big[\left(\nu + \nu_\tau\right)\nabla\overline{u}\Big] \tag{3.2}$$

where $\overline{u}$ is the resolved velocity (m/s), $\overline{p}$ is the resolved pressure (Pa), ρ is the fluid density (kg/m^3), ν is the kinematic viscosity (m^2/s) and ν_τ is the anisotropic eddy viscosity (m^2/s).
A novel component in the implementation of the standard LES equations within **Fluidity** is the anisotropic eddy viscosity tensor ν_τ defined by equation 3.3.

$$\nu_\tau = C_S^2 l^2 |\overline{S}| \tag{3.3}$$

C_S is the Smagorinsky coefficient (usually taken equal to 0.1), l is the Smagorinsky length-scale which depends on the local element size and $|\overline{S}|$ is the strain rate expressed as in equation 3.4.

$$|\overline{S}| = (2\overline{S}_{ij}\overline{S}_{ij})^{1/2} \tag{3.4}$$

where $\overline{S}_{ij}$ is the local strain rate defined by equation 3.5.

$$\overline{S}_{ij} = \frac{1}{2}\left(\frac{\partial \overline{u}_i}{\partial x_j} + \frac{\partial \overline{u}_i}{\partial x_i}\right) \tag{3.5}$$

3.1.2 Advection-Diffusion equation

The transport of a scalar field c (i.e, a passive tracer) having the unit $unit_c$ is expressed using a classic advection-diffusion equation with a source term (equation 3.6).

$$\frac{\partial c}{\partial t} + \nabla.(\mathbf{u}c) = \nabla.\left(\overline{\overline{\kappa}}\nabla c\right) + F \tag{3.6}$$

where $\mathbf{u}$ is the velocity vector (m/s), $\overline{\overline{\kappa}}$ is the diffusivity tensor (m^2/s) and F represents the source terms ($unit_c$/s).
In the case where the scalar c is the temperature in Kelvin, then the source term F is expressed by equation 3.7

$$F = \frac{Q}{\rho c_p} \tag{3.7}$$

where Q is a power density expressed in W/m^3.
In the case where the scalar c is the species concentration in kg/m^3, then the source term F is expressed by equation 3.8 or equation 3.9:

$$F = \frac{\dot{m}}{V} \tag{3.8}$$

where $\dot{m}$ is a mass flow rate expressed in kg/s and V is the volume of the source in m^3;

$$F = \frac{Q\rho}{V} \tag{3.9}$$

where Q is a volumetric flow rate expressed in m^3/s and V is the volume of the source in m^3.

3.1.3 Boussinesq approximation

Under certain conditions, one can assume that density does not vary greatly about a mean reference density, that is, the density at a position $\mathbf{x}$ can be written as:

$$\rho(\mathbf{x}, t) = \rho_0 + \rho'(\mathbf{x}, t) \tag{3.10}$$

where $\rho' \ll \rho_0$. Such an approximation is named the Boussinesq approximation. This assumption ignores density differences except when they are multiplied by g, the acceleration due to gravity.

3.2 Numerical methods

3.2.1 Discretisation

For indoor-outdoor exchange simulations or urban environment simulations, the following discretisation are recommended:

- **Navier-Stokes equations:** The Navier-Stokes equations, under the Boussinesq approximation, are solved using a continuous Galerkin finite element discretisation, while a Crank-Nicolson time discretisation approach is adopted.
- **Advection-diffusion equation:** The advection-diffusion is solved using a control volume - finite element space discretisation, while a Crank-Nicolson time discretisation approach is adopted.

3.2.2 CFL number

To avoid crashes in simulations, the time step can be adaptive using a Courant-Friedrichs-Lewy (CFL) condition. This option allows the time step Δt to vary throughout the run, depending on the CFL number. The maximum CFL number $C_{\max}$ is set by the user as shown in Figure 5.2. The CFL condition is a necessary condition for convergence while solving certain partial differential equations and has the following form:

$$C = \frac{u\Delta t}{\Delta x} \leq C_{\max} \tag{3.11}$$

where C is the dimensionless CFL number, $C_{\max}$ is the maximum CFL number given by the user, u is the magnitude of the velocity (m/s), Δt is the time step (s) and Δx is the length interval, i.e taken as the edge element in the mesh (m).
It is commonly say that the maximum value of $C_{\max}$ should be 1. However, in **Fluidity**, this value can be increased further (until 5-10) without convergence issues. However, it is recommended to start the simulations with a value of 1 and then increase this value incrementally checking if the accuracy of the results are not affected. A too high CFL number might prematurely kill the turbulence.

3.2.3 Solver: PETSc

The solver used in **Fluidity** is the open-source solver toolbox **PETSc**. The user can refer to https://www.mcs.anl.gov/petsc/ for more information.

Chapter 4

Boundary and initial conditions

4.1 Introduction

This section shows examples of boundary conditions that can be used to set up a wide range of indoor simulations. They all rely on the geometry described previously which is a box with two openings in the middle of a wider computational domain. In this chapter, the fluid is air, with properties defined in Table 4.1. Gravity ($g = 9.81$ m/s^2) is taken into account. The Navier-Stokes equations, under the Boussinesq approximation, are solved for the fluid, while the advection-diffusion equation is solved for the heat transfers. The mesh and the time step are fixed and the simulations are run in serial.
Important note: The simulations with constant time steps work with the geometry file provided, i.e. if the element sizes have not been changed (see Section 2.3.2). If the mesh has been refined (i.e. the element size decreased), the simulations may crash. In that case, the time step has to be decreased under the option `timestepping/timestep` or the user can use an adaptive time step (option `timestepping/adaptive_timestep`) and use a CFL condition (see Section 3.2.2).
In the next sections, different common and useful boundary conditions will be tested. The following will however remain fixed:

- **Outlet (Dirichlet boundary condition):** A zero stress conditions is imposed at the outlet which sets $p = 0$. It must noted that at least one pressure boundary

Thermal Diffusivity	$\kappa = 2.12 \times 10^{-5}$ m^2/s
Thermal Conductivity	$\lambda = 2.597 \times 10^{-2}$ W/m/K
Kinematic Viscosity	$\nu = 1.5 \times 10^{-5}$ m^2/s
Reference Density	$\rho_0 = 1.225$ kg/m^3
Thermal Expansion coefficient	$\alpha = 3.43 \times 10^{-3}$K^{-1}
	at $T = 293$ K
Specific Heat Capacity	$c_p = 1000$ J/kg/K

Table 4.1: Properties of the air used in the simulations.

condition is required as a reference for **Fluidity** to run. See Section 4.6.

- **Sides and top of the domain (Dirichlet boundary condition):** A perfect slip boundary condition is imposed on the sides and top of the domain which sets the normal component of velocity equal to zero.
- **Ground of the domain and walls (Dirichlet boundary condition):** A zero velocity boundary condition is prescribed on the floor of the domain, the floor of the box and the walls of the box which sets the three components of velocity equal to zero. This boundary condition is discussed in details in Section 4.5.3.

Table 4.2 summarises the different simulations presented in the next sections.

4.2 Quick start

Running a simulation

Running a simulation with **Fluidity** consists of the following steps:

- **Step 1:** Set up the **Fluidity** options in *3d_Case.flml* using the graphical interface **Diamond** running `diamond 3d_Case.flml &`
- **Step 2:** Run **Fluidity** using `<<FluiditySourcePath>>/bin/fluidity -l -v3 3d_Case.flml &`
- **Step 3:** Visualise the **Fluidity** log file during the simulation using the command `tail -f fluidity.log-0` in a terminal.
- **Step 4:** Open the **Fluidity** error file using the command `gedit fluidity.err-0 &` in a terminal.

Command 4.1 is the basic command line to run a simulation with **Fluidity**. One can notice two options:

- `-l`: This option writes the terminal log and errors in the files `fluidity.log-0` and `fluidity.err-0`, respectively, instead of writing them directly in the terminal.
- `-v3`: This is the degree of verbosity that the user wants. The user can choose between `-v1`, `-v2` and `-v3`, where `-v1` will be less verbose than `-v3`.

```
user@mypc:~$ <<FluiditySourcePath>>/bin/fluidity -l -v3 3d_Case.flml &
```

Command 4.1: Command to run a simulation with **Fluidity**.

Case Nbr	**Time Step**	T_{init}	**Floor BC**	u_{init} **(m/s)**	**Inlet velocity (m/s)**	**Section**
1a	1s	293 K	Dirichlet BC $T_f = 298$ K	0	0	4.3.1
1b	1s	293 K	Dirichlet BC $T_f = f(x)$	0	0	4.3.1
1c	1s	293 K	Dirichlet BC $T_f = f(t)$	0	0	4.3.1
1d	1s	293 K	Dirichlet BC $T_f = f(x,t)$	0	0	4.3.1
2a	1s	293 K	Neumann BC $\phi_f = 10$ W/m^2	0	0	4.3.2
2b	1s	293 K	Neumann BC $\phi_s = 10^3$ W/m^2	0	0	4.3.2
2c	1s	293 K	Neumann BC $\phi_f = f(x,t)$	0	0	4.3.2
3	1s	293 K	Robin BC $T_\infty = 25$ °C $h = 5$ W/m^2/K	0	0	4.3.3
4	1s	Outside: 293 K Inside: 298 K	/	0	0	4.4
5a	1s	Outside: 293 K Inside: 298 K	/	1	1	4.5.1
5b	1s	Outside: 293 K Inside: 298 K	/	Log-profile	Log-profile	4.5.1
5c	1s	Outside: 293 K Inside: 298 K	/	1	Turbulent inlet	4.5.2
5d	1s	Outside: 293 K Inside: 298 K	/	Log profile	Turbulent inlet	4.5.2

Table 4.2: Summary of the simulations presented in the following sections of Chapter 4. Subscript f stands for *floor* (ground of the box + the source) and subscript s stands for *source* only. All these simulations are for a fixed mesh.

Killing a simulation

At any time, to kill a simulation, the following can be done in a terminal:

- Run the command `top`. All the processes currently running on the machine are listed, including the **Fluidity** simulations. Note the `ProcID` that you want to kill, then press the key `q` to quit.
- As the user can have several simulations running in different folders, the command `pwdx ProcID` can be use to determine where the `ProcID` is currently running. This command will provide the path where the simulation was launched.
- Once the user is sure that the simulation to kill has the ID `ProcID`, then the command `kill -9 ProcID` can be run in a terminal to kill the simulation.

4.3 Thermal boundary conditions

4.3.1 Dirichlet boundary condition: Constant temperature

Constant floor temperature

In *3dBox_Case1a.flml*, the floor of the box is set to a constant temperature of 298K (Figure 4.1b) using a Dirichlet boundary condition. The initial and the ambient temperatures are set to 293 K (Figure 4.1a). The initial and inlet velocity are set to 0 m/s (Figure 4.1c and Figure 4.1d). This simulation can be run using the command:

```
user@mypc:~$ <<FluiditySourcePath>>/bin/fluidity -l -v3 3dBox_Case1a.flml &
```

A snapshot of the result obtained at 60 s is shown in Figure 4.2. Go to Chapter 10 to learn how to visualise the results using **ParaView**.

Floor temperature as a function of space and/or time: python script

In some cases, the user might want to prescribe a Dirichlet boundary that is space and/or time dependent. This can be done in **Diamond** using a python script. The following examples show how to prescribe these kinds of boundary conditions.

- **Space dependent boundary condition:** In *3dBox_Case1b.flml*, as shown in Figure 4.3a, the python script Code 4.1 is used.

```
1 def val(X, t):
2   # Function code
3   if X[0]<9.0:
4     val = 298.0
5   else:
6     val = 303.0
7   return val # Return value
```

Code 4.1: Space dependent Dirichlet boundary condition for temperature.

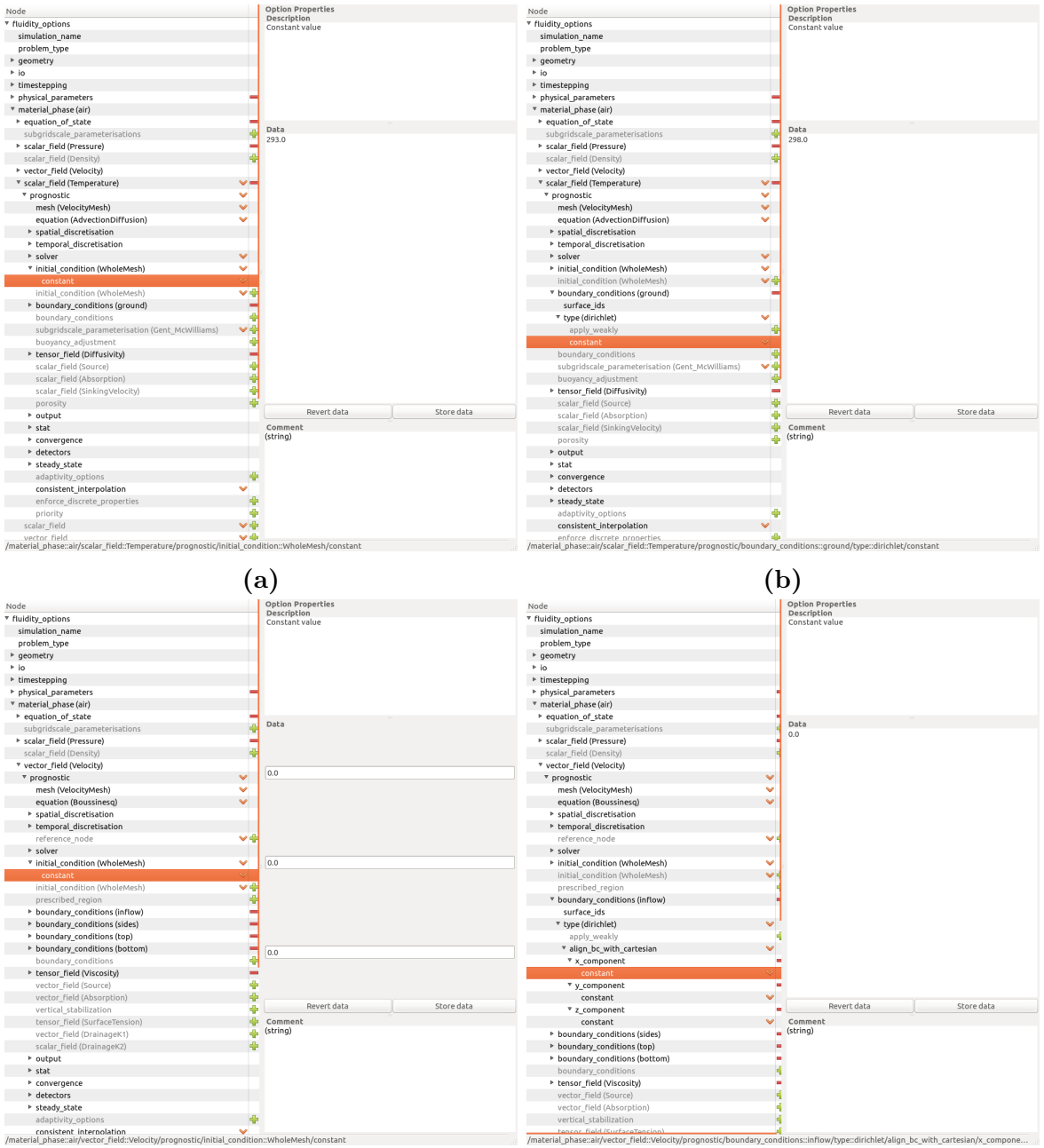


Figure 4.1: Options used in *3dBox_Case1a.flml*. (a) Initial temperature, (b) Thermal boundary condition for the floor, (c) Initial velocity and (d) Inlet boundary condition for the velocity.

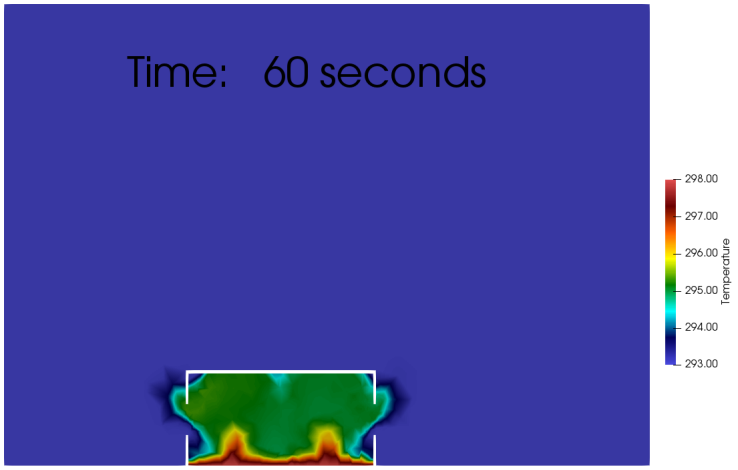


Figure 4.2: Temperature field within the box in example *3dBox_Case1a.fml* with ground temperature set at 298 K.

- **Time dependent boundary condition:** In *3dBox_Case1c.fml*, as shown in Figure 4.3b, the python script Code 4.2 is used.

```
def val(X, t):
  # Function code
  if t<60.0:
    val = 303.0
  else:
    val = 298.0
  return val # Return value
```

Code 4.2: Time dependent Dirichlet boundary condition for temperature.

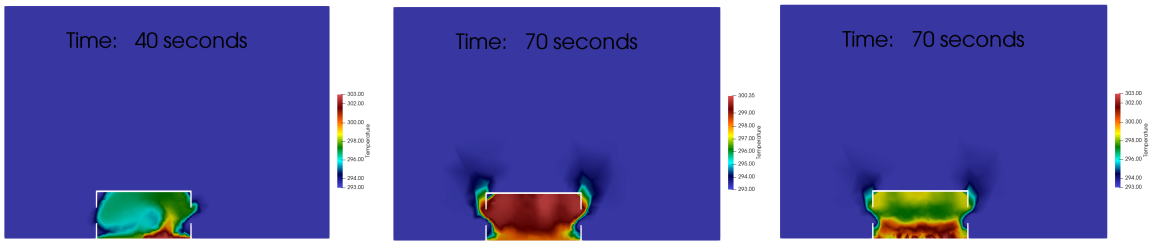
- **Space and time dependent boundary condition:** In *3dBox_Case1d.fml*, as shown in Figure 4.3c, the python script Code 4.3 is used.

```
def val(X, t):
  # Function code
  if t<60.0:
    if X[1] < 9.0:
      val = 298.0
    else:
      val = 303.0
  else:
    if X[1] < 9.0:
      val = 303.0
    else:
      val = 298.0
  return val # Return value
```

Code 4.3: Space and time dependent Dirichlet boundary condition for temperature.

(a) *3dBox_Case1b.flml* **(b)** *3dBox_Case1c.flml* **(c)** *3dBox_Case1d.flml*

Figure 4.3: Space and/or time dependent Dirichlet boundary condition for the temperature. (a) Space dependent boundary condition, (b) time dependent boundary condition and (c) space and time dependent boundary condition.



(a) *3dBox_Case1b.flml* **(b)** *3dBox_Case1c.flml* **(c)** *3dBox_Case1d.flml*

Figure 4.4: Temperature field within the box when using (a) a space dependent, (b) a time dependent or (c) a space and time dependent Dirichlet boundary condition for the ground of the box.

These examples can be run using the commands:

```
user@mypc:~$ <<FluiditySourcePath>>/bin/fluidity -l -v3 3dBox_Case1b.flml &
user@mypc:~$ <<FluiditySourcePath>>/bin/fluidity -l -v3 3dBox_Case1c.flml &
user@mypc:~$ <<FluiditySourcePath>>/bin/fluidity -l -v3 3dBox_Case1d.flml &
```

Snapshots of the results obtained from these three simulations are shown in Figure 4.4. Go to Chapter 10 to learn how to visualise the results using **ParaView**.

4.3.2 Neumann boundary condition: Heat flux

Heat flux from the ground

Case *3dBox_Case2a.flml* is similar to the previous one, except a heat flux is now applied at the bottom, effectively changing the Dirichlet boundary condition to a Neumann one as shown in Figure 4.5a. The ambient and the initial temperatures are set to 293 K and u is set equal to 0 m/s. In **Fluidity**, the value of the heat flux, specified in **Diamond**, is given by equation 4.1:

$$\phi_{fluidity} = \frac{\phi_{floor}}{\rho_0 c_p} \tag{4.1}$$

where $\phi_{fluidity}$ (Km/s) is the value that needs to be set into **Diamond**, ϕ_{floor} (W/m^2) is the actual heat flux that the user wants to prescribe, ρ_0 (kg/m^3) is the reference density and c_p (J/kg/K) is the heat capacity of the fluid.
In example *3dBox_Case2a.flml*, the heat flux ϕ_{floor} is equal to 10 W/m^2, hence the value $\frac{\phi_{floor}}{\rho_0 c_p} = \frac{10}{1{,}225 \times 1000} = 0.00816$ is set up in **Diamond** as shown in Figure 4.5a. The 10 W/m^2 heat flux is applied to the box's floor having a surface equal to $6 \times 6 = 36$ m^2: the flux is then equal to 360 W.
This example can be run using the command:

```
user@mypc:~$ <<FluiditySourcePath>>/bin/fluidity -l -v3 3dBox_Case2a.flml &
```

A snapshot of the result obtained at 994 s is shown in Figure 4.6a. Go to Chapter 10 to learn how to visualise the results using **ParaView**.

Heat flux from the source only

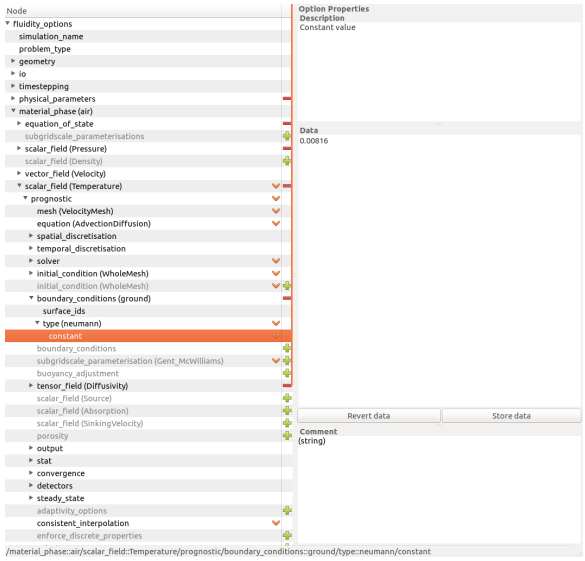
Using the physical IDs previously defined (see Section 2.3.5), the heat flux boundary condition can be changed to include only a section of the floor, defined as the source. Based on Section 2.3.5, the ID of the floor of the box (without the source) is 7 and the ID of the source only is 8. In the previous example *3dBox_Case2a.flml*, the surface IDs, where the Neumann boundary condition were applied, are 7 (the floor) and 8 (the source) (see Figure 4.5b): in that case, the heat flux is applied everywhere on the floor. In example *3dBox_Case2b.flml*, the surface ID where the Neumann boundary condition is applied is 8 only (the source) (see Figure 4.5c). Therefore the heat flux is applied at the source only.
In case *3dBox_Case2b.flml*, the initial and the ambient temperatures are set to 293 K and u is set equal to 0 m/s. The heat flux applied at the source ϕ_{source} is equal to 1000 W/m^2, hence $\phi_{fluidity}$ set up in **Diamond** is equal to 0.8163 according to equation 4.1. The surface of the heat source is 0.2×0.2 m^2: the flux applied at the source is then equal to 40 W.
This example can be run using the command:

```
user@mypc:~$ <<FluiditySourcePath>>/bin/fluidity -l -v3 3dBox_Case2b.flml &
```

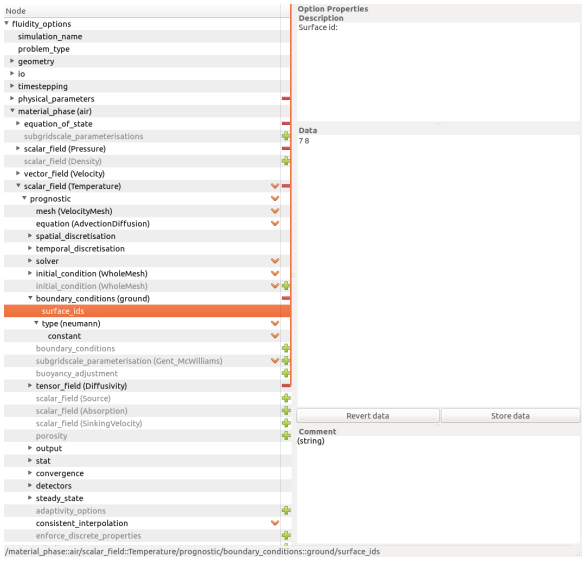
A snapshot of the result obtained at 712 s is shown in Figure 4.6b. Go to Chapter 10 to learn how to visualise the results using **ParaView**.

Heat flux as a function of space or time: python script

In some cases, the user might want to prescribe a Neumann boundary that is space and/or time dependent. This can be done in **Diamond** using a python script as shown in Figure 4.5d.



(a) *3dBox_Case2a.flml*

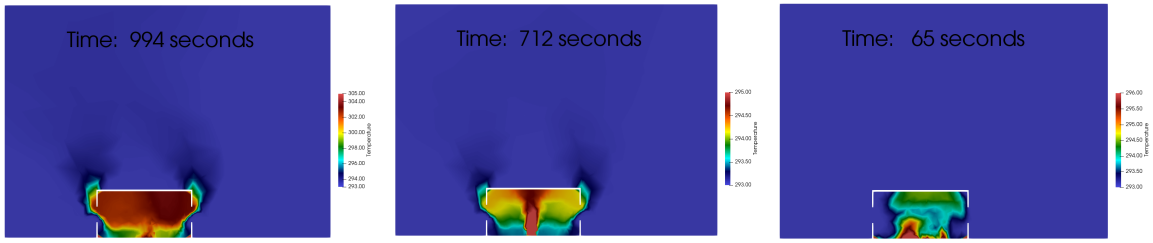


(b) *3dBox_Case2a.flml*

(c) *3dBox_Case2b.flml*

(d) *3dBox_Case2c.flml*

Figure 4.5: Neumann boundary condition (a) Value of $\phi_{fluidity}$, (b) List of IDs to prescribe a heat flux on the overall floor box, (c) The heat flux is applied at the source only and (d) The heat flux is space and time dependent and is prescribed using a python script.



(a) *3dBox_Case2a.flml* **(b)** *3dBox_Case2b.flml* **(c)** *3dBox_Case2c.flml*

Figure 4.6: Temperature field within the box when using (a) heat flux on the ground, (b) a heat flux in the middle of the box only and (c) a space and time dependent heat flux on the ground.

In example *3dBox_Case2c.flml*, the python script Code 4.4 is used. Note that in this example, the choice was made to calculate the heat flux $\phi_{fluidity}$ directly in the python script.

```
def val(X, t):
  # Function code
  phi_1 = 10.0    # W/m2
  phi_2 = 20.0    # W/m2
  Cp    = 1000.0
  rho   = 1.225

  if t<60.0:
    if X[0] < 9.0:
      val = phi_1/(rho*Cp)
    else:
      val = phi_2/(rho*Cp)
  else:
    if X[0] < 9.0:
      val = phi_2/(rho*Cp)
    else:
      val = phi_1/(rho*Cp)

  return val # Return value
```

Code 4.4: Space and time dependent Neumann boundary condition for temperature field in example *3dBox_Case2c.flml*.

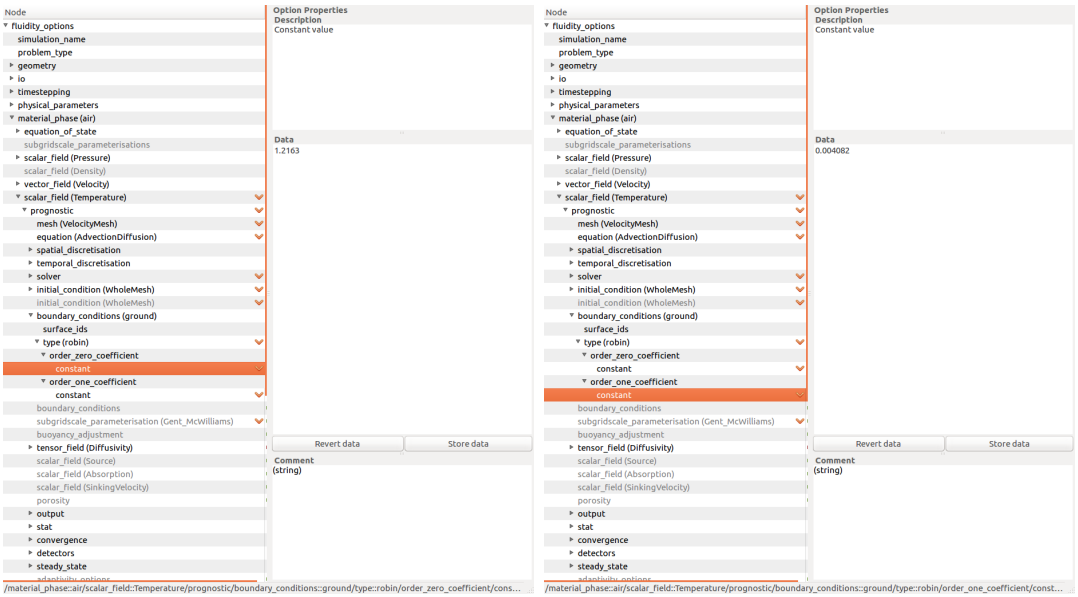
This example can be run using the command:

```
user@mypc:~$ <<FluiditySourcePath>>/bin/fluidity -l -v3 3dBox_Case2c.flml &
```

A snapshot of the result obtained at 65 s is shown in Figure 4.6c. Go to Chapter 10 to learn how to visualise the results using **ParaView**.

4.3.3 Robin boundary condition

In example *3dBox_Case3.flml*, a Robin boundary condition (equation 4.2) is applied between the box's floor and the air as shown in Figure 4.7. Generally this boundary



(a) C_0 coefficient **(b)** C_1 coefficient

Figure 4.7: Robin boundary condition used in example *3dBox_Case3.fml*.

condition is used to model the heat exchange by convection between a fluid and a solid surface.

$$-(\overline{\overline{\kappa}}\nabla T)\cdot\mathbf{n} = \frac{h}{\rho_0 c_p}(T - T_\infty) \tag{4.2}$$

where $\overline{\overline{\kappa}}$ is the thermal diffusivity (m^2/s) of the fluid, h is the convective heat transfer coefficient ($W/m^2/K$) and T_∞ is the ground temperature (K).
In **Fluidity**, the Robin boundary condition is specified using the equation 4.3.

$$C_1 T + \mathbf{n}\cdot(\overline{\overline{\kappa}}\nabla T) = C_0 \tag{4.3}$$

Hence, the coefficients C_0 and C_1 are given by equation 4.4 and equation 4.5, respectively.

$$C_0 = \frac{h}{\rho_0 c_p} T_\infty \tag{4.4}$$

$$C_1 = \frac{h}{\rho_0 c_p} \tag{4.5}$$

where C_0 is in Km/s and C_1 is in m/s. Note that if C_1 is equal to 0, then the Robin boundary condition leads to a Neumann boundary condition.
In example *3dBox_Case3.fml*, the heat transfer coefficient between the ground and the air is assumed to be equal to 5 $W/m^2/K$ and the ground temperature T_∞ is taken equal to 298 K. Hence, the value of C_0 and C_1 are equal to 1.2163 Km/s and 0.004082 m/s,

Figure 4.8: Temperature field within the box in example *3dBox_Case3.flml* using a Robin condition.

respectively as shown in Figure 4.7. The initial temperature is set to 293 K and u is set equal to 0 m/s.
This example can be run using the command:

```
user@mypc:~$ <<FluiditySourcePath>>/bin/fluidity -l -v3 3dBox_Case3.flml &
```

A snapshot of the result obtained at 150 s is shown in Figure 4.8. Go to Chapter 10 to learn how to visualise the results using **ParaView**.

4.4 Initial conditions for temperature

The initial temperature can be set using a python script to prescribe different initial values in different regions. In example *3dBox_Case4.flml*, the interior of the box is set to 298 K while the outside remains at ambient temperature, i.e. 293 K. The python script in Code 4.5 is used as shown in Figure 4.9. No particular thermal boundary condition is prescribed for the floor of the box and u is set to 0 m/s.

```
def val(X, t):
  # Function code
  xmin = 6.0
  xmax = 12.0
  ymin = 6.0
  ymax = 12.0
  zmax = 3.0

  val = 293.0  # outside of the box

  if X[2] <= zmax:
    if (X[1] >= ymin) and (X[1] <= ymax):
      if (X[0] >= xmin) and (X[0] <= xmax):
        val = 298.0  # inside of the box

  return val # Return value
```

Code 4.5: Python script to prescribe different initial temperatures inside and outside the box.

This example can be run using the command:

```
user@mypc:~$ <<FluiditySourcePath>>/bin/fluidity -l -v3 3dBox_Case4.flml &
```

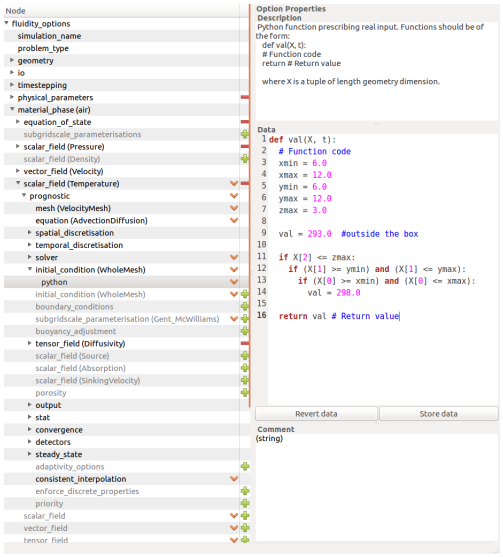


Figure 4.9: Example *3dBox_Case4.flml*: python script to prescribe different initial temperatures.

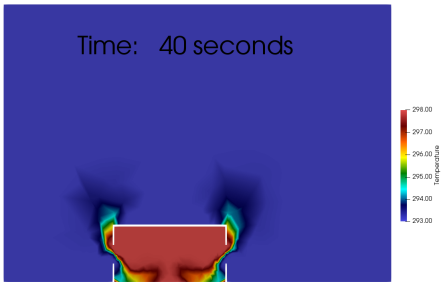


Figure 4.10: Temperature field in example *3dBox_Case4.flml* with an initial temperature in the box.

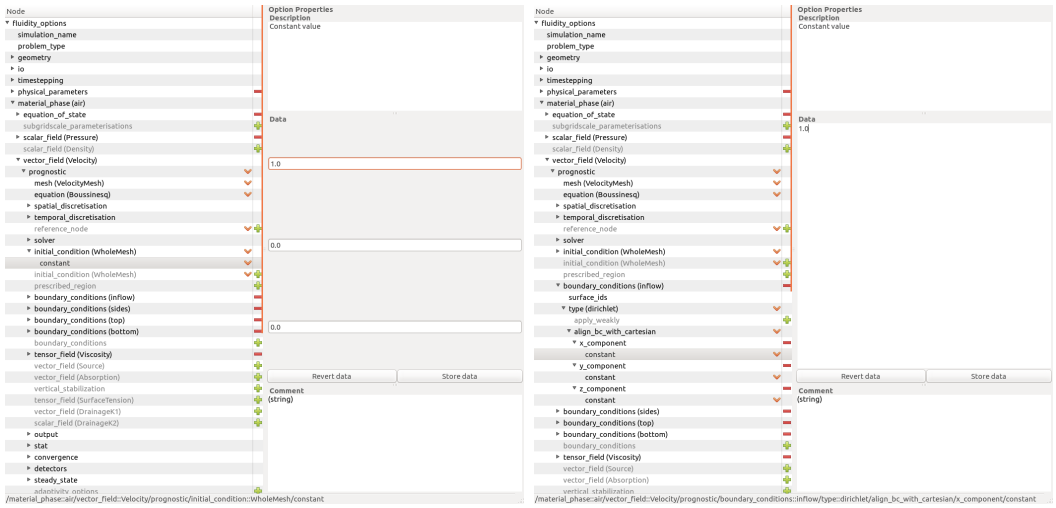
A snapshot of the result obtained at 40 s is shown in Figure 4.10. Go to Chapter 10 to learn how to visualise the results using **ParaView**.

4.5 Velocity boundary conditions

4.5.1 Dirichlet boundary condition: Constant and uniform inlet wind

Uniform inlet velocity

In addition to setting boundary or initial values of temperature, the boundary condition for velocity can also be specified. In example *3dBox_Case5a.flml*, the initial and inlet velocities (u, v, w) are set to $(1, 0, 0)$ m/s (Figure 4.11) and the interior of the box is set to 298 K while the outside remains at ambient temperature 293 K (Code 4.5). The time step is kept equal to 1 s in this example. However, the results of the first 10 time steps are not totally accurate. To avoid this, a value of 0.01 s is recommended.



(a) Initial velocity **(b)** Inlet velocity

Figure 4.11: (a) Initial and (b) inlet velocity prescribed in example *3dBox_Case5a.flml*.

This example can be run using the command:

```
user@mypc:~$ <<FluiditySourcePath>>/bin/fluidity -l -v3 3dBox_Case5a.flml &
```

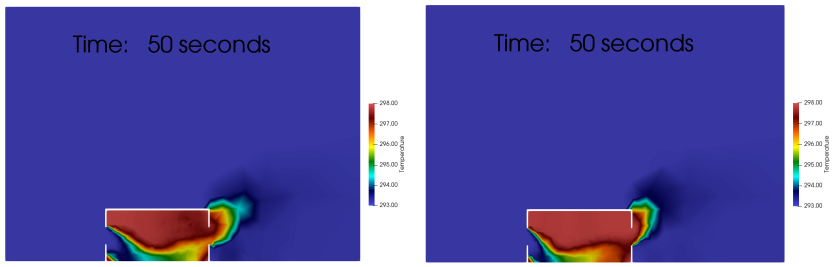
A snapshot of the result obtained at 50 s is shown in Figure 4.12a. Go to Chapter 10 to learn how to visualise the results using **ParaView**.

Prescribing a velocity profile: python script

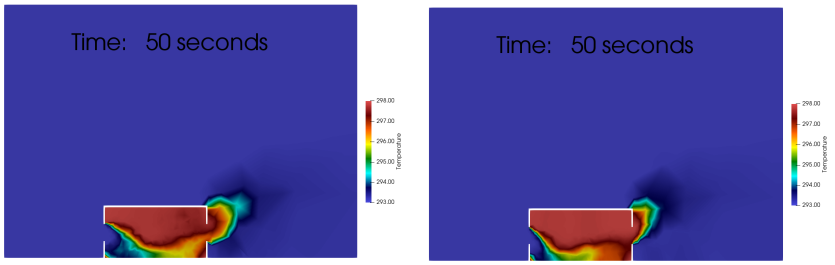
In example *3dBox_Case5b.flml*, the u-component of the initial and inlet velocity are set using a log-profile and the python scripts in Code 4.6 and Code 4.7 are used (Figure 4.13).The interior of the box is set to 298 K while the outside remains at ambient temperature 293 K (Code 4.5).

```
def val(X, t):
  # Function code
  import numpy as np

  ustar = 0.06
  kappa = 0.41
  z0    = 0.02

  val = 0.0
  if X[2] > z0:
    val = (ustar/kappa) * np.log(X[2]/z0)

  return [val,0.0,0.0] #Return value
```

Code 4.6: Python script to prescribe an initial log-profile for the velocity.



(a) *3dBox_Case5a.flml* **(b)** *3dBox_Case5b.flml*



(c) *3dBox_Case5c.flml* **(d)** *3dBox_Case5d.flml*

Figure 4.12: Temperature field at 50 s when using (a) a uniform and constant inlet velocity, (b) a log-profile inlet velocity, (c) a turbulent inlet velocity with uniform profiles and (d) a turbulent inlet velocity with a log-profile mean velocity.

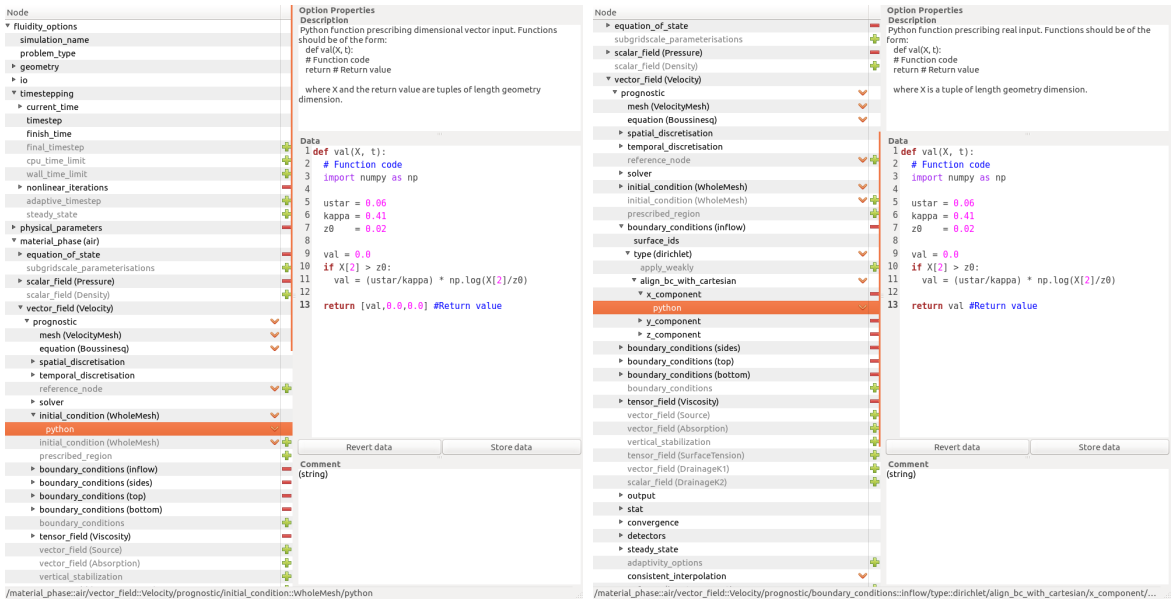
```
def val(X, t):
  # Function code
  import numpy as np

  ustar = 0.06
  kappa = 0.41
  z0    = 0.02

  val = 0.0
  if X[2] > z0:
    val = (ustar/kappa) * np.log(X[2]/z0)

  return val #Return value
```

Code 4.7: Python script to prescribe an inlet log-profile for the velocity.

This example can be run using the command:

```
user@mypc:~$ <<FluiditySourcePath>>/bin/fluidity -l -v3 3dBox_Case5b.flml &
```

A snapshot of the result obtained at 50 s is shown in Figure 4.12b. Go to Chapter 10 to learn how to visualise the results using **ParaView**.



(a) Initial velocity **(b)** Inlet velocity

Figure 4.13: (a) Initial and (b) inlet log-profile velocity in example *3dBox_Case5b.flml* prescribed using python scripts.

4.5.2 Synthetic eddy method: Turbulent inlet velocity

Constant values

Finally, the last interesting velocity boundary condition is called the `Synthetic eddy method` and mimics a turbulent inlet velocity. For more details, the user can refer to [5]. This boundary condition is used to reproduced the behaviour of the atmospheric boundary layer and the 4 following variables need to be defined by the user for each velocity component:

- **Number of eddies:** this number has to be large enough to ensure the Gaussian behaviour of the fluctuating component. Usually this value is taken to be 4000.
- **Turbulence lengthscale:** the turbulence lengthscale is in meters and is defined by equation 4.6.
- **Mean profile:** the mean velocity profiles of each velocity component in m/s.
- **Reynolds stresses profile:** the Reynolds stresses profile of the components $\overline{u'u'}$, $\overline{v'v'}$ and $\overline{w'w'}$ (in m^2/s^2) are prescribed assuming that the remaining stresses are negligible as in equation 4.7.

$$\mathbf{L} = \begin{pmatrix} L_u & 0 & 0 \\ 0 & L_v & 0 \\ 0 & 0 & L_w \end{pmatrix} \tag{4.6}$$

$$\mathbf{Re} = \begin{pmatrix} \overline{u'u'} & 0 & 0 \\ 0 & \overline{v'v'} & 0 \\ 0 & 0 & \overline{w'w'} \end{pmatrix} \tag{4.7}$$

In example *3dBox_Case5c.flml*, the interior of the box is set to 298 K while the outside remains at ambient temperature 293 K (Code 4.5). The initial velocity and the inlet velocity (u, v, w) are set to $(1, 0, 0)$ m/s. The number of eddies is taken as 4000 and the turbulence lengthscale is equal to 5 m. The $\overline{u'u'}$-component of the Reynolds stresses is taken to be to 0.8, while $\overline{v'v'}$ and $\overline{w'w'}$ are equal to 0.3. For brevity, the options set up for the u-component only are shown in Figure 4.14.
This example can be run using the command:

```
user@mypc:~$ <<FluiditySourcePath>>/bin/fluidity -l -v3 3dBox_Case5c.flml &
```

A snapshot of the result obtained at 50 s is shown in Figure 4.12c. Go to Chapter 10 to learn how to visualise the results using **ParaView**.

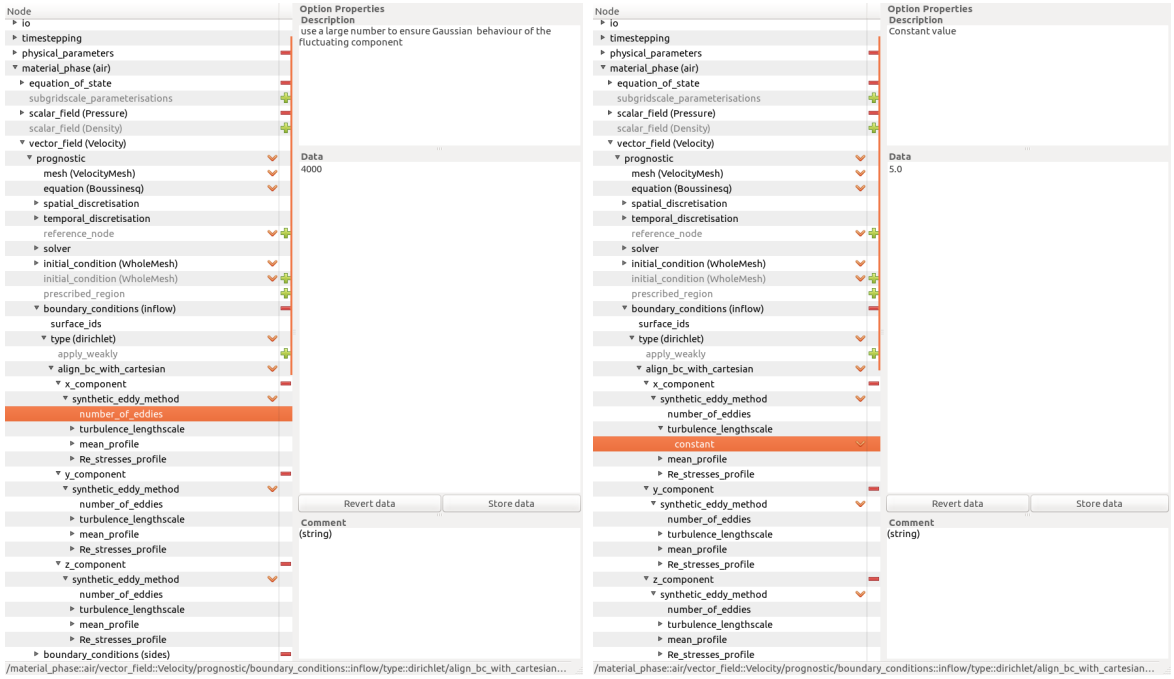
Using python scripts

The initial velocity, the turbulence lengthscale, the mean velocity and the Reynolds stresses profiles can also be prescribed using python scripts if the user wants to use real profiles found in literature. In example *3dBox_Case5d.flml*, the interior of the box is set to 298 K while the outside remains at ambient temperature 293 K (Code 4.5). The initial velocity is prescribed using Code 4.6. The turbulent inlet options are defined as follows (see also Figure 4.15):

- **Turbulence lengthscale:** Assuming a linear relationship between the lengthscale and the height, the python script in Code 4.8 is used for the three velocity components as shown in Figure 4.15a.

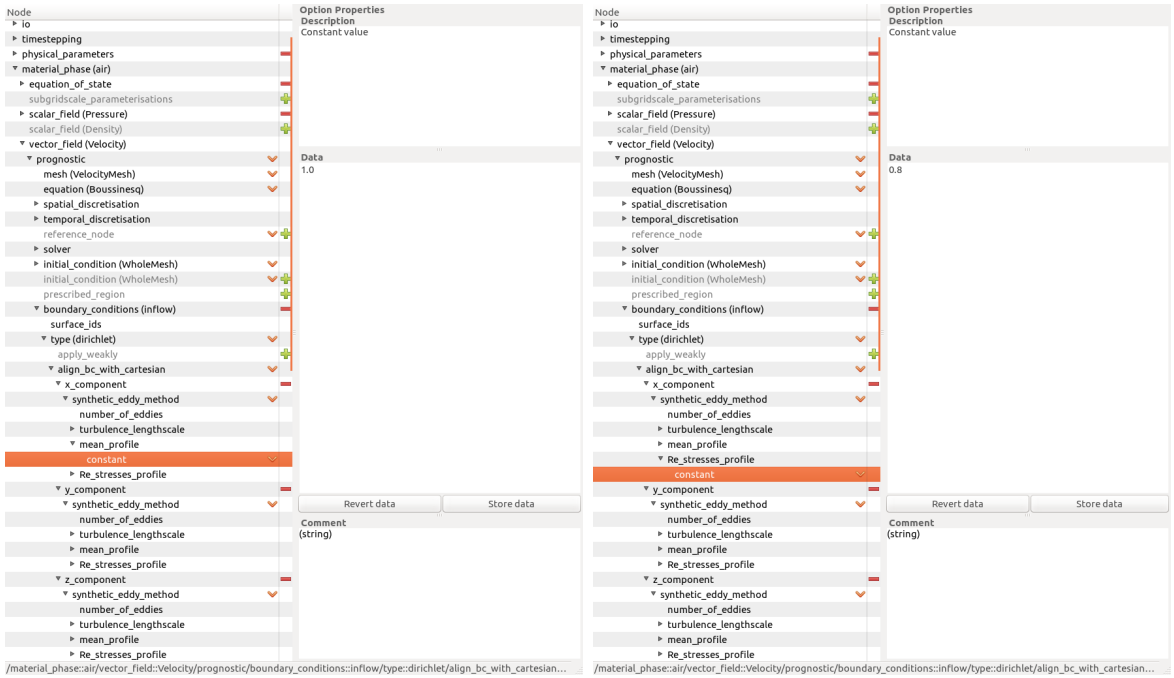
```
def val(X, t):
  # Function code
  import numpy as np

  zmin = 1.0
  zmax = 15.0
  Lmin = 1.0
  Lmax = 5.0

  a = (Lmax-Lmin)/(zmax-zmin)
  b = Lmin - a * zmin

  val = a * X[2] + b

  return val #Return value
```

Code 4.8: Python script to prescribe a turbulence lengthscale profile.



(a) Number of eddies

(b) Lengthscale



(c) Mean profile

(d) Reynolds stresses

Figure 4.14: Options used for the turbulent inlet velocity in example *3dBox_Case5c.flml*.

- **Mean velocity:** Assuming a log-profile, the python script in Code 4.7 is prescribed to the u-component of the velocity, while 0 m/s is prescribed to the v and w-components.
- **Reynolds Stresses:** The $\overline{u'u'}$-component of the Reynolds stresses are prescribed using the python script in Code 4.9 (Figure 4.15b). The $\overline{v'v'}$ and $\overline{w'w'}$ components of the Reynolds stresses is prescribed using the python script in Code 4.10 (Figure 4.15c). A linear relationship between the Reynolds stresses and the height is assumed.

```
def val(X, t):
  # Function code
  import numpy as np

  zmin = 1.0
  zmax = 15.0
  Remin = 0.8
  Remax = 0.1

  a = (Remax-Remin)/(zmax-zmin)
  b = Remin - a * zmin

  val = a * X[2] + b

  return val #Return value
```

Code 4.9: Python script to prescribe the Reynolds stresses $\overline{u'u'}$.

```
def val(X, t):
  # Function code
  import numpy as np

  zmin = 1.0
  zmax = 15.0
  Remin = 0.3
  Remax = 0.1

  a = (Remax-Remin)/(zmax-zmin)
  b = Remin - a * zmin

  val = a * X[2] + b

  return val #Return value
```

Code 4.10: Python script to prescribe the Reynolds stresses $\overline{v'v'}$ and $\overline{w'w'}$.

This example can be run using the command:

```
user@mypc:~$ <<FluiditySourcePath>>/bin/fluidity -l -v3 3dBox_Case5d.flml &
```

A snapshot of the result obtained at 50 s is shown in Figure 4.12d. Go to Chapter 10 to learn how to visualise the results using **ParaView**.

(a) Lengthscale **(b)** Reynolds stresses $\overline{u'u'}$ **(c)** Reynolds stresses $\overline{v'v'}$

Figure 4.15: Python scripts used to prescribe a turbulent inlet velocity in *3dBox_Case5d.flml*.

Case Nbr	BC type	From	Aligned with	BCs aligned with surface	Work?
4	Dirichlet: No-slip	Strong	Cartesian	N/A	YES
13a	Dirichlet: No-slip	Strong	Surface	1	YES
13b	Dirichlet: No-slip	Strong	Surface	2	NO
13c	Dirichlet: No-slip	Weak	Cartesian	N/A	YES
13d	Dirichlet: No-slip	Weak	Surface	1	YES
13e	Dirichlet: No-slip	Weak	Surface	2	YES
13f	Dirichlet: Slip	Strong	Surface	1	YES
13g	Dirichlet: Slip	Weak	Cartesian	N/A	YES
13h	Dirichlet: Slip	Weak	Surface	1	NO
13i	No normal flow: Slip	Weak	N/A	N/A	YES

Table 4.3: Summary of the simulations using different Dirichlet velocity boundary condition for solid surfaces.

4.5.3 Dirichlet boundary condition on solids

Note: This section is particularly important and it is recommended to read it carefully. This section is also summarised in Section 8.4 due to its importance. The option `align_bc_with_surface` in the Dirichlet type boundary condition is not well-implemented in **Fluidity** and not always work properly. This section describes in details in which case it works or not. In any case, this option should be avoided if possible. The simulations presented in that section are based on *3dBox_Case4.flml* and are summarised in Table 4.3.

Boundary condition `align_bc_with_cartesian` or `align_bc_with_surface`?

It exists two options available to apply a Dirichlet boundary condition in **Fluidity**:

- `align_bc_with_cartesian`: the three components of the velocity are assigned.

- `align_bc_with_surface`: the normal and the two tangential components of the velocity are assigned.

The second option can be really useful when the surfaces of the geometry are not aligned with Cartesian coordinates system for very complex geometry. However, this functionality does not always work properly in **Fluidity** as detailed in the following:

- Example *3dBox_Case4.flml* uses the option `align_bc_with_cartesian` to apply a no-slip boundary condition (the three components x, y and z of the velocity are equal to zero) on the solid surfaces.

- Example *3dBox_Case13a.flml* is a replicate of example *3dBox_Case4.flml*, excepted that the velocity boundary condition on the solid surfaces is now applied using the `align_bc_with_surface` option, i.e. the normal and the two tangential components of the velocity are now equal to zero.

  ⇒ Examples *3dBox_Case4.flml* and *3dBox_Case13a.flml* run correctly and give the same results - that was actually expected...

- In *3dBox_Case13b.flml*, the no-slip boundary condition `align_bc_with_surface` is now dissociated into two no-slip boundary conditions `align_bc_with_surface`: one for the ground of the domain and the walls; and one for the ground of the box only.

  ⇒ If the user runs example *3dBox_Case13b.flml*, the simulation will crash and the error in Command 4.13 will be raised.

```
user@mypc:~$ Inside create_rotation_matrix
*** ERROR ***
Error message:  Two rotated boundary condition specifications for the same
node.
```

Command 4.13: Error occurring when two strongly applied Dirichlet boundary conditions using `align_bc_with_surface` are defined.

Unfortunately, if several strong boundary conditions (see next section for discussion about the strong form) `align_bc_with_surface` are really wanted, there is not tricks to avoid this error in **Fluidity**. Only one `align_bc_with_surface` Dirichlet boundary condition strongly applied is allowed by **Fluidity**, which can be problematic when dealing with complex geometries.

Boundary condition applied strongly or weakly?

The only way to avoid the error previously described (when more than one `align_bc_with_surface` no-slip Dirichlet boundary condition is used) is to apply the boundary conditions weakly.

It is to be noted that when boundary conditions are applying weakly, the discrete solution will not satisfy the boundary condition exactly. Instead the solution will converge to the correct boundary condition along with the solution in the interior as the mesh is refined. An alternative way of implementing boundary conditions is to strongly imposed boundary conditions. Although this guarantees that the Dirichlet boundary condition will be satisfied exactly, it does not at all mean that the discrete solution converges to the exact continuous solution more quickly than it would with weakly imposed boundary conditions. Strongly imposed boundary conditions may sometimes be necessary if the boundary condition needs to be imposed strictly for physical reasons. Unlike the strong form of the Dirichlet conditions, weak Dirichlet conditions do not force the solution on the boundary to be point-wise equal to the boundary condition.
If boundary conditions are applied weakly, then the following options need to be turned on in **Diamond**:

- Under the Pressure field: `spatial_discretisation/continuous_galerkin/integrate_continuity_by_parts`
- Under the Velocity field: `spatial_discretisation/continuous_galerkin/advection_terms/integrate_advection_by_parts`

Examples *3dBox_Case13c.flml*, *3dBox_Case13d.flml* and *3dBox_Case13e.flml* use a no-slip boundary condition applied weakly. The time-step was reduce to 0.01 second to avoid divergence of the simulation and the options `integrate_*_by_parts` are turned on.

- Example *3dBox_Case13c.flml* is equivalent to *3dBox_Case4.flml*, excepted that the velocity boundary condition on solid surfaces is now applied weakly instead of strongly, still using `align_bc_with_cartesian`.

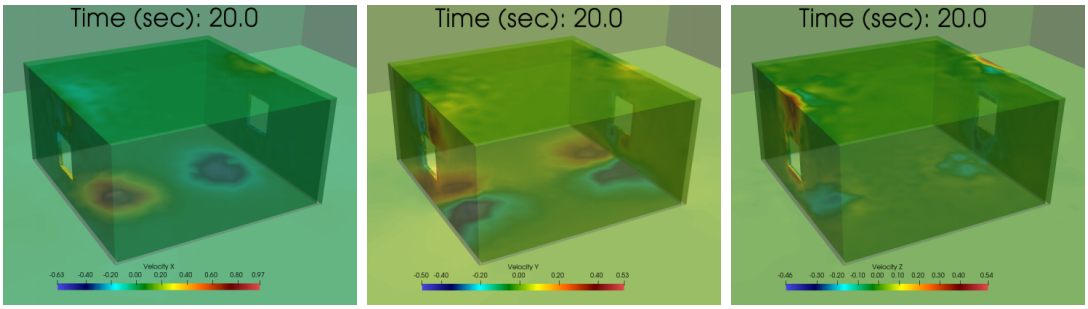
  ⇒ As shown in Figure 4.16, the velocity is not equal to zero on solid walls for the reason explained above, i.e. because the boundary condition is applied weakly.

- Example *3dBox_Case13d.flml* is the same than *3dBox_Case13c.flml*, excepted that the velocity boundary condition on solid surfaces, still applied weakly, is now `align_bc_with_surface`.

  ⇒ The results obtained from example *3dBox_Case13d.flml* are the same than the ones from *3dBox_Case13c.flml*.

- Finally, example *3dBox_Case13e.flml* is the same than *3dBox_Case13b.flml* (which was previously crashing because of two strong `align_bc_with_surface` boundary type), excepted that the two velocity boundary conditions are now applied weakly.

  ⇒ Contrary to *3dBox_Case13b.flml*, example *3dBox_Case13e.flml* runs and does not crashed. As expected, results are the same than in *3dBox_Case13c.flml* and *3dBox_Case13d.flml*.



(a) $x-$velocity **(b)** $y-$velocity **(c)** $z-$velocity

Figure 4.16: (a) $x-$, (b) $y-$ and (c) $z-$ components of the velocity in the box. A weak no-slip boundary condition is applied on solid surfaces. Example *3dBox_Case13c.flml*.

No-slip or slip boundary condition on solid?

This section will discuss the use of slip or no-slip boundary condition on solid surfaces. One can argue that a no-slip is more appropriate, while other will prone the use of a slip boundary condition. A no-slip boundary condition is defined by the three components of the velocity being equal to zero, while a slip boundary condition corresponds to the normal component of the velocity only being equal to zero.
The following examples use a slip boundary condition on solid surfaces and for comparison results are shown in Figure 4.17, Figure 4.18 and Figure 4.19.

- Example *3dBox_Case13f.flml* prescribes a slip boundary condition on solid surfaces applied strongly using a Dirichlet type `align_bc_with_surface`.

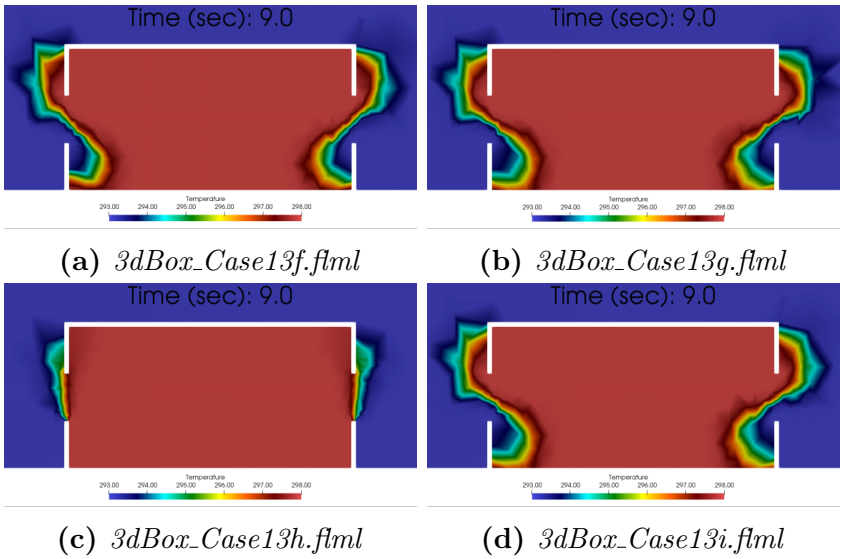
  ⇒ This case works perfectly as long as only one `align_bc_with_surface` is used. Results are shown in Figure 4.17a, Figure 4.18a and Figure 4.19a.

- Examples *3dBox_Case13g.flml* and *3dBox_Case13h.flml* prescribe a slip boundary condition applied weakly using the option `align_bc_with_cartesian` and `align_bc_with_surface`, respectively.

  ⇒ While *3dBox_Case13g.flml* runs like a charm (Figure 4.17b, Figure 4.18b and Figure 4.19b), example *3dBox_Case13h.flml* gives weird results (Figure 4.17c, Figure 4.18c and Figure 4.19c) and finally crashes. Indeed, the option `align_bc_with_surface`, when a slip boundary condition is weakly applied, does not work in **Fluidity** and the user should instead use the `no_normal_flow` option.

- The option `no_normal_flow` is used in example *3dBox_Case13i.flml*: this option apply automatically a weak slip boundary condition on any surfaces specified.

  ⇒ This case runs and results are shown in Figure 4.17d, Figure 4.18d and Figure 4.19d.



(a) *3dBox_Case13f.flml* **(b)** *3dBox_Case13g.flml*

(c) *3dBox_Case13h.flml* **(d)** *3dBox_Case13i.flml*

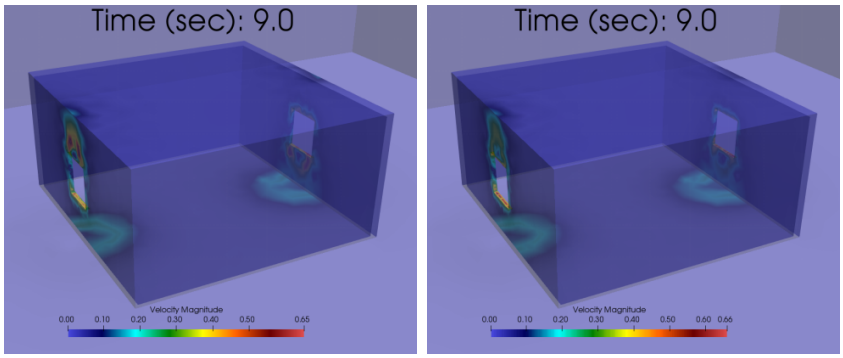
Figure 4.17: Temperature field in the box when a slip boundary condition is applied on solid walls. The boundary condition is applied (a) strongly `align_bc_with_surface`; (b) weakly `align_bc_with_cartesian`, (c) weakly `align_bc_with_surface` and (d) weakly using `no_normal_flow`. Note that example (c) *3dBox_Case13h.flml* does not work properly.

In summary

In summary:

- The option `align_bc_with_cartesian` should always be preferred if possible.
- Only one no-slip Dirichlet `align_bc_with_surface` applied strongly is allowed, while several can be used when applied weakly.
- For a slip boundary condition weakly applied, `align_bc_with_cartesian` type for simple geometry or `no_normal_flow` type for any geometry should be used. The Dirichlet `align_bc_with_surface` type does not work.

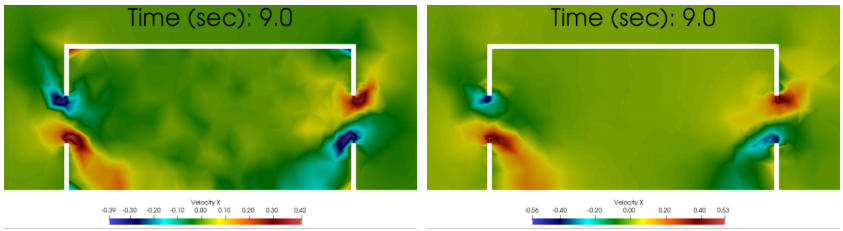
Finally, when defining the velocity boundary conditions at a wall, it is recommended to use a slip boundary condition (normal component only equal to 0) instead of a no-slip condition (all components are set to 0 at the wall) if the boundary layer is not going to be fully resolved with the chosen mesh. Using a no-slip condition can notably be problematic near a heat source and will generate wide variations in the expected temperature. The temperature fields obtained from examples *3dBox_Case4.flml*, *3dBox_Case13c.flml*, *3dBox_Case13f.flml* and *3dBox_Case13g.flml* are shown in Figure 4.20. One can noticed that the temperature stays hot in the lower corners of the box when a no-slip strongly applied boundary condition is used, while this hot spots disappear when a slip boundary condition is used or when the boundary condition is applied weakly (which is basically more or less the same...).



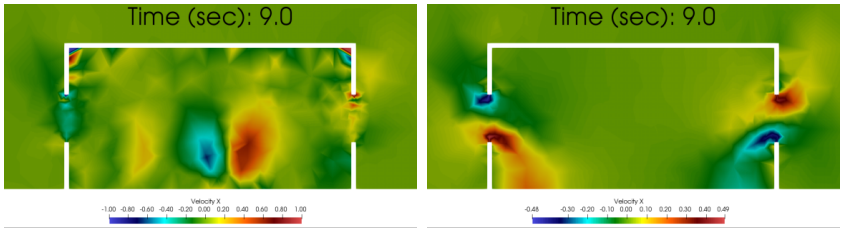
(a) *3dBox_Case13f.flml* **(b)** *3dBox_Case13g.flml*

(c) *3dBox_Case13h.flml* **(d)** *3dBox_Case13i.flml*

Figure 4.18: Velocity magnitude when a slip boundary condition is applied on solid surfaces of the domain. The boundary condition is applied (a) strongly `align_bc_with_surface`; (b) weakly `align_bc_with_cartesian`; (c) weakly `align_bc_with_surface` and (d) weakly using `no_normal_flow`. Note that example (c) *3dBox_Case13h.flml* does not work properly.

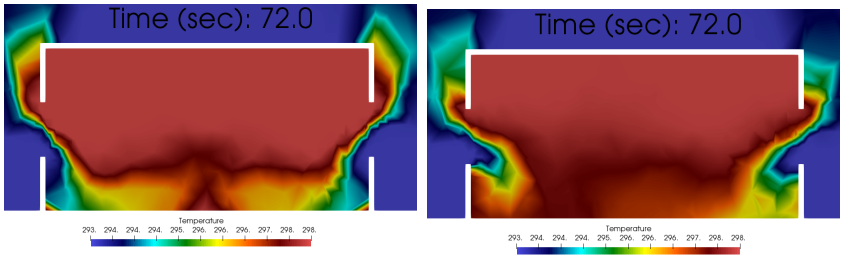


(a) *3dBox_Case13f.fml* **(b)** *3dBox_Case13g.fml*

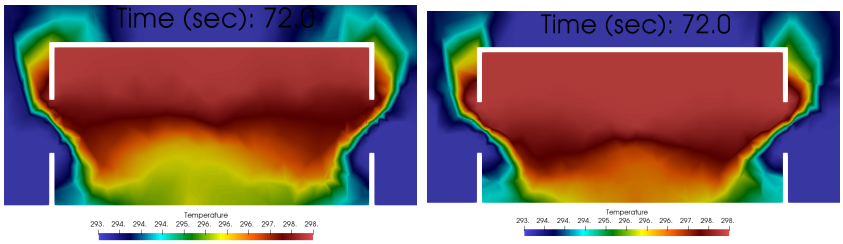


(c) *3dBox_Case13h.fml* **(d)** *3dBox_Case13i.fml*

Figure 4.19: x-component of the velocity when a slip boundary condition is applied on solid surfaces. The boundary condition is applied (a) strongly `align_bc_with_surface`; (b) weakly `align_bc_with_cartesian`; (c) weakly `align_bc_with_surface` and (d) weakly using `no_normal_flow`. Note that example (c) *3dBox_Case13h.fml* does not work properly.

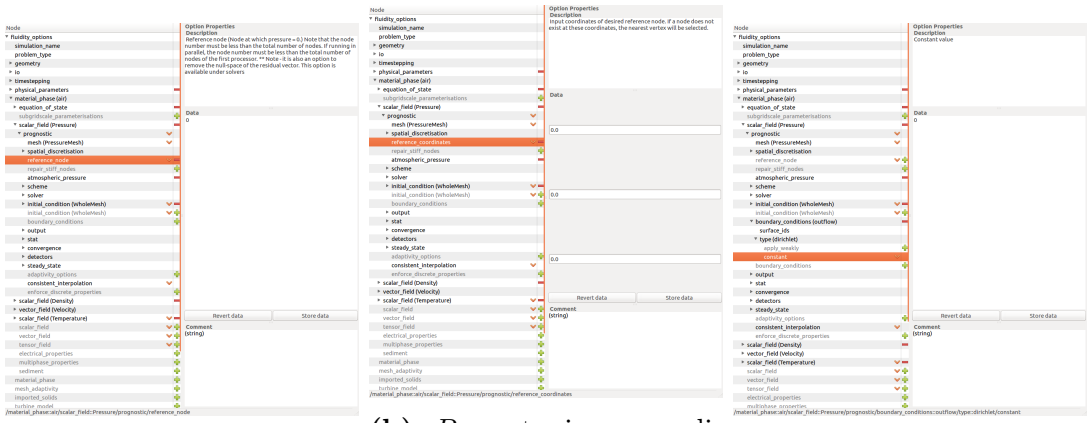


(a) *3dBox_Case4.fml* **(b)** *3dBox_Case13c.fml*



(c) *3dBox_Case13f.fml* **(d)** *3dBox_Case13g.fml*

Figure 4.20: Temperature field in the box with a (a) no-slip strongly applied; (b) no-slip weakly applied; (c) slip strongly applied and (d) slip weakly applied boundary condition on solid surfaces.



(a) P_{ref} at node ID

(b) P_{ref} at given coordinates

(c) P_{ref} on outlet surface

Figure 4.21: The three different ways to assign a reference pressure in **Fluidity**.

4.6 Reference pressure

In every simulations, a reference pressure needs to be given. In **Fluidity**, there are three different ways to assign the reference pressure:

- The reference pressure is given at a specific node
  - defined by one node's ID `reference_node` (Figure 4.21a)
  - defined by one node's coordinates `reference_coordinates` (Figure 4.21b)
- The reference pressure is given as a `boundary_conditions` using a Dirichlet type, usually imposed equal to 0 at the outlet surface (Figure 4.21c).

The last option (reference pressure given as a boundary condition) is recommended.

4.7 Common errors

If the simulation crashes, the user can have a look at the file `fluidity-err.0`, which will give information about the reasons for the crash. Usually, the main and recurrent errors are:

- **Mesh errors**: The mesh is not consistent and this might be caused by the user not following the steps in Chapter 2.
- **Python script errors**: The Python language is sensitive to indentation. As such the indentation needs to be checked in the python scripts.
- **Non-convergence of the solver**: This is frequently caused by the time step being too large. The user should reduce the time step and/or the CFL number.

See also section 8.4 for other tricks.

Chapter 5

Mesh adaptivity

5.1 Explanation and tricks

5.1.1 Explanations

One of the key aspects of **Fluidity** is its mesh adaptivity capability with unstructured meshes, making it a unique tool that enhances and provides detailed and accurate information at high resolutions within the computational domain. The aim of this section is not to describe the theory behind mesh adaptivity but to explain, from a user point of view, how to set up mesh adaptivity options. The user can refer to [1] and [3] for more details regarding the theory. Different mesh adaptivity algorithms exist and the one used in this document is the `hr-adaptivity` one based on the change of the connectivity of the mesh and the relocation of the vertices of the mesh while retaining that same connectivity, as described in [3].
The mesh adaptivity process refines automatically the mesh in regions where significant physical processes are happening, which implies that the mesh adaptivity process is field-specific. The mandatory options that need to be turned on for mesh adaptivity are the following:

- **In the `Field` of interest:** As the mesh adaptivity is field-specific, the option `adaptivity_options` in the field of interest needs to be turned on as shown in Figure 5.1a and the `error_bound_interpolation` value has to be set (see Section 5.1.2). Moreover, the option `p_norm` can also be enabled and set to 2. Historically, the interpolation error was first controlled in the L_∞ norm. The metric formulation which controls the L_∞ norm is the simplest, and remains the default in **Fluidity** (option `p_norm` is turned off by default). However the L_∞ norm can have a tendency to focus the resolution entirely on the dynamics with the largest magnitude. Therefore, the L_p norm, which also includes the influence of the dynamics with smaller magnitudes, can be used. Empirical experience indicates that choosing $p = 2$, and hence the L_2 norm, generally gives better results. For that reason we recommend it as default for all adaptivity configurations (Figure 5.1b). However, this option can also tend to focus excessively the resolution on dynamics

of very small magnitudes. The user should do a prior sensibility analysis to figure out which option is more appropriate for the case considered. See sections 7.5.1 and 7.5.2 of the **Fluidity** manual [1] for more details.

- **In the `Mesh_adaptivity` options:**
  - **Period:** defines how often the mesh should be adapted. This can be set in number of simulation seconds `period`, or in number of time steps `period_in_timesteps`. Note that mesh adaptivity has a certain computational cost and a trade-off has to be found between how often the mesh is adapted and the total simulation time. It is recommended that adaptation happens every 10-20 time steps.
  - **Maximum number of nodes:** sets the maximum possible number of nodes `maximum_number_of_nodes` in the domain (see Section 5.1.2 to know how). In parallel, by default, this is the global maximum number of nodes. If the mesh adaptivity algorithm wants to place more nodes than this, the desired mesh is coarsened everywhere in space until it fits within this limit. In general, the error tolerances should be set so that this is never reached; it should only be a safety catch. If the simulation runs in parallel, make sure that the maximum number of nodes specified is at least $Nbr_{Proc} \times 50,000$ nodes.
  - **Gradation:** In numerical simulations, a smooth transition from small elements to large elements is generally important for mesh quality. Therefore, a mesh gradation algorithm is applied to smooth out sudden variations in the mesh sizing function. Various mesh gradation algorithms have been introduced to solve this problem and the one recommended is the `anisotropic_gradation`, with 0.75 prescribed on the diagonal and 0 otherwise, as shown in Figure 5.1c.
  - **Minimum edge length:** is the minimum edge length of an element allowed in the mesh (in meters). The input to this quantity is a tensor allowing one to impose different limits in different directions (see Figure 5.1d). See Section 5.1.2 to know how to find the appropriate value. This condition is not a hard constraint and the user may observe the constraint being (slightly) broken in places.
  - **Maximum edge length:** is the maximum edge length of an element allowed in the mesh (in meters). The input to this quantity is a tensor allowing one to impose different limits in different directions. See Section 5.1.2 to know how to find the appropriate value. This condition is not a hard constraint and the user may observe the constraint being (slightly) broken in places.

The minimum and maximum edge lengths and the maximum number of nodes, in combination with the interpolation error bound, will define how the resolution of the mesh varies with adaptation.

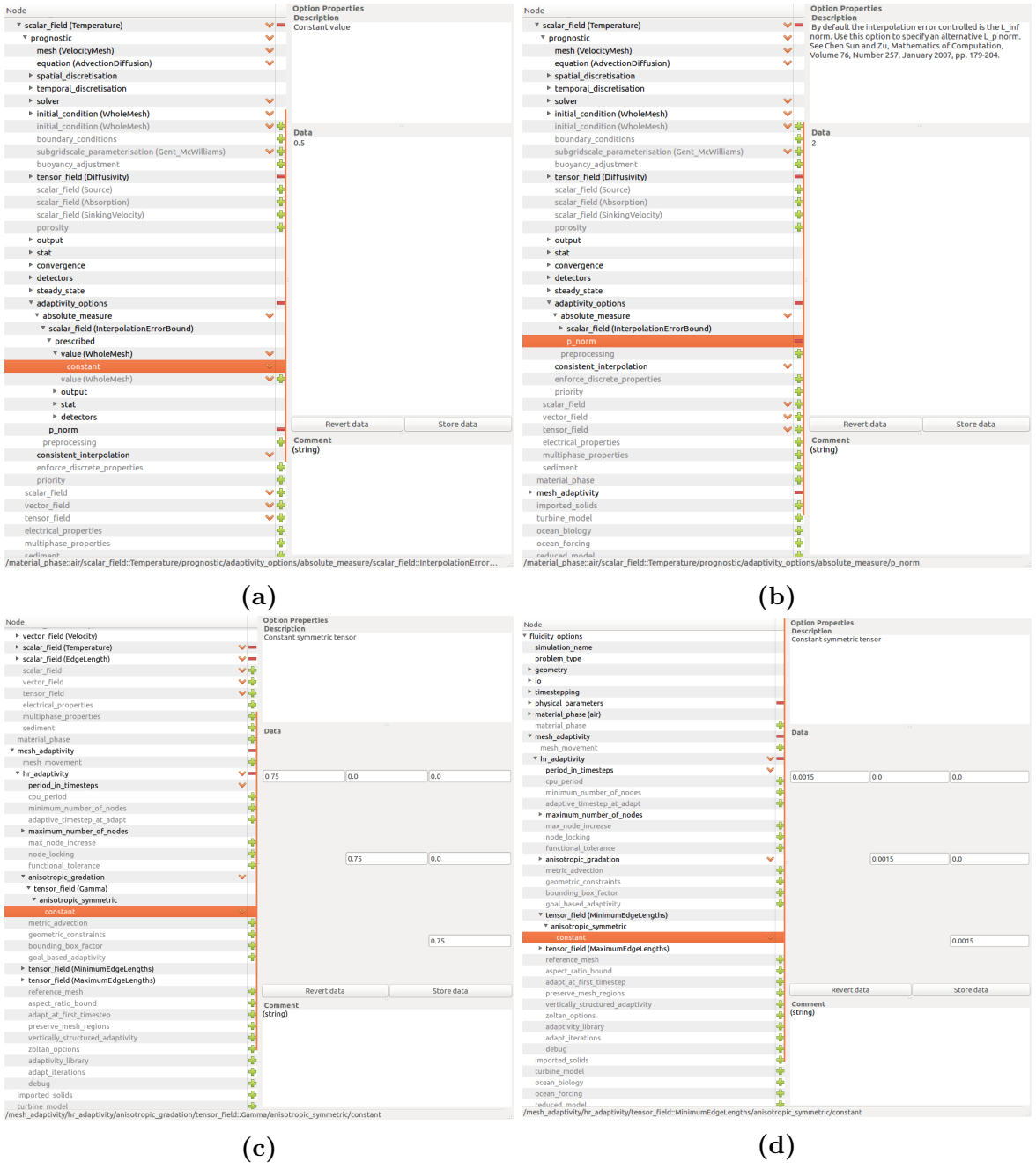


Figure 5.1: Options that need to be turned on in **Diamond** for mesh adaptivity.

5.1.2 Tricks to set up mesh adaptivity

Setting up the correct parameters needed for mesh adaptivity is not trivial and there are no universal rules. The user needs to experiment with the three main parameters which are: `Interpolation_error_bound`, `Minimum_edge_length` and `Maximum_edge_length`. However, here are some basic rules that can be followed.

- **Maximum number of nodes:** As a start, the user is suggested to use a relatively small number of maximum nodes to test all the options: between $100,000$ and $200,000$ is recommended. This value can be increased later.
- **Minimum edge length:** The minimum edge length should be quite large to start with. The value $H/1000$, where H is the height of the domain OR the value $L/100$, where L is a characteristic length of your geometry (here, the height of the openings for example), are recommended. This value can be progressively decreased afterwards to reach the resolution needed.
- **Maximum edge length:** The maximum edge length should be quite large to start with and the value $H/10$, where H is the height of the domain, is recommended.
- **Interpolation error bound:** The general advice would be to start with a high interpolation error, 10% of the range of the field considered being a good rule of thumb. As this value will certainly be too high, it is then recommended to reduce this value by small increments until reaching a refinement able to represent the desired dynamics. In any case, the interpolation error bound value should be the main parameter to vary to control the resolution of the adapted meshes. The value of `p_norm` should be equal to 2 as a first try. However, using $p = 2$ might also tend to focus the resolution on dynamics of too small magnitudes. The user should do a prior sensibility analysis with and without the `p_norm` function to figure out which option is more appropriate for the case considered.

Python scripts can be used to vary the specified lengths over the domain, allowing finer resolutions over areas of interest for instance. This will be discussed in Section 5.4.
Important note: The velocity field and/or the temperature (or any scalar field) can be adapted. Several field can be taken into account during adaptation. However, it is not recommended to adapt the pressure field: for cases involving indoor-outdoor exchanges and/or the urban environment, one might even say it is forbidden!

5.2 Summary of the simulations

Table 5.1 summarises the different simulations presented in the next sections.

Case Nbr	Initial Test Case Nbr	Field adapted	Interpolation error bound	Advected mesh	Section
6a	5a	Temperature	0.5	No	5.3.2
6b	5a	Temperature	0.3	No	5.3.2
6c	5a	Temperature	0.1	No	5.3.2
6d	5a	Temperature	0.05	No	5.3.2
7a	5a	Velocity	0.5	No	5.3.3
7b	5a	Velocity	0.25	No	5.3.3
7c	5a	Velocity	0.15	No	5.3.3
7d	5a	Velocity	0.1	No	5.3.3
8	5a	Temperature Velocity	0.15 0.15	No	5.3.4
9	2b	Temperature Velocity	075 0.045	No	5.4
10	5a	Temperature	0.1	Yes	5.5

Table 5.1: Summary of the simulations presented in the following sections of the Chapter 5.

5.3 Field specific adaptation

5.3.1 Set-up of examples

Boundary conditions

In examples *3dBox_Case6a.flml* to *3dBox_Case7d.flml*, the initial velocity and the inlet velocity (u, v, w) are set to $(1, 0, 0)$ m/s and the interior of the box is set to 298 K, while the outside remains at ambient temperature 293 K. These examples are similar to example *3dBox_Case5a.flml* which is set up without mesh adaptivity, i.e on a fixed mesh.

CFL number

To avoid any crash of the simulations, the time step is now also adaptive using a CFL condition as described in Section 3.2.2 and the CFL number is taken equal to 2 in the following examples (Figure 5.2). This value can be increased later on to speed up the simulations. However, it is recommended to the user to do a sensibility analysis of the results as a function of the CFL number to ensure that important information is not missing.

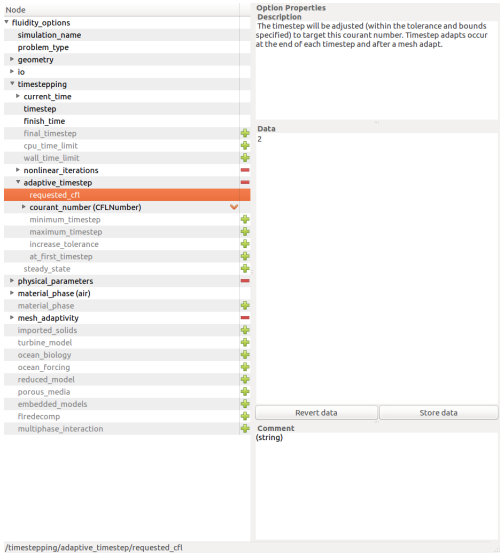


Figure 5.2: Adaptive time step.

General mesh adaptivity options

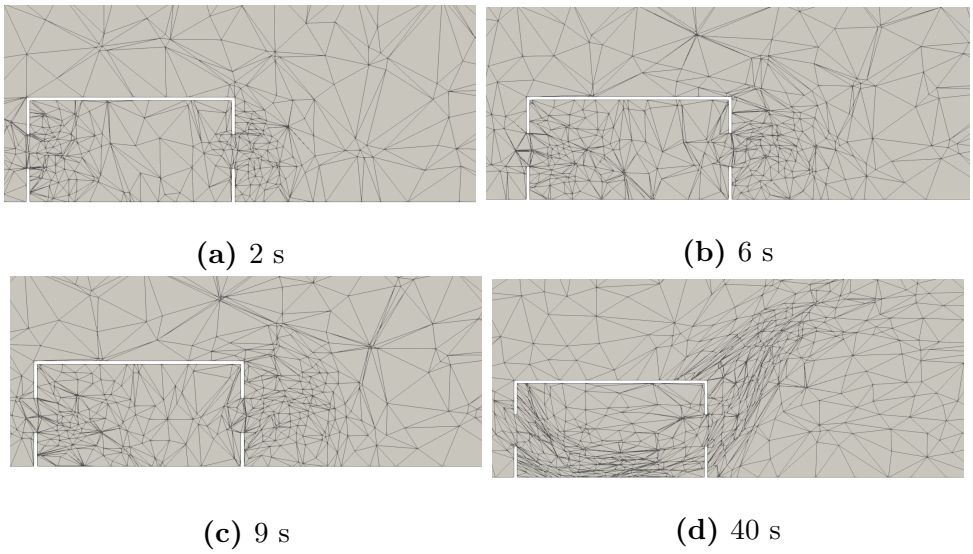
In the following sections, mesh adaptivity will be performed based on the temperature field only (Section 5.3.2), the velocity field only (Section 5.3.3) and both the velocity and temperature fields (Section 5.3.4). When the user wants to adapt several fields, it is recommended firstly to analyse each field independently as done in the following sections.
The maximum number of nodes is set equal to $200,000$ and the mesh is adapted every 10 time steps.
The characteristic length L of the domain is taken to be the windows opening, i.e. 1 m: the minimum edge length is set up to $L/100$, i.e. 0.01 m. The height H of the domain is 21 m: the maximum edge length is set up to $H/10$, i.e 2.1 m.

5.3.2 Adaptation based on the temperature field

In this section, the mesh adaptivity process is prescribed based on the temperature field only.

Mesh adaptivity options

The range of the temperature is between 293 K and 298 K, i.e. a difference of 5 K. The `error_bound_interpolation` is in a first run set up at 10% of this temperature range: the value $5 \times 10\% = 0.5$ is used in example *3dBox_Case6a.flml*. Then the `error_bound_interpolation` is progressively decreased to values equal to 0.3 (6% of the temperature range) in *3dBox_Case6b.flml*, 0.1 (2% of the temperature range) in *3dBox_Case6c.flml* and 0.05 (1% of the temperature range) in *3dBox_Case6d.flml*.



(a) 2 s **(b)** 6 s

(c) 9 s **(d)** 40 s

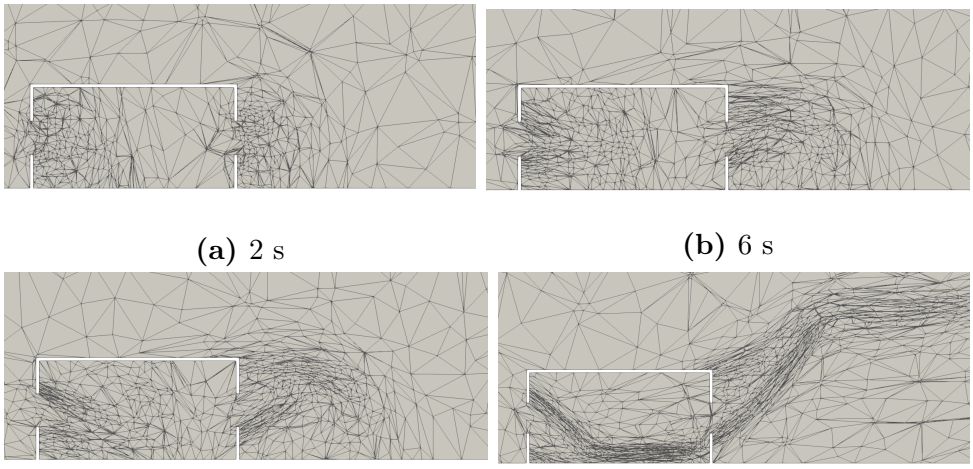
Figure 5.3: Meshes at different instant for example *3dBox_Case6a.flml*. The temperature field only is adapted with an `error_bound_interpolation` equal to 0.5.

These examples can be run using the commands:

```
user@mypc:~$ <<FluiditySourcePath>>/bin/fluidity -l -v3 3dBox_Case6a.flml &
user@mypc:~$ <<FluiditySourcePath>>/bin/fluidity -l -v3 3dBox_Case6b.flml &
user@mypc:~$ <<FluiditySourcePath>>/bin/fluidity -l -v3 3dBox_Case6c.flml &
user@mypc:~$ <<FluiditySourcePath>>/bin/fluidity -l -v3 3dBox_Case6d.flml &
```

Results and discussion

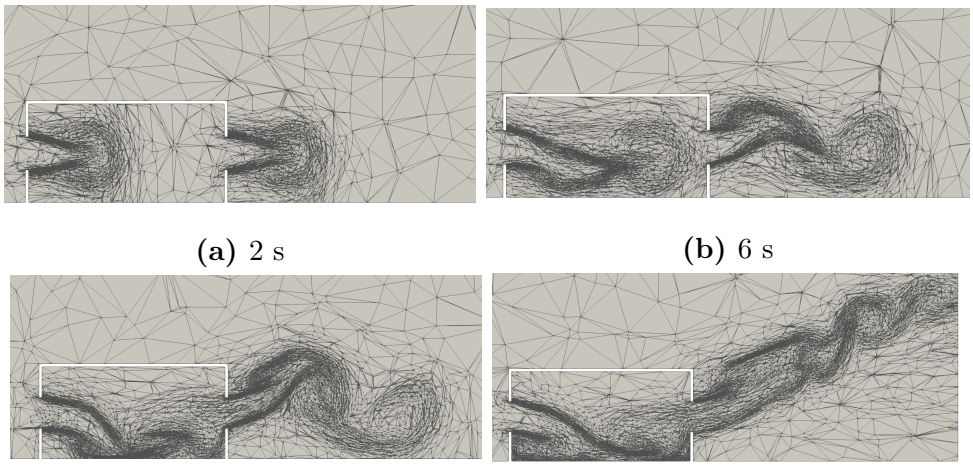
Snapshots of the meshes are shown in Figure 5.3, Figure 5.4, Figure 5.5 and Figure 5.6. Snapshots of the temperature field are shown in Figure 5.7, Figure 5.8, Figure 5.9 and Figure 5.10. Snapshots of the velocity field are shown in Figure 5.11, Figure 5.12, Figure 5.13 and Figure 5.14. Go to Chapter 10 to learn how to visualise the results using **ParaView**.
For a given `error_bound_interpolation`, as shown in Figure 5.3, Figure 5.4, Figure 5.5 and Figure 5.6 the mesh is adapting based on the temperature field, i.e. mainly within the box and at the outlet of the box. Indeed, decreasing the value of the `error_bound_interpolation` results in finer mesh in those regions. However, it is important to mention that the computational time is by consequence larger, see Section 5.3.5. Choosing an `error_bound_interpolation` higher to 0.3 seems to lead to poor mesh quality (in that particular case). Even with small `error_bound_interpolation` and if the temperature field is well resolved, the velocity field is not properly captured due to a poor mesh quality, especially around the box.



(a) 2 s **(b)** 6 s

(c) 9 s **(d)** 40 s

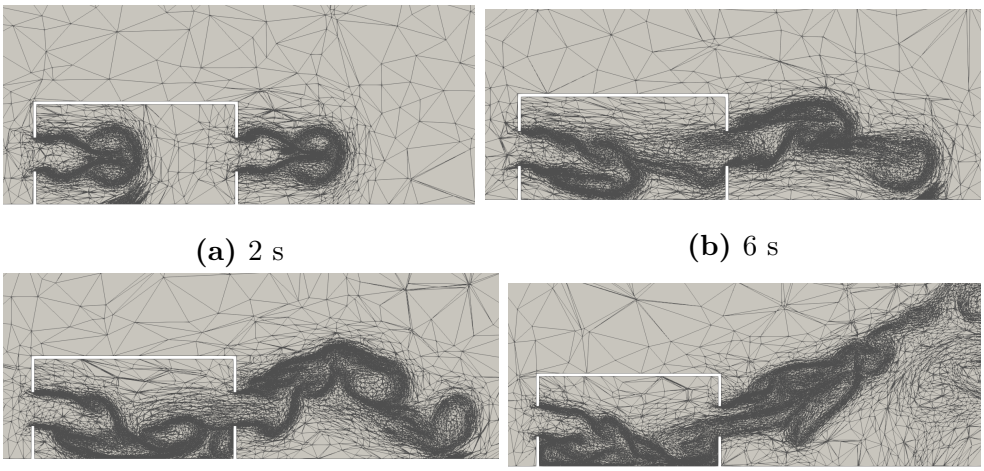
Figure 5.4: Meshes at different instant for example *3dBox_Case6b.fml*. The temperature field only is adapted with an `error_bound_interpolation` equal to 0.3.



(a) 2 s **(b)** 6 s

(c) 9 s **(d)** 40 s

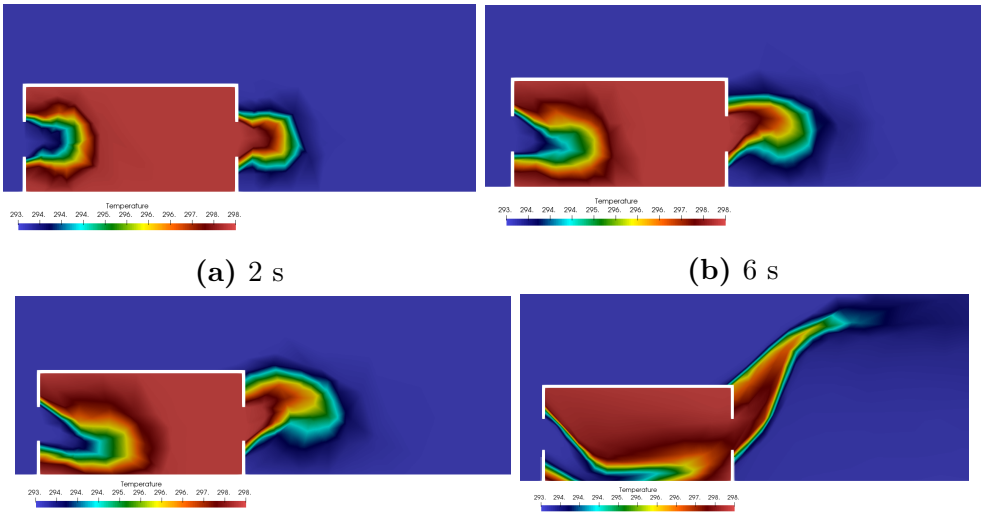
Figure 5.5: Meshes at different instant for example *3dBox_Case6c.fml*. The temperature field only is adapted with an `error_bound_interpolation` equal to 0.1.



(a) 2 s **(b)** 6 s

(c) 9 s **(d)** 30 s

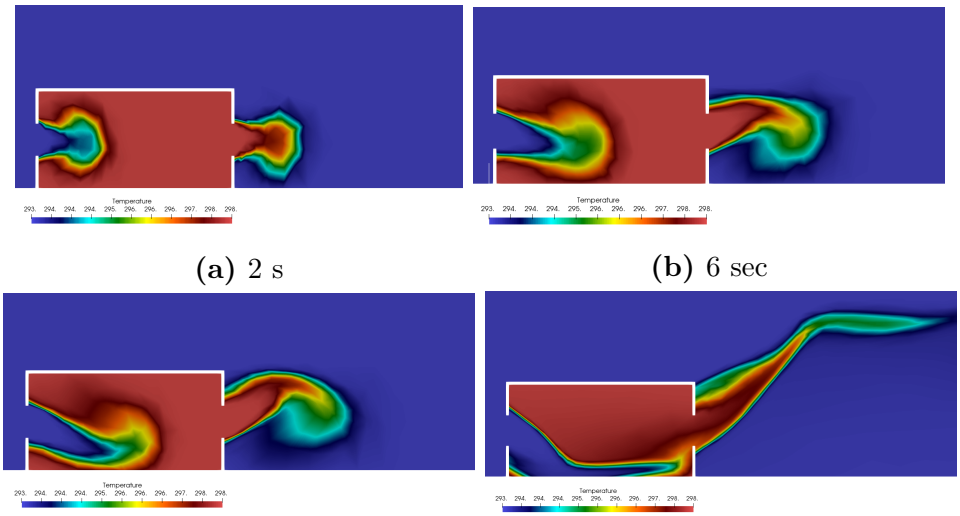
Figure 5.6: Meshes at different instant for example *3dBox_Case6d.fml*. The temperature field only is adapted with an `error_bound_interpolation` equal to 0.05.



(a) 2 s **(b)** 6 s

(c) 9 s **(d)** 40 s

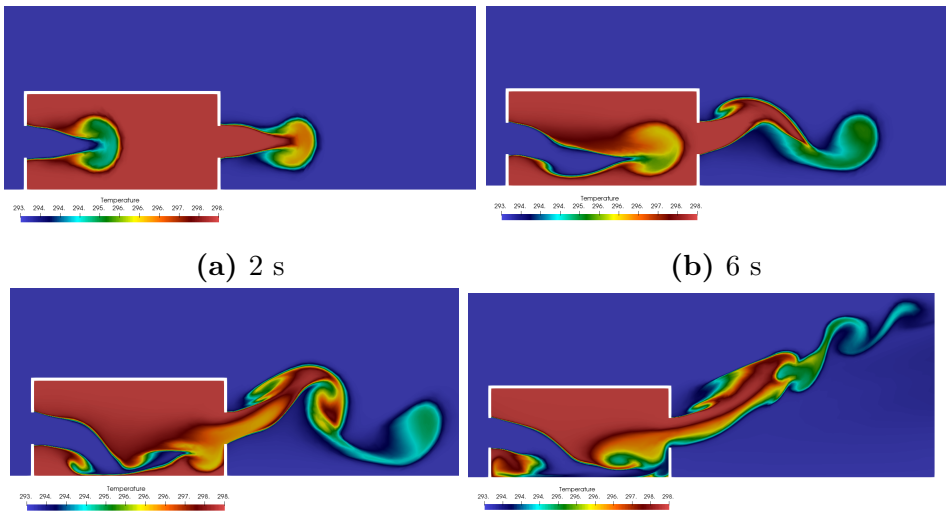
Figure 5.7: Temperature field at different instant for the simulation *3dBox_Case6a.fml*. The temperature field only is adapted with an `error_bound_interpolation` equal to 0.5.



(a) 2 s **(b)** 6 sec

(c) 9 sec **(d)** 40 sec

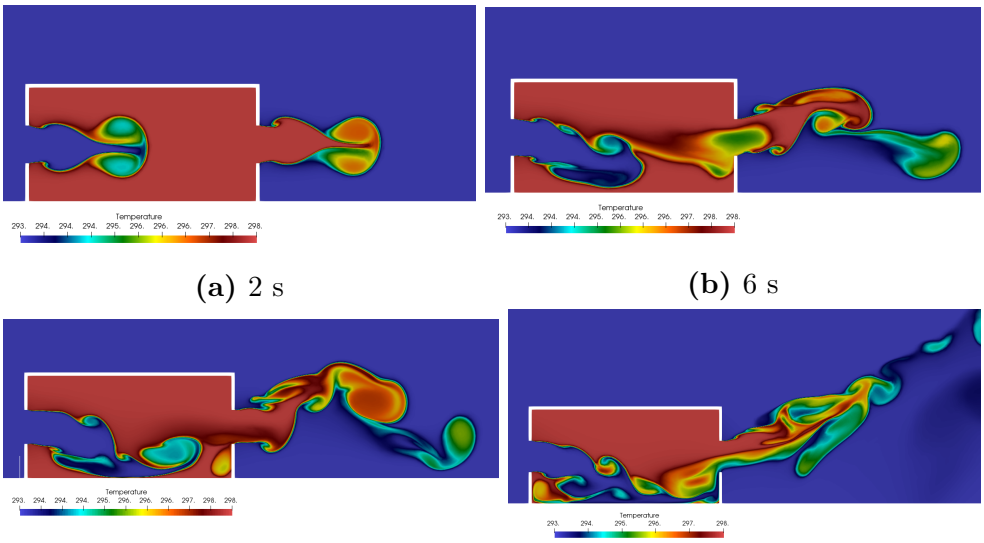
Figure 5.8: Temperature field at different instant for the simulation *3dBox_Case6b.fml*. The temperature field only is adapted with an `error_bound_interpolation` equal to 0.3.



(a) 2 s **(b)** 6 s

(c) 9 s **(d)** 40 s

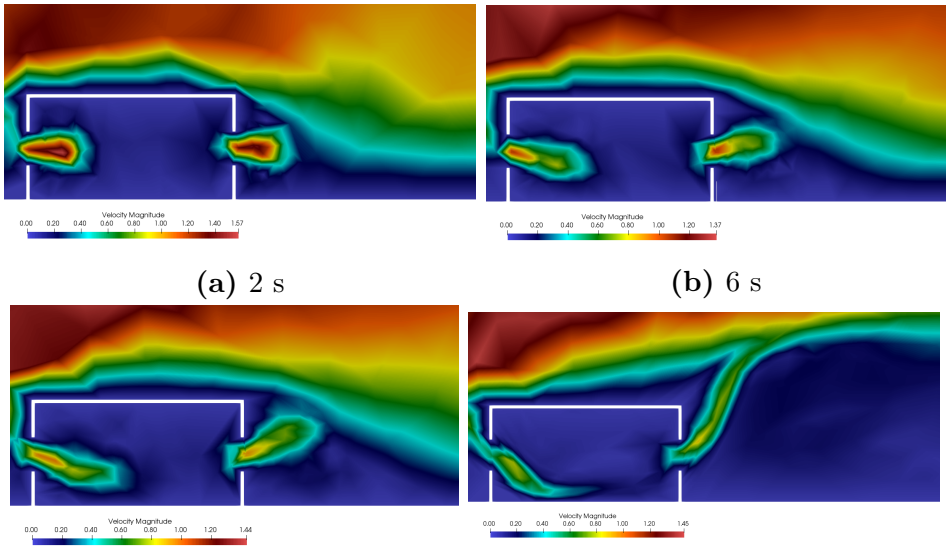
Figure 5.9: Temperature field at different instant for the simulation *3dBox_Case6c.fml*. The temperature field only is adapted with an `error_bound_interpolation` equal to 0.1.



(a) 2 s **(b)** 6 s

(c) 9 s **(d)** 30 s

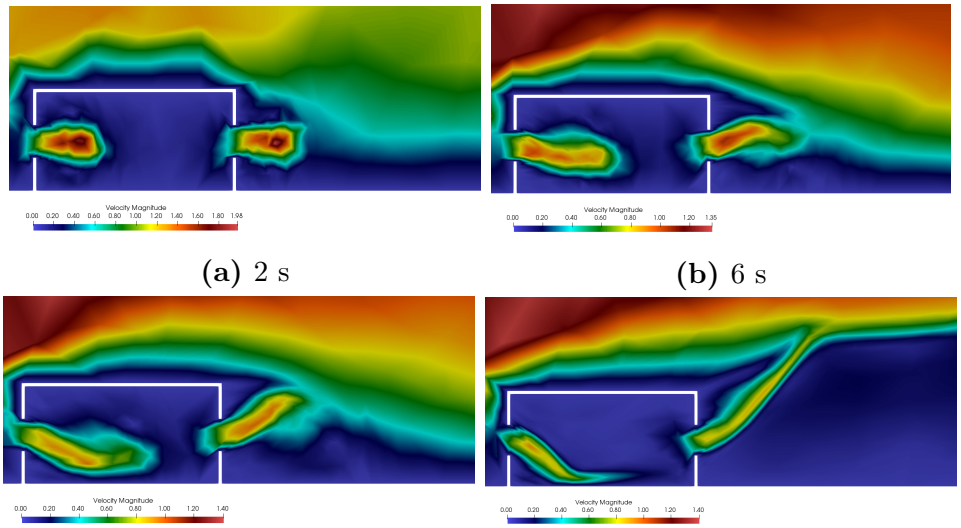
Figure 5.10: Temperature field at different instant for the simulation *3dBox_Case6d.fml*. The temperature field only is adapted with an `error_bound_interpolation` equal to 0.05.



(a) 2 s **(b)** 6 s

(c) 9 s **(d)** 40 s

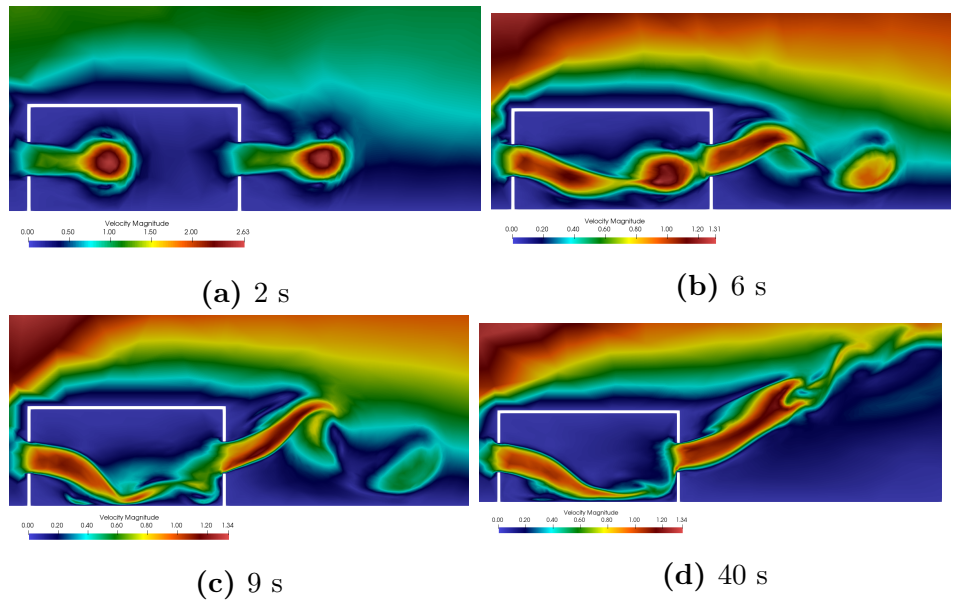
Figure 5.11: Velocity field at different instant for the simulation *3dBox_Case6a.fml*. The temperature field only is adapted with an `error_bound_interpolation` equal to 0.5.



(a) 2 s **(b)** 6 s

(c) 9 s **(d)** 40 s

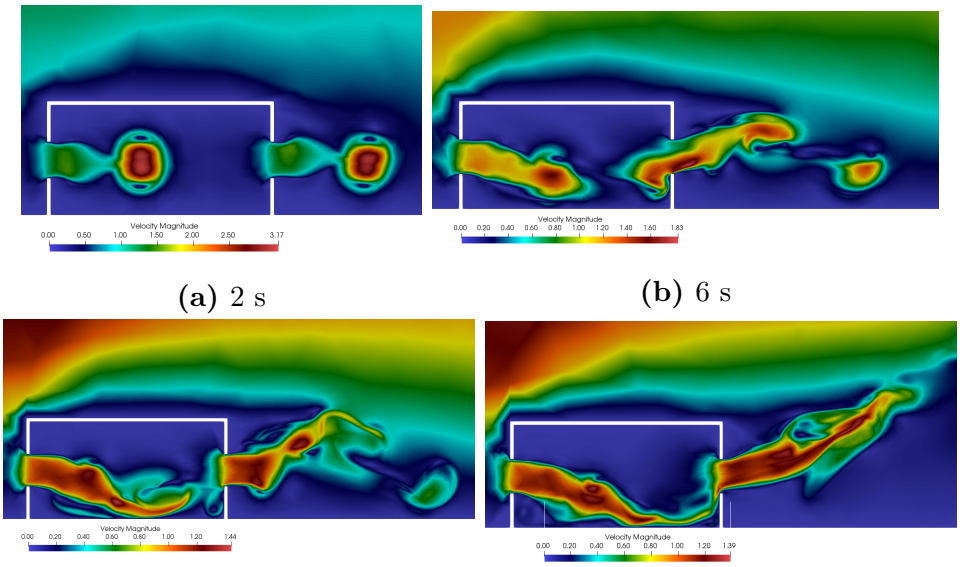
Figure 5.12: Velocity field at different instant for the simulation *3dBox_Case6b.fml*. The temperature field only is adapted with an `error_bound_interpolation` equal to 0.3.



(a) 2 s **(b)** 6 s

(c) 9 s **(d)** 40 s

Figure 5.13: Velocity field at different instant for the simulation *3dBox_Case6c.fml*. The temperature field only is adapted with an `error_bound_interpolation` equal to 0.1.



(a) 2 s **(b)** 6 s

(c) 9 s **(d)** 30 s

Figure 5.14: Velocity field at different instant for the simulation *3dBox_Case6d.flml*. The temperature field only is adapted with an `error_bound_interpolation` equal to 0.05.

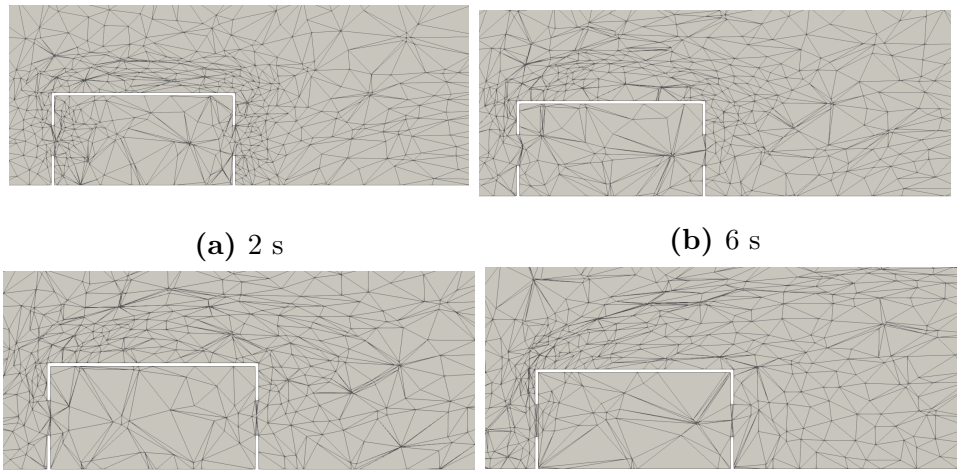
5.3.3 Adaptation based on the velocity field

In this section, the mesh adaptivity process is prescribed based on the velocity field only.

Mesh adaptivity options

Even if the initial inlet velocity is prescribed equal to 1 m/s, it is not recommended to use 1 m/s as the upper bound to determine the `error_bound_interpolation`. Indeed, the velocity magnitude in the domain will probably be higher than this value and estimate the `error_bound_interpolation` based on 1 m/s will lead to a too small value as a first guess. Therefore, based on the run performed in examples *3dBox_Case6*.flml*, the velocity range seems to be between 0 m/s and approximately 5 m/s, i.e. a difference of 5 m/s. The `error_bound_interpolation` is, in a first run, set up at 10% of this velocity range: the value $5 \times 10\% = 0.5$ is used in example *3dBox_Case7a.flml*. Then the `error_bound_interpolation` is progressively decreased to values equal to 0.25 (5% of the velocity range) in *3dBox_Case7b.flml*, 0.15 (3% of the velocity range) in *3dBox_Case7c.flml* and 0.1 (2% of the velocity range) in *3dBox_Case7d.flml*.
These examples can be run using the commands:

```
user@mypc:~$ <<FluiditySourcePath>>/bin/fluidity -l -v3 3dBox_Case7a.flml &
user@mypc:~$ <<FluiditySourcePath>>/bin/fluidity -l -v3 3dBox_Case7b.flml &
user@mypc:~$ <<FluiditySourcePath>>/bin/fluidity -l -v3 3dBox_Case7c.flml &
user@mypc:~$ <<FluiditySourcePath>>/bin/fluidity -l -v3 3dBox_Case7d.flml &
```



(a) 2 s **(b)** 6 s

(c) 9 s **(d)** 40 s

Figure 5.15: Meshes at different instant for example *3dBox_Case7a.flml*. The velocity field only is adapted with an `error_bound_interpolation` equal to 0.5.

Results and discussion

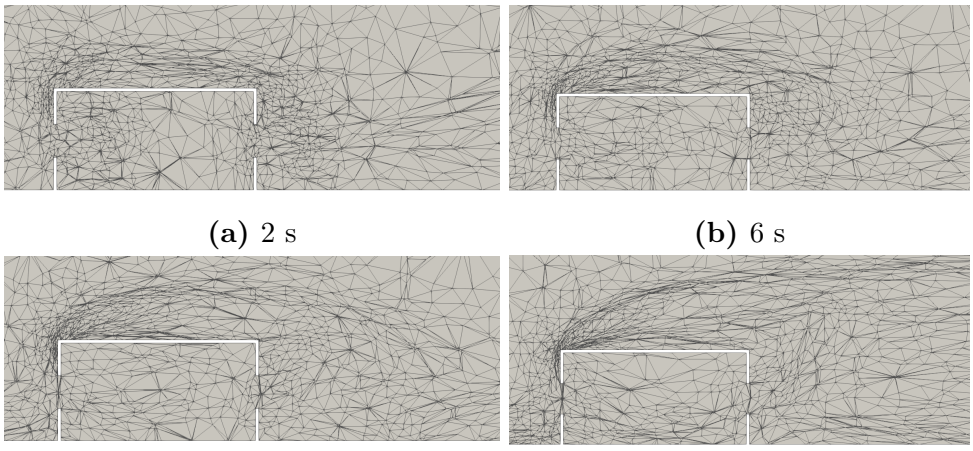
Snapshots of the meshes are shown in Figure 5.15, Figure 5.16, Figure 5.17 and Figure 5.18. Snapshots of the temperature field are shown in Figure 5.19, Figure 5.20, Figure 5.21 and Figure 5.22. Snapshots of the velocity field are shown in Figure 5.23, Figure 5.24, Figure 5.25 and Figure 5.26. Go to Chapter 10 to learn how to visualise the results using **ParaView**.
For a given `error_bound_interpolation`, as shown in Figure 5.15, Figure 5.16, Figure 5.17 and Figure 5.18 the mesh is adapting based on the velocity field, i.e. mainly at the openings and around the exterior surfaces of the box. Indeed, decreasing the value of the `error_bound_interpolation` results in finer mesh in those regions. Choosing an `error_bound_interpolation` higher to 0.15 seems to lead to poor mesh quality (in that particular case). Even with small `error_bound_interpolation` and if the velocity field is well resolved, the temperature field is not properly captured due to a poor mesh quality, especially within the box.

5.3.4 Adaptation based on the velocity and the temperature fields

In this section, the mesh adaptivity process is prescribed based on both the velocity field and the temperature field.

Mesh adaptivity options

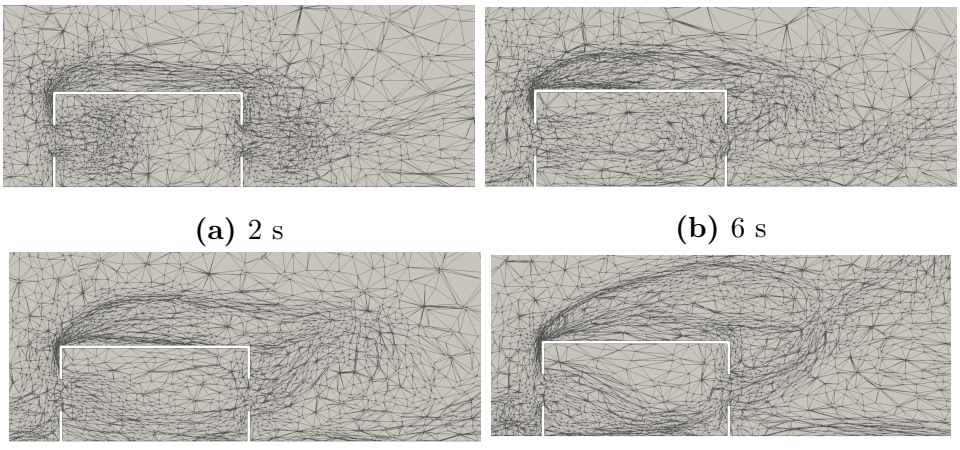
Based on the run performed in examples *3dBox_Case6*.flml* and *3dBox_Case7*.flml*, the `error_bound_interpolation` values for the temperature and the velocity are cho-



(a) 2 s **(b)** 6 s

(c) 9 s **(d)** 40 s

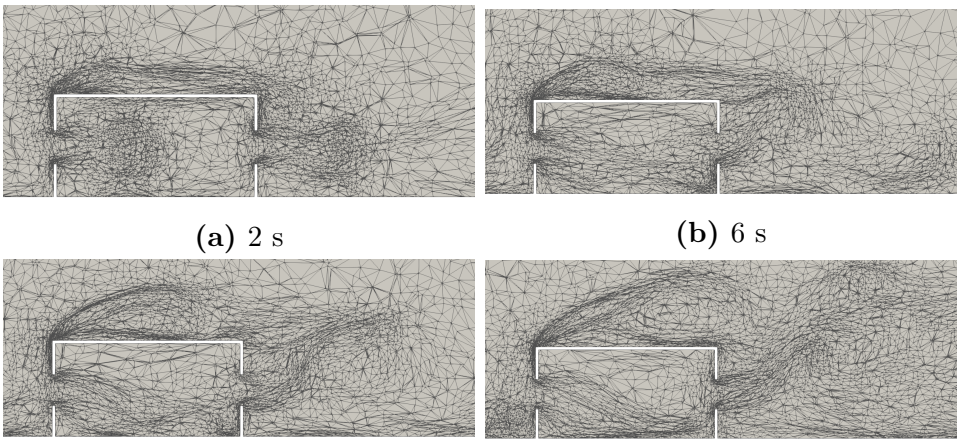
Figure 5.16: Meshes at different instant for example *3dBox_Case7b.fml*. The velocity field only is adapted with an `error_bound_interpolation` equal to 0.25.



(a) 2 s **(b)** 6 s

(c) 9 s **(d)** 40 s

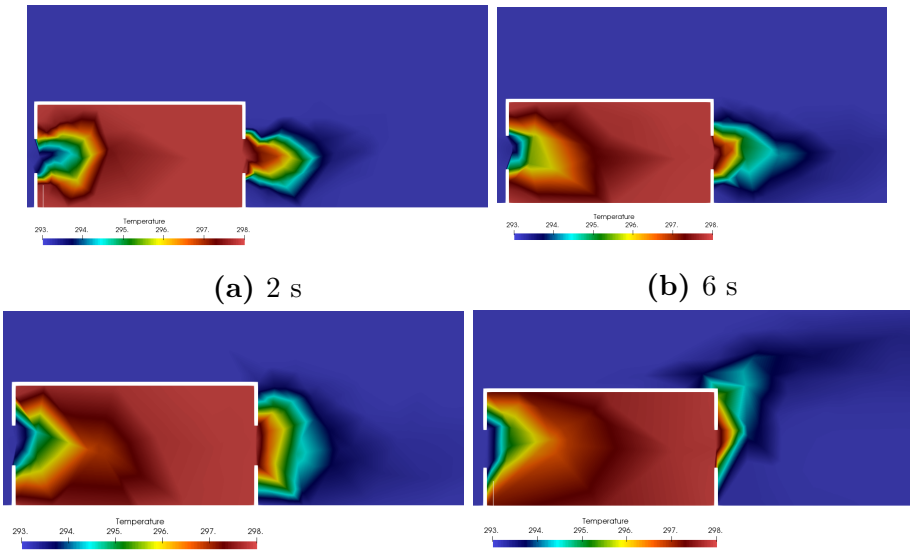
Figure 5.17: Meshes at different instant for example *3dBox_Case7c.fml*. The velocity field only is adapted with an `error_bound_interpolation` equal to 0.15.



(a) 2 s **(b)** 6 s

(c) 9 s **(d)** 40 s

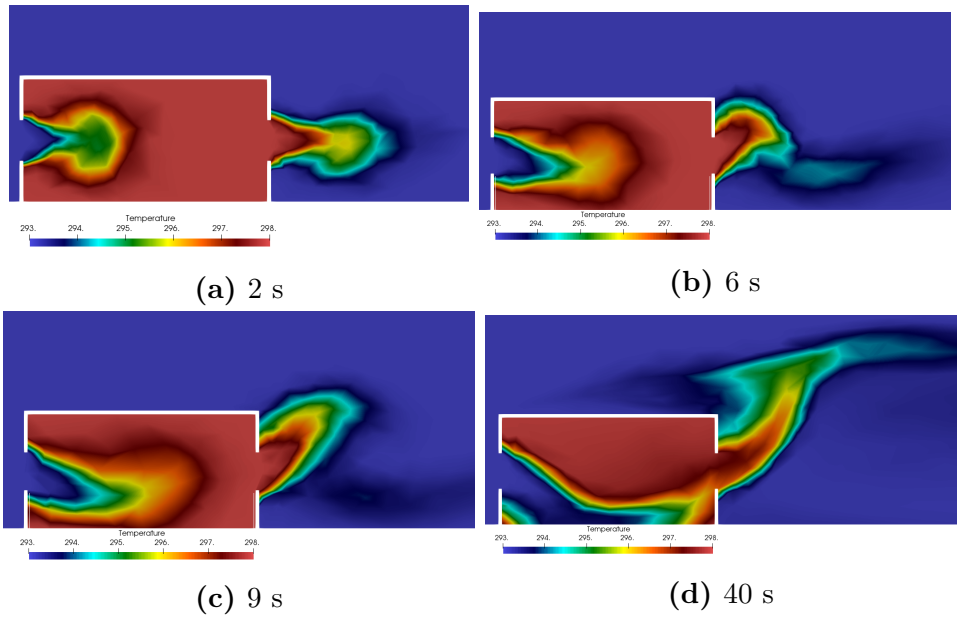
Figure 5.18: Meshes at different instant for example *3dBox_Case7d.fml*. The velocity field only is adapted with an `error_bound_interpolation` equal to 0.1.



(a) 2 s **(b)** 6 s

(c) 9 s **(d)** 40 s

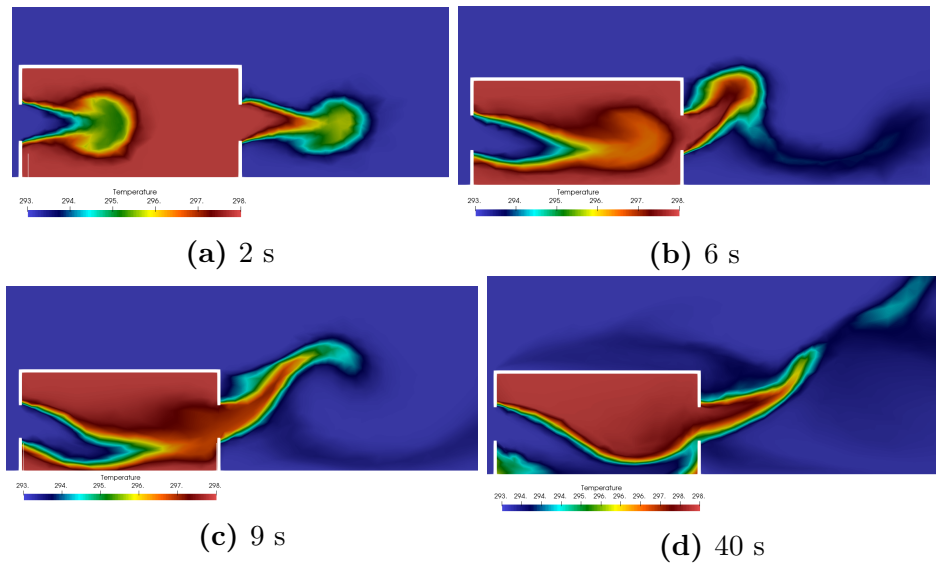
Figure 5.19: Temperature field at different instant for example *3dBox_Case7a.fml*. The velocity field only is adapted with an `error_bound_interpolation` equal to 0.5.



(a) 2 s (b) 6 s

(c) 9 s (d) 40 s

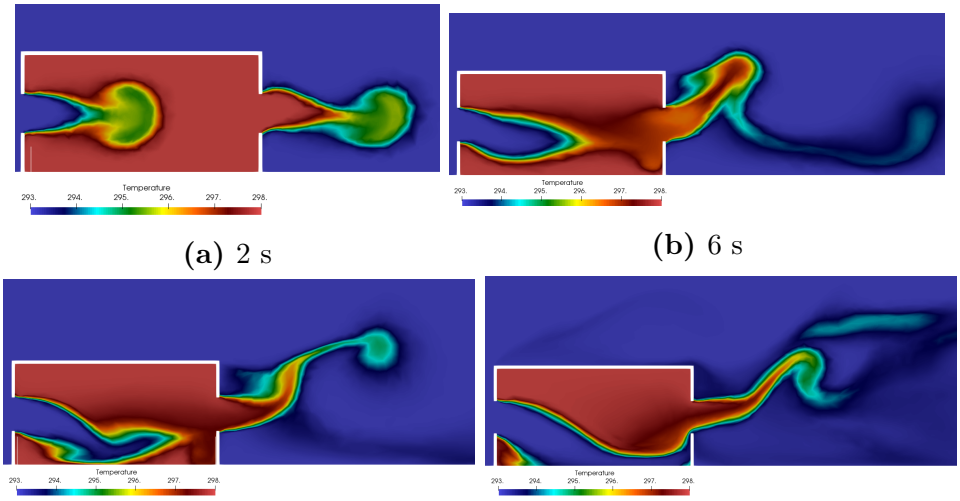
Figure 5.20: Temperature field at different instant for example *3dBox_Case7b.fml*. The velocity field only is adapted with an `error_bound_interpolation` equal to 0.25.



(a) 2 s (b) 6 s

(c) 9 s (d) 40 s

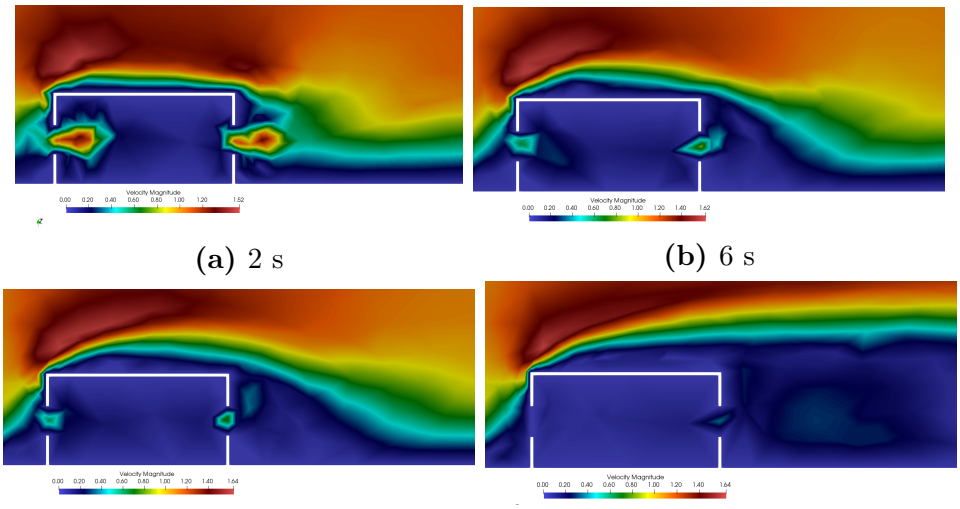
Figure 5.21: Temperature field at different instant for the simulation *3dBox_Case7c.fml*. The velocity field only is adapted with an `error_bound_interpolation` equal to 0.15.



(a) 2 s **(b)** 6 s

(c) 9 s **(d)** 40 s

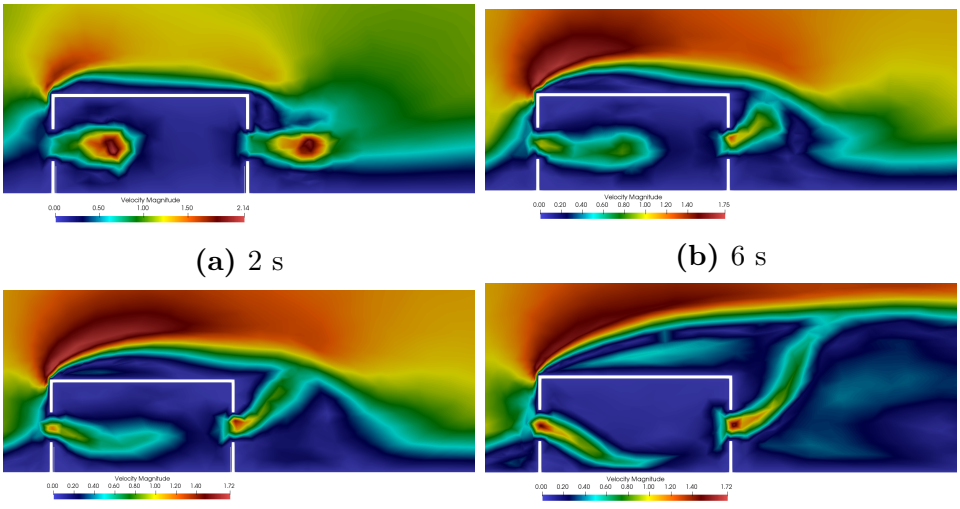
Figure 5.22: Temperature field at different instant for the simulation *3dBox_Case7d.fml*. The velocity field only is adapted with an `error_bound_interpolation` equal to 0.1.



(a) 2 s **(b)** 6 s

(c) 9 s **(d)** 40 s

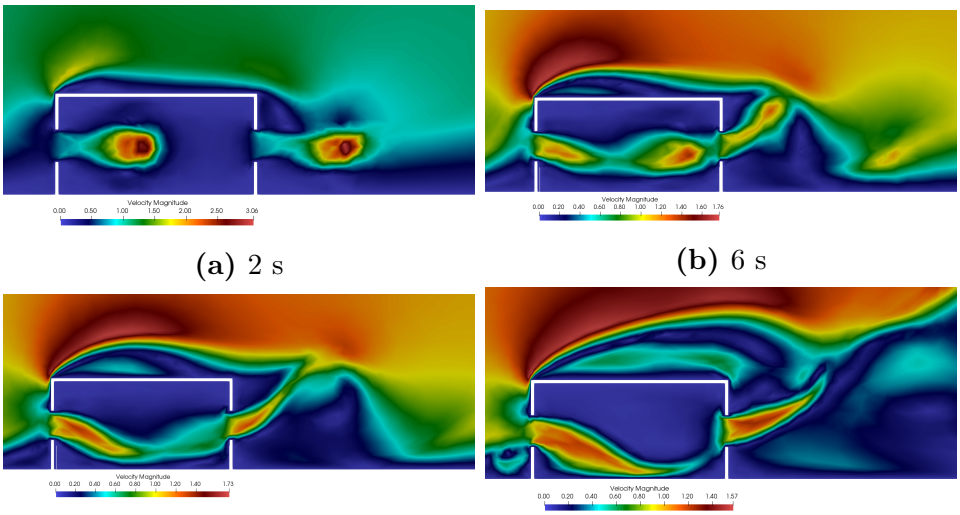
Figure 5.23: Velocity field at different instant for the simulation *3dBox_Case7a.fml*. The velocity field only is adapted with an `error_bound_interpolation` equal to 0.5.



(a) 2 s **(b)** 6 s

(c) 9 s **(d)** 40 s

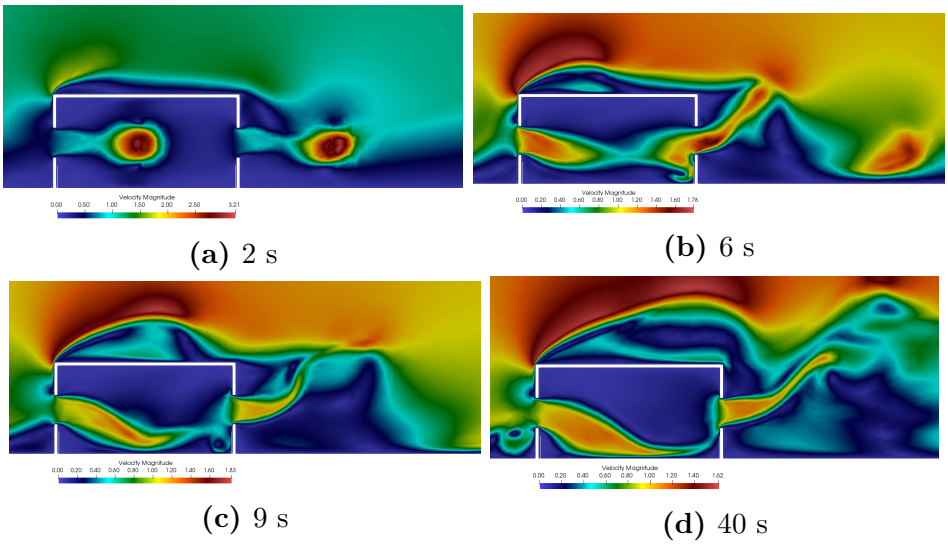
Figure 5.24: Velocity field at different instant for the simulation *3dBox_Case7b.fml*. The velocity field only is adapted with an `error_bound_interpolation` equal to 0.25.



(a) 2 s **(b)** 6 s

(c) 9 s **(d)** 40 s

Figure 5.25: Velocity field at different instant for the simulation *3dBox_Case7c.fml*. The velocity field only is adapted with an `error_bound_interpolation` equal to 0.15.



(a) 2 s **(b)** 6 s **(c)** 9 s **(d)** 40 s

Figure 5.26: Velocity field at different instant for the simulation *3dBox_Case7d.flml*. The velocity field only is adapted with an `error_bound_interpolation` equal to 0.1.

sen to be both equal to 0.15 in example *3dBox_Case8.flml*. Note that using the same value is a coincidence, and these values can be of course different. These values were chosen to capture properly both the temperature and the velocity fields, while keeping an acceptable computational time for the purpose of this manual. It is therefore recommended to use 0.1 for both field to fully capture the dynamics.
This example can be run using the command:

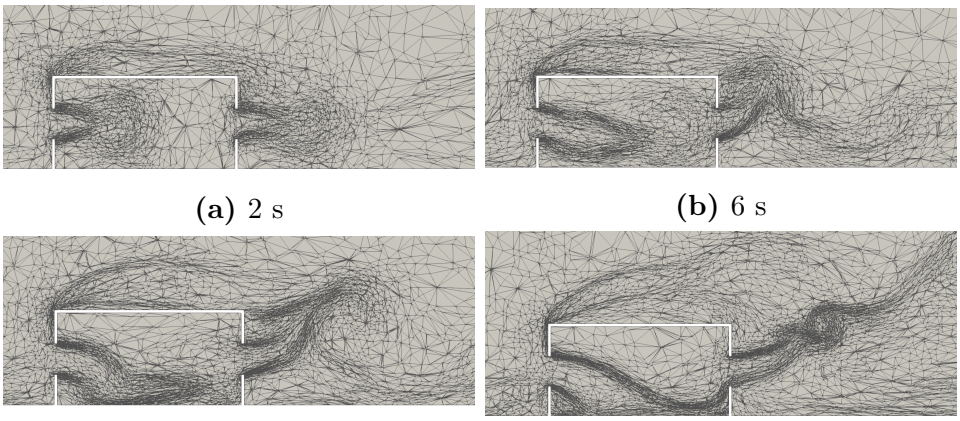
```
user@mypc:~$ <<FluiditySourcePath>>/bin/fluidity -l -v3 3dBox_Case8.flml &
```

Results and discussion

Snapshots of the meshes are shown in Figure 5.27. Snapshots of the temperature field are shown in Figure 5.28. Snapshots of the velocity field are shown in Figure 5.29. Go to Chapter 10 to learn how to visualise the results using **ParaView**.
As shown in Figure 5.27 the mesh is well-adapted based on the velocity field, i.e. at the openings and around the exterior surfaces of the box and based on the temperature field, i.e. within the box. In other words, the mesh is not only adapted in the interior or the exterior of the box but in both regions, thus capturing the full dynamics of the velocity field and the temperature field.

5.3.5 Computation time

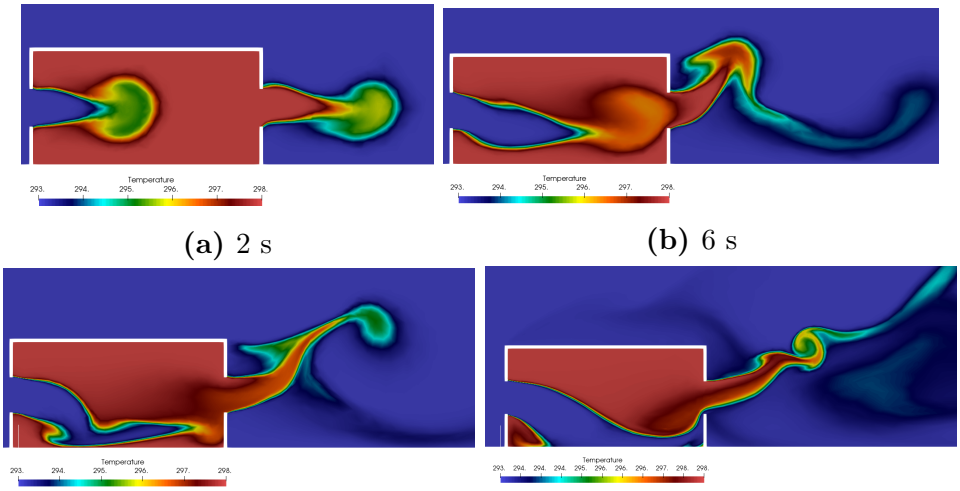
The computation time for all the simulations is reported in Table 5.2, highlighting that refining the mesh, i.e. decreasing the `error_bound_interpolation`, drastically increases the computational time. Therefore, a trade-off has to be made between the accuracy desired and an acceptable computational time.



(a) 2 s **(b)** 6 s

(c) 9 s **(d)** 40 s

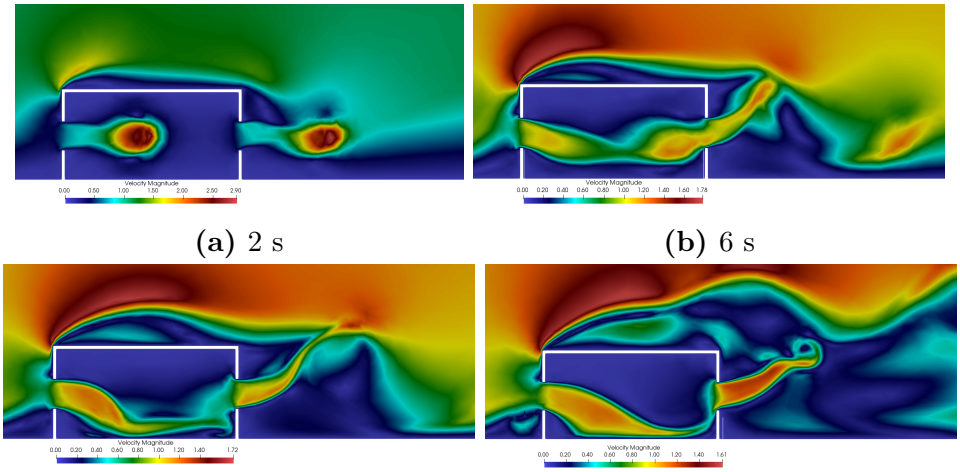
Figure 5.27: Meshes at different instant for the simulation *3dBox_Case8.fml*. Temperature and velocity fields are both adapted with `error_bound_interpolation` values equal to 0.15.



(a) 2 s **(b)** 6 s

(c) 9 s **(d)** 40 s

Figure 5.28: Temperature field at different instant for example *3dBox_Case8.fml*. Temperature and velocity fields are both adapted with `error_bound_interpolation` values equal to 0.15.



(a) 2 s **(b)** 6 s

(c) 9 s **(d)** 40 s

Figure 5.29: Velocity field at different instant for example *3dBox_Case8.fml*. Temperature and velocity fields are both adapted with `error_bound_interpolation` values equal to 0.15.

Case Nbr	**Simulation time: 2 s**	**Simulation time: 6 s**	**Simulation time: 9 s**	**Simulation time: 40 s**
6a	00H 01min 05s	00H 01min 33s	00H 01min 53s	00H 02min 08s
6b	00H 01min 35s	00H 02min 59s	00H 04min 27s	00H 32min 29s
6c	00H 25min 12s	01H 24min 33s	02H 11min 44s	16H 51min 14s
6d	03H 43min 19s	10H 28min 17s	19H 19min 28s	Too long...
7a	00H 02min 39s	00H 03min 38s	00H 04min 12s	00H 09min 56s
7b	00H 07min 37s	00H 11min 42s	00H 16min 45s	01H 21min 22s
7c	00H 25min 37s	00H 58min 26s	01H 34min 29s	08H 25min 53s
7d	01H 04min 17s	02H 35min 45s	03H 56min 29s	31H 04min 48s
8	00H 32min 27s	01H 10min 05s	01H 50min 02s	11H 08min 00s

Table 5.2: Computation time for the simulations with mesh adaptivity at different instants.

5.4 Ensuring enough resolution in specific region

5.4.1 Python script to refine zone

Boundary conditions

For the cases *3dBox_Case9a.flml* and *3dBox_Case9b.flml*, the initial and the ambient temperatures are set to 293 K and u is set to 0 m/s. The heat flux applied at the source ϕ_{source} is equal to 1000 W/m^2, hence $\phi_{fluidity}$, set up in **Diamond**, is equal to 0.8163 according to equation 4.1. The surface of the heat source is 0.2×0.2 m^2: the flux applied at the source is then equal to 40 W. This example is similar to *3dBox_Case2b.flml* which is set up without mesh adaptivity, i.e on a fixed mesh.

CFL number

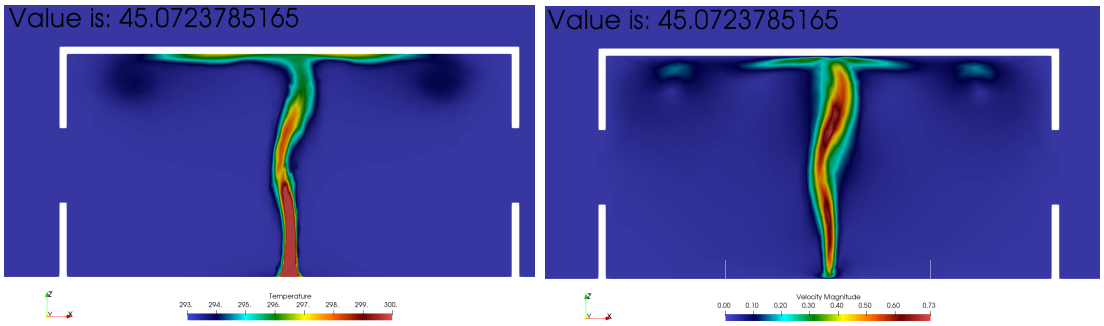
To avoid any crash of the simulations, the time step is now also adaptive using a CFL condition as described in Section 3.2.2, with the CFL number taken as 2 in the following example. This value can be increased later on to speed up the simulations. However, it is recommended to do a sensibility analysis of the results as a function of the CFL number to ensure that no important information is missed. Moreover, a maximum time step is prescribed equal to 1 s: at the beginning of the simulation, the velocity within the domain is almost equal to 0 m/s. As a consequence, based on the CFL number, the computed time step will be unreasonably very large (see equation 3.11) causing the simulation to crash.

General mesh adaptivity options

In the following sections, mesh adaptivity will be performed based on the temperature and the velocity fields. The maximum number of nodes is set to $200,000$ and the mesh is adapted every 10 time steps.
Based on the results of *3dBox_Case2b.flml*, the velocity is estimated to be approximately between 0 m/s and 0.45 m/s. The velocity `error_bound_interpolation` is taken to be equal to 10% of the velocity range, i.e equal to 0.045. Based on the results of *3dBox_Case2b.flml*, the temperature is estimated to be approximately between 293 K and 333 K. However, the highest temperatures are located near the source only: the rest of the inner box is much cooler, i.e. between 293 K and approximately 300 K. The choice is then made not to take into account the entire temperature range, but only the one of interest, i.e. between 293 K and 300 K. The temperature `error_bound_interpolation` is taken to be equal to 10% of the interesting temperature range, i.e of 7 K. Therefore, the `error_bound_interpolation` is set to 0.7.

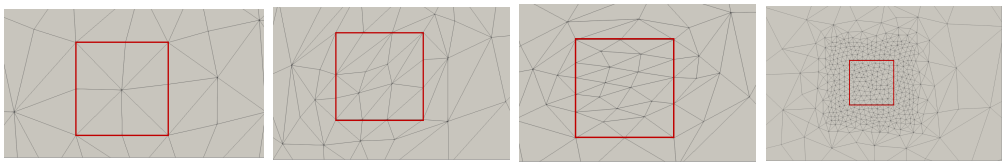
Minimum and maximum edge lengths

The characteristic length L of the domain is taken to be the windows opening, i.e. $1m$: the minimum edge length is set up to $L/100$, i.e. 0.01 m. The height H of the domain



(a) **(b)**

Figure 5.30: (a) Temperature and (b) Velocity fields at 45 s for the simulation *3dBox_Case9a.fiml*. The temperature and the velocity fields are both adapted with `error_bound_interpolation` values equal to 0.7 and 0.045, respectively.



(a) 20 sec **(b)** 45 sec **(c)** 70 sec **(d)**

Figure 5.31: Meshes at the source location (a), (b) and (c) at different instant and for the simulation *3dBox_Case9a.fiml* when no constraint is imposed on the mesh at the source and (d) meshes at the source location for the simulation *3dBox_Case9b.fiml* when refinement is enforced around the source. The red squares depict the location of the source.

is 21 m: the maximum edge length is set up to $H/10$, i.e 2.1 m.
As shown in Figure 5.30, these `error_bound_interpolation` values gives acceptable results as a first run. However, zooming on the source, Figure 5.31 shows that the region near the source is not well resolved. It is commonly assumed that at least 10-20 elements should define a source, which is clearly not the case in *3dBox_Case9a.fiml*.
Reducing the `error_bound_interpolation` value for the temperature will have a tendency to overly increase the resolution near the source at the expense of the rest of the plume. One shortcut, to ensure a well resolved source, is to use a python script to vary the specified minimum and the maximum edge lengths over the domain, constraining finer resolutions over areas of interest, in this case the source. It is worth noting that this technique can also be used to ensure refinement near openings for example. In example *3dBox_Case9b.fiml*, the python scripts in Code 5.1 and Code 5.2 are used to set up the minimum and the maximum edge lengths. The refined region of the mesh near the source is twice as large as the source itself and at least 20 elements are forced in that region. The mesh obtained near the source is shown in Figure 5.31d.
These two python scripts can be used for a square/cubic source. For a circular/spherical/ellipsoidal source, a python script similar to the one in Code 5.3 can be used.

```
1 def val(X, t):
```

```
  # Function code
  # Geometry variables
  x_source = 9.0 # x-position of the center of the source
  y_source = 9.0 # y-position of the center of the source
  z_source = 0.0 # z-position of the center of the source

  lx = 0.4 # x dimension of the refinement region (twice the source)
  ly = 0.4 # y dimension of the refinement region (twice the source)
  lz = 0.2 # z dimension of the refinement region

  xmin = x_source - (lx/2.)
  xmax = x_source + (lx/2.)
  ymin = y_source - (ly/2.)
  ymax = y_source + (ly/2.)
  zmin = z_source - (lz/2.)
  zmax = z_source + (lz/2.)

  # Values of the edge length
  s_domain = 0.01   # L/100, L: windows opening
  s_source = 0.002  # lx/100

  val = [[s_domain,0.0,0.0],[0.0,s_domain,0.0],[0.0,0.0,s_domain]]

  if (X[2] >= zmin) and (X[2] <= zmax):
    if (X[1] >= ymin) and (X[1] <= ymax):
      if (X[0] >= xmin) and (X[0] <= xmax):
        val = [[s_source,0.0,0.0],[0.0,s_source,0.0],[0.0,0.0,s_source
           ]]

  return val #Return value
```

Code 5.1: Python script to prescribed different minimum edge length in different region used in *3dBox_Case9b.fml*.

```
def val(X, t):
  # Function code
  # Geometry variables
  x_source = 9.0 # x-position of the center of the source
  y_source = 9.0 # y-position of the center of the source
  z_source = 0.0 # z-position of the center of the source

  lx = 0.4 # x dimension of the refinement region (twice the source)
  ly = 0.4 # y dimension of the refinement region (twice the source)
  lz = 0.2 # z dimension of the refinement region

  xmin = x_source - (lx/2.)
  xmax = x_source + (lx/2.)
  ymin = y_source - (ly/2.)
  ymax = y_source + (ly/2.)
  zmin = z_source - (lz/2.)
  zmax = z_source + (lz/2.)

```

```
  # Values of the edge length
  b_domain = 2.1   # H/10, H: domain height
  b_source = 0.02  # lx/20

  val = [[b_domain,0.0,0.0],[0.0,b_domain,0.0],[0.0,0.0,b_domain]]

  if (X[2] >= zmin) and (X[2] <= zmax):
    if (X[1] >= ymin) and (X[1] <= ymax):
      if (X[0] >= xmin) and (X[0] <= xmax):
        val = [[b_source,0.0,0.0],[0.0,b_source,0.0],[0.0,0.0,b_source
           ]]

  return val #Return value
```

Code 5.2: Python script to prescribed different maximum edge length in different region used in *3dBox_Case9b.flml*.

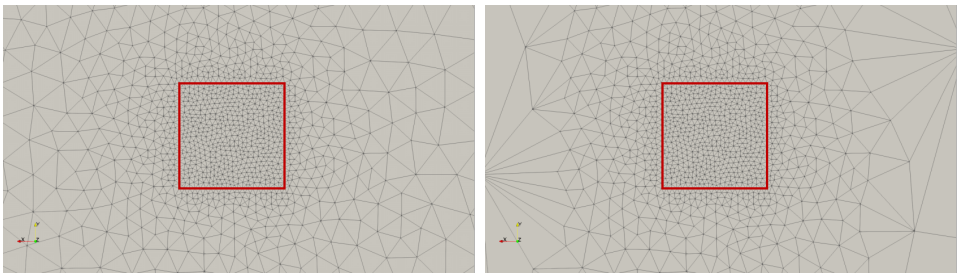
```
def val(X, t):
  # Function code
  # Geometry variables
  x_source = 9.0 # x-position of the center of the source
  y_source = 9.0 # y-position of the center of the source
  z_source = 0.0 # z-position of the center of the source

  dx = 0.4 # x radius of the refinement region (twice the source)
  dy = 0.4 # y radius of the refinement region (twice the source)
  dz = 0.2 # z radius of the refinement region

  # Values of the edge length
  b_domain = 2.1   # H/10, H: domain height
  b_source = 0.02  # lx/20

  val = [[b_domain,0.0,0.0],[0.0,b_domain,0.0],[0.0,0.0,b_domain]]

  if(((X[0]-x_source)**2/dx**2)+((X[1]-y_source)**2/dy**2)+((X[2]-
     z_source)**2/dz**2)<=1.0):
        val = [[b_source,0.0,0.0],[0.0,b_source,0.0],[0.0,0.0,b_source
           ]]

  return val #Return value
```

Code 5.3: Python script to prescribed different edge length in different region in the case of an ellipsoidal source.

These examples can be run using the commands:

```
user@mypc:~$ <<FluiditySourcePath>>/bin/fluidity -l -v3 3dBox_Case9a.flml &
user@mypc:~$ <<FluiditySourcePath>>/bin/fluidity -l -v3 3dBox_Case9b.flml &
```

Go to Chapter 10 to learn how to visualise the results using **ParaView**.



(a) Initial mesh from *Box.msh* **(b)** Mesh after the 1st adaptation

Figure 5.32: Meshes at the source location fro example *3dBox_Case9c.flml*. (a) Initial mesh generated by **GMSH** from file *Box.geo*. (b) Mesh obtained after the first adaptation using mesh adaptivity in **Fluidity**. The red squares depict the location of the source.

5.4.2 Locking nodes

Set-up of example *3dBox_Case9c.flml* is the same than example *3dBox_Case9a.flml*. In example *3dBox_Case9c.flml*, the *Box.geo* and by consequence *Box.msh* files were modified to initially assign an higher resolution near the source as shown in Figure 5.32a. In the mesh adaptivity option, the option `node_locking` (Figure 5.33) is turned on to specify that nodes around the source are locked using Code 5.4. This option prevent the mesh to be adapted where specified and thus allow to ensure that the desire resolution in specific regions are kept. Once the simulation is running, it can be observed that the mesh is preserved at the source location after the adaptation process (Figure 5.32b). However, this option can sometimes lead to weird meshes.
This example can be run using the command:

```
user@mypc:~$ <<FluiditySourcePath>>/bin/fluidity -l -v3 3dBox_Case9c.flml &
```

Go to Chapter 10 to learn how to visualise the results using **ParaView**.

```python
def val(X, t):
    # Function code
    zmax = 0.01
    xmin = 8.9
    xmax = 9.1
    ymin = 8.9
    ymax = 9.1
    tol  = 0.2

    val = 0
    if X[2] < zmax:
        if (X[1] > (ymin-tol)) and (X[1] < (ymax+tol)):
            if (X[0] > (xmin-tol)) and (X[0] < (xmax+tol)):
                val = 1

    return val # Return value
```

Code 5.4: Python script to lock nodes and prevent mesh adaptation near the source.

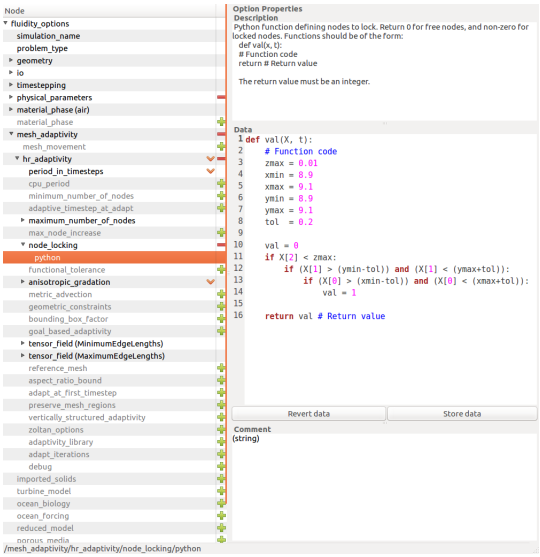


Figure 5.33: Options to lock nodes and prevent mesh adaptation in specific region in **Diamond**.

5.5 Advection of the mesh

Metric advection is a technique that uses the current flow velocity to advect the metric forward in time over the period until the next mesh adapt. With metric advection, mesh resolution is pushed ahead of the flow such that, between mesh adapts, the dynamics of interest are less likely to propagate out of the region of higher resolution. This leads to a larger area that requires refinement and, therefore, an increase in the number of nodes. However, metric advection can allow the frequency of adapt to be reduced whilst maintaining a good representation of the dynamics.

The options for metric advection can be found under the `mesh_adaptivity` options as shown in Figure 5.34. The advection equation is discretised with a control volume method. For spatial discretisation, a first order upwind scheme and non-conservative (`conservative_advection`=0) form are generally recommended. For temporal discretisation a semi-implicit discretisation in time is recommended, i.e `theta`=0.5. The time step is controlled by the choice of CFL number under the option `temporal_discretisation/maximum_courant_number_per_subcycle` and the value set should be the same as the one specified under the option `timestepping /adaptive_timestep/requested_cfl`.

The case *3dBox_Case10.fml* is similar to the case *3dBox_Case6c.fml* with the mesh advection turned on. Difference between the meshes generated at different times for both cases is shown in Figure 5.35 and Figure 5.36. Figure 5.35 shows the meshes and the temperature field just after the second adaptation and just before the third adaptation. The region where the mesh is refined in Figure 5.35a is clearly much smaller than in Figure 5.35b. Therefore, just before the next adaptation, the temperature starts to propagate out of the region with higher resolution when mesh advection is not used,

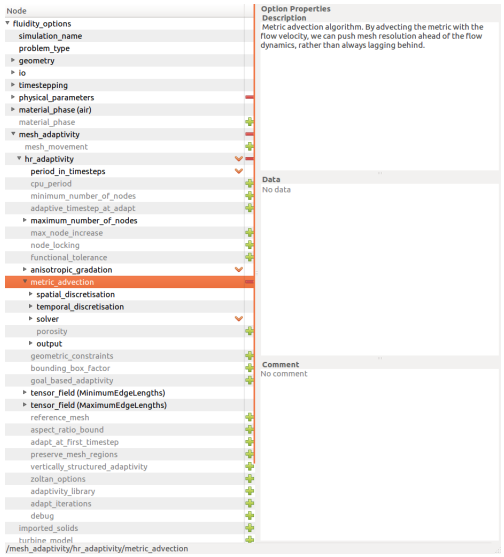
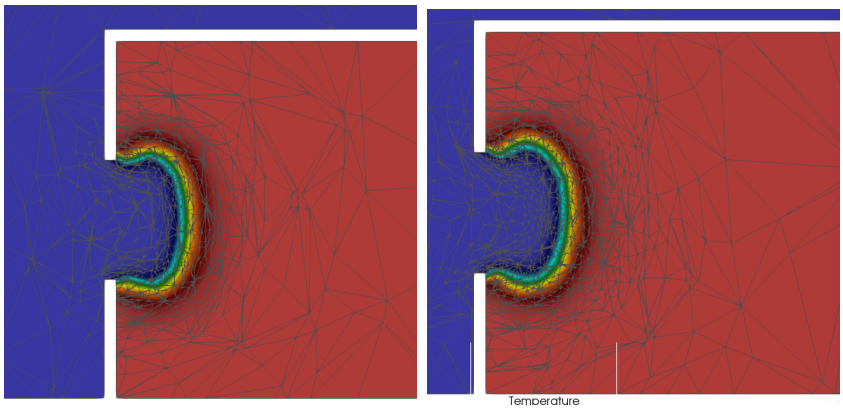


Figure 5.34: Options to advect the mesh in **Diamond**.

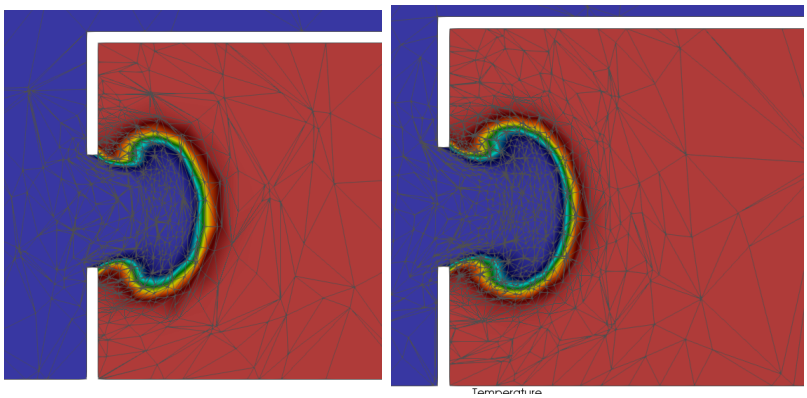
as shown in Figure 5.35c. However, the temperature is maintained in the finer region when using the mesh advection option as shown in Figure 5.35d.
Figure 5.36 shows the temperature field at 1 s. As the advection of the mesh allows the field of interest to remain in the fine region, there should be less artificial diffusion due to the presence of coarse mesh elements as shown in Figure 5.36.

5.6 Common errors

All errors are listed in the `fluidity-err.0` file, including those linked to mesh adaptivity. Some might only be warnings and if the simulation is still running they can be safely ignored. However, if something went wrong during the adaptation process, the simulation will automatically crash. This is primarily caused by the user pushing the adaptation parameters too far... Finally, the user should be reminded that it is not recommended to adapt the pressure field.

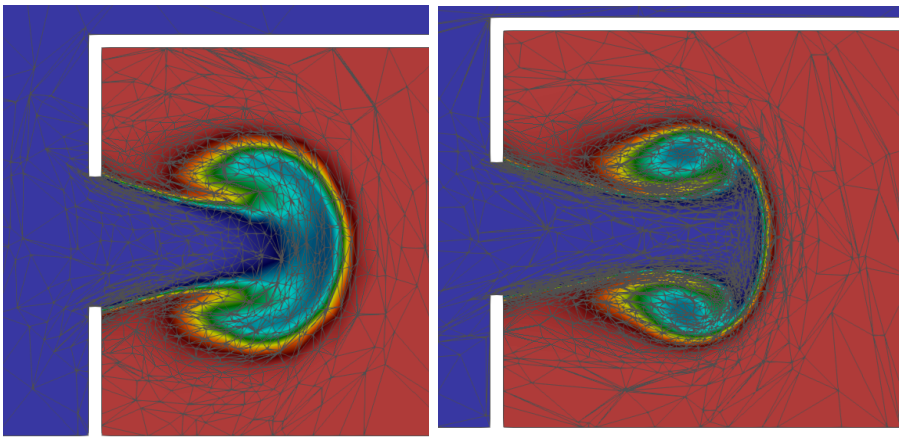


(a) After the 2nd adaptation **(b)** After the 2nd adaptation



(c) Before the 3rd adaptation **(d)** Before 3rd adaptation

Figure 5.35: Temperature field and meshes for (a), (c) *3dBox_Case6c.flml* when the mesh is not advected and (b), (d) *3dBox_Case10.flml* when the mesh is advected.



(a) *3dBox_Case6c.flml* **(b)** *3dBox_Case10.flml*

Figure 5.36: Temperature field and meshes for (a) *3dBox_Case6c.flml* when the mesh is not advected and (b) *3dBox_Case10.flml* when the mesh is advected at $t = 1$ s.

Chapter 6

Other fields

6.1 Case set-up

Example *3dBox_Case11.flml* is based on example *3dBox_Case8.flml*, apart from the following properties that were changed to speed-up the simulation:

- CFL number is now equal to 5.
- Mesh adaptivity options:
  - Temperature: `error_bound_interpolation`=0.2
  - Velocity: `error_bound_interpolation`=0.17
  - The mesh is advected.

The mesh is also refined at the openings of the box, using a python script in the maximum edge length field under the adaptivity option, to be sure that the flow is well-captured (Figure 6.1c).
A number of other fields can be added in **Diamond** and some are described below. Example *3dBox_Case11.flml* contains all the interesting fields discussed in this chapter and that the user might want to use. The fields in *3dBox_Case11.flml* are the following:

- Prognostic fields:
  - Pressure
  - Velocity
  - Temperature
  - Tracer
- Diagnostic fields:
  - Density
  - VelocityAverage: time-average of the velocity

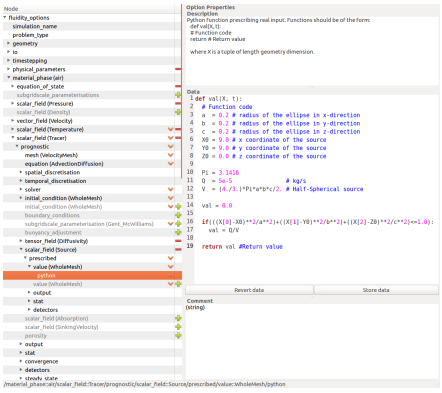
- u: u', fluctuation term of the u-component of the velocity
- v: v', fluctuation term of the v-component of the velocity
- w: w', fluctuation term of the w-component of the velocity
- uu: $u'u'$, squared fluctuation term of the u-component of the velocity
- vv: $v'v'$, squared fluctuation term of the v-component of the velocity
- ww: $w'w'$, squared fluctuation term of the w-component of the velocity
- uuAverage: $\overline{u'u'}$, u-component of the Reynolds stresses (time-average)
- vvAverage: $\overline{v'v'}$, v-component of the Reynolds stresses (time-average)
- wwAverage: $\overline{w'w'}$, w-component of the Reynolds stresses (time-average)
- PressureAverage: time-average of the pressure
- TemperatureAverage: time-average of the temperature
- TracerAverage: time-average of the passive tracer
- CFLNumber: CLF number in the mesh
- EdgeLength: edge length in the domain

6.2 Passive tracer

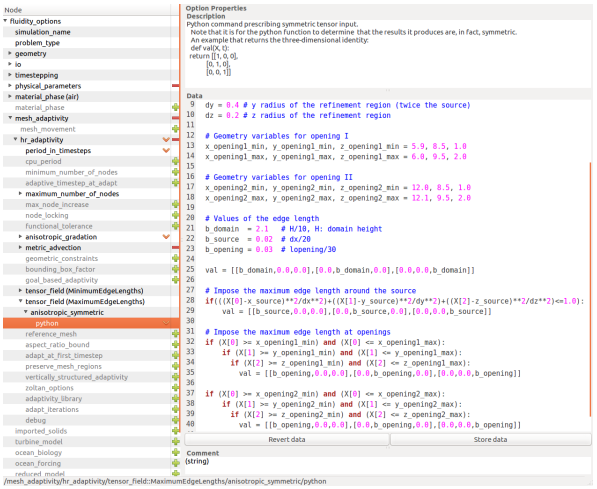
A passive tracer field can notably be added as shown in Figure 6.1. In example *3dBox_Case11.flml*, the passive tracer has a source located in the middle of the box. Let's assume that the passive tracer is NO_2, the diffusion coefficient of NO_2 in air is equal to 1.54×10^{-5} m^2/s. A source, located in the middle of the box, is assumed to release NO_2 with a mass flow rate equal to 5×10^{-5} kg/s. The volume of the source is assumed to be half a sphere with a radius of 0.2 m. Therefore, based on equation 3.6 and equation 3.8, the python script in Code 6.1 is assigned to the source scalar field in the Tracer field. Moreover, the mesh in the vicinity of the source is forced to be refined using python scripts, as previously described.

```
def val(X, t):
  # Function code
  a  = 0.2 # radius of the ellipse in x-direction
  b  = 0.2 # radius of the ellipse in y-direction
  c  = 0.2 # radius of the ellipse in z-direction
  X0 = 9.0 # x coordinate of the source
  Y0 = 9.0 # y coordinate of the source
  Z0 = 0.0 # z coordinate of the source

  Pi = 3.1416
  Q  = 5e-5                  # kg/s
  V  = (4./3.)*Pi*a*b*c/2. # Half-Spherical source

  val = 0.0
```

(a) Tracer field



(b) Source of the tracer



(c) Refinement of the source and openings

Figure 6.1: (a) Addition of a tracer field in **Diamond**. (b) The tracer has a source located in the middle of the box near the ground. (c) The mesh is refinement using a python script to ensure that the source and flow through openings are well-resolved.

```
15
16  if(((X[0]-X0)**2/a**2)+((X[1]-Y0)**2/b**2)+((X[2]-Z0)**2/c**2)<=1.0)
        :
17      val = Q/V
18
19  return val #Return value
```

Code 6.1: Python script to prescribe a source term in the advection-diffusion equation.

6.3 Diagnostic fields in Diamond

Some interesting diagnostic fields can also be added in **Diamond**. Diagnostic fields are calculated from other fields without solving a partial differential equation. Note that scalar, vector and tensor diagnostic field can be added, but only the interesting scalar and vector ones are discussed here.

6.3.1 Density field

The density field is automatically available in **Diamond** like the Pressure and the Velocity ones, except it is turned off by default. The user can turn on this field if wanted.

6.3.2 Diagnostic fields

See Chapter 9 of **Fluidity** manual [1] for more details.
As shown in Figure 6.2, already implemented diagnostic fields can be found in several locations in **Diamond**:

- **Internal diagnostic fields:** Directly under the scalar or vector fields: when the user wants to add a new scalar or vector field, it is possible to directly choose already implemented fields from a drop down list (see Figure 6.2a and Figure 6.2b).
- **Diagnostic algorithms:** Add a new scalar or vector field, then open the option tree and choose `diagnostic` instead of `prognostic`. Under the `diagnostic` option, the user will see the `algorithm`, set by default to `internal`. Here, the algorithm can be changed into another using the drop down list as shown in Figure 6.2c and Figure 6.2d.

Internal diagnostic fields

The scalar field to output the CFL number is for example already implemented as a scalar field as shown in 6.2a. In the same list, the user can notice that it is also possible to output the grid Reynolds number and the grid Peclet number.

Diagnostic algorithms

Once a new scalar or vector filed is added and `diagnostic` is chosen, the user can notice other interesting diagnostic fields (Figure 6.2c and Figure 6.2d) such as:

- `time_averaged_scalar`: calculates the time-average of a scalar field over the duration of a simulation. A spin-up time can be added: the average will start after the set-up value (value in second).
- `time_averaged_vector`: calculates the time-average of a vector field over the duration of a simulation. A spin-up time can be added: the average will start after the set-up value (value in second).
- `scalar_edge_lengths`: outputs the edge lengths of the mesh.
- `scalar_python_diagnostic`: allows direct access to the internal **Fluidity** data structures in the computation of a scalar diagnostic field.
- `vector_python_diagnostic`: allows direct access to the internal **Fluidity** data structures in the computation of a vector diagnostic field.

Some diagnostic algorithms need a source field attribute defining the field used to compute the diagnostic (for example the field used to compute the time-average). The name of the field as to be set appropriately, see Figure 6.3a for example.
By selecting the `scalar_python_diagnostics` or `vector_python_diagnostic` options, a python script can be used to calculate a new field from existing fields. Under the option `depends`, the user can specify dependencies manually. Any field specified here will be calculated before the python diagnostic field. An example is shown in Figure 6.3b where the instantaneous $u'u'$ component is calculated directly from the velocity field and its time-average. The python code to compute the instantaneous value $u'u'$ is shown in Code 6.2. Then, applying the `time_averaged_scalar` to this field will give the $\overline{u'u'}$-component of the Reynolds stresses.

```
uvw   = state.vector_fields["Velocity"]
uvw_m = state.vector_fields["VelocityAverage"]

for i in range(field.node_count):
    uu = (uvw.node_val(i)[0] - uvw_m.node_val(i)[0]) * (uvw.node_val(i
        )[0] - uvw_m.node_val(i)[0])
    field.set(i, uu)
```

Code 6.2: Python script to compute $u'u'$ from the velocity and the time-averaged velocity fields.

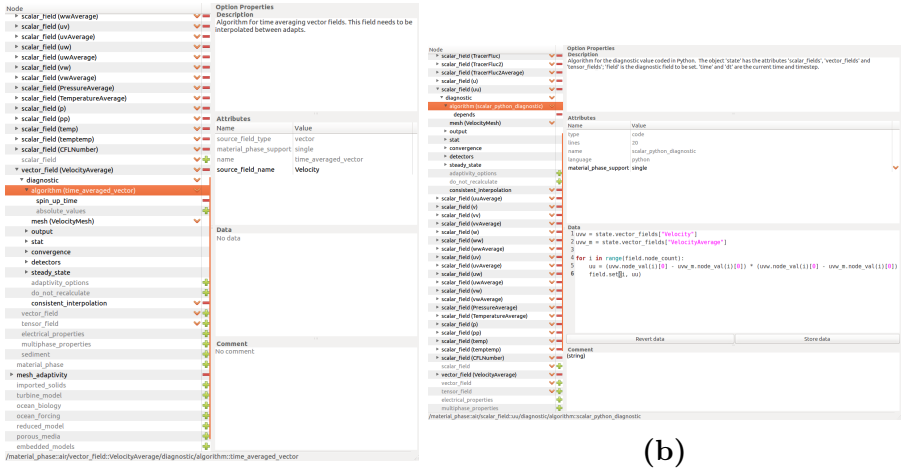
6.3.3 Note about the time-averaged field

Note that there is currently a bug in **Fluidity** concerning the time-averaged field: when a simulation is run from a checkpoint the value of the previous time-average is

(a) Scalar field **(b)** Vector field

(c) Algorithm scalar field **(d)** Algorithm vector field

Figure 6.2: All the different diagnostic fields available in **Diamond** for the scalar and the vector fields.



(a) **(b)**

Figure 6.3: (a) Time-average of the Velocity field using an internal diagnostic algorithm in **Diamond**. (b) Use of a python script to compute $u'u'$.

not properly read from the checkpointed files implying that the average is not correct. This will later be fixed but for now it is recommended to the user to specify a spin-up time higher than the checkpoint time to start a new time-average. See Section 8.7 for more details about checkpointing.

Chapter 7

Details of options

A number of options for the simulation are available to be set up in **Diamond**. Some are detailed here and most are described in the manual too [1]. For simplicity a screen shot of the drop down menu found in **Diamond** is shown in Figure 7.1. The name of the simulation is inputted in `simulation_name` and the problem type is defined as `fluids` for the cases considered here.

7.1 Geometry

The first part of the options defines the geometry used for the simulations as shown in Figure 7.2. The file used for the mesh needs to be inputted in `mesh (CoordinateMesh) /from_file`.

7.2 Input-Output

The options for the inputs and outputs are defined in the `io` menu shown in Figure 7.3. In these options, `dump_period_in_timesteps` defines how often **ParaView** files (**.vtu*) should be outputted. This can be defined as a function of time (in second) or time steps.
The checkpointing options are also defined in this section. They will determine how often checkpoints are made. Checkpoints will become useful if a simulation needs to be restarted from a particular point in time. See Section 8.7 for more details.

7.3 Time stepping

The options for time stepping are then defined in the `timestepping` menu shown in Figure 7.4. They comprise the initial, current and final time of the simulation as well as the time step requested, and are all defined in seconds. In the case of an adaptive time step, this is the initial time step. The adaptive time step can be turned on by

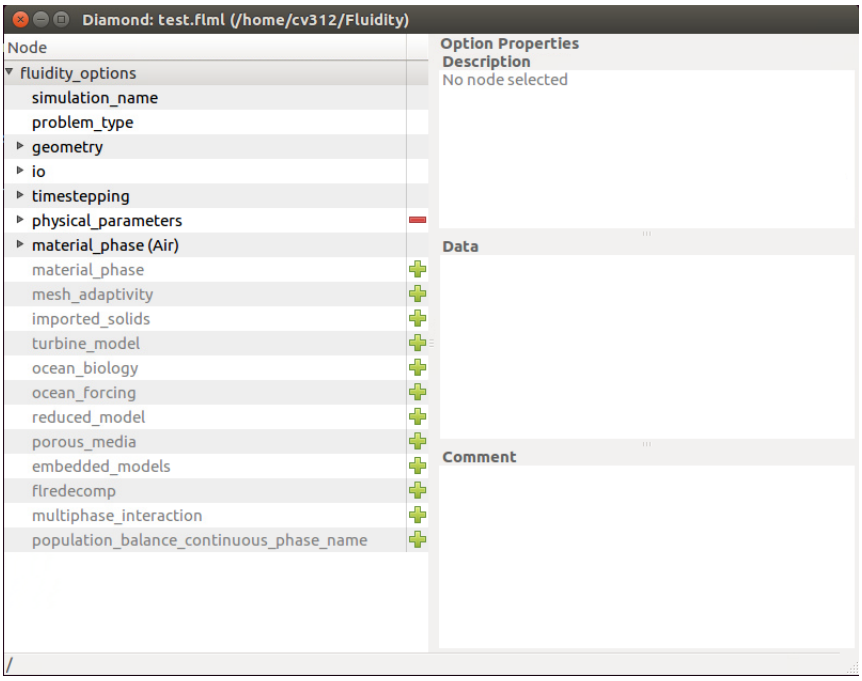


Figure 7.1: Drop down menu of the options available in **Diamond**.

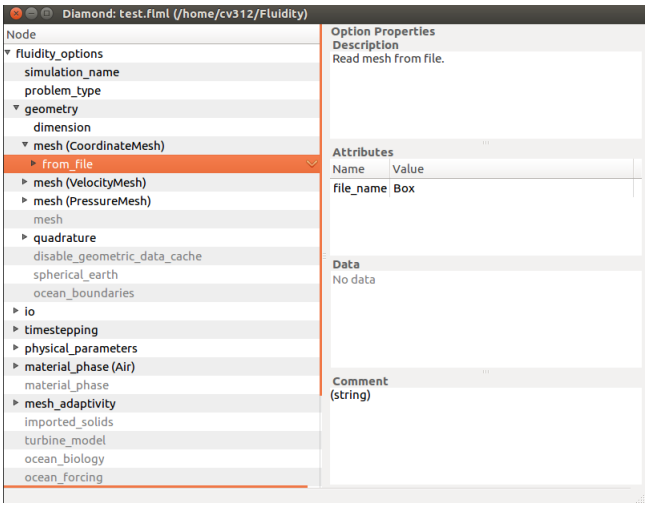


Figure 7.2: Geometry options in **Diamond**.

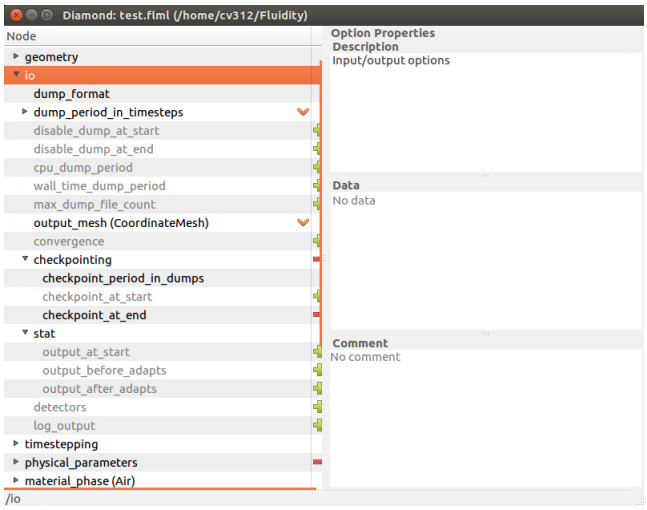


Figure 7.3: Input-output options in **Diamond**.

selecting the option and choosing a CFL number under requested CFL. The non-linear iteration parameter has to be set equal to 2.

7.4 Physical parameters

The magnitude and direction of gravity is defined in the drop down menu of the physical parameters shown in Figure 7.5. It is valuable to check whether the value of gravity corresponds to the coordinate system used. For example, the magnitude is usually set to 9.81 (if you are not on Mars) and the `GravityDirection` to $(0, 0, -1)$ if the z-axis corresponds to the height pointing upwards.

7.5 Material phase

All the fields used for a given fluid are defined in `material_phase/`, this include their initial and boundary conditions. In a case where different materials are used multiple `material_phase/` sections will have to be added. In the cases presented here however, only air is present.

7.5.1 Equation of state

The equation of state options, shown in Figure 7.6, define the dependency between temperature and density. This is also where the reference values for temperature and density are defined. The option `subtract_out_hydrostatic_level` has to be turned on if the Boussinesq approximation is used, which is the case in all the examples presented in this manual.

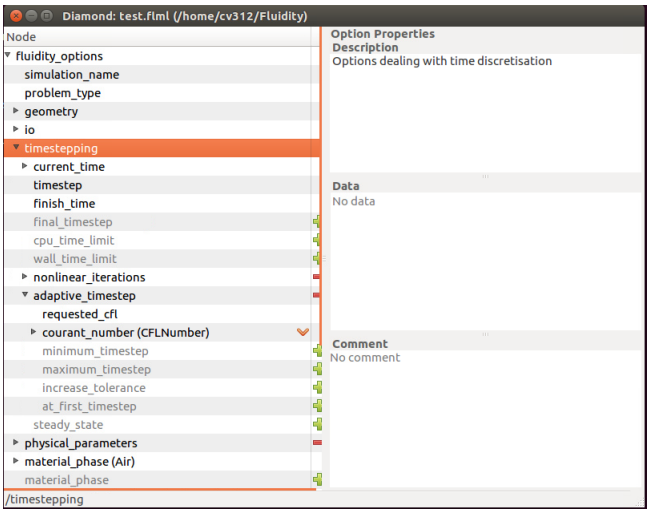


Figure 7.4: Time stepping options in **Diamond**.

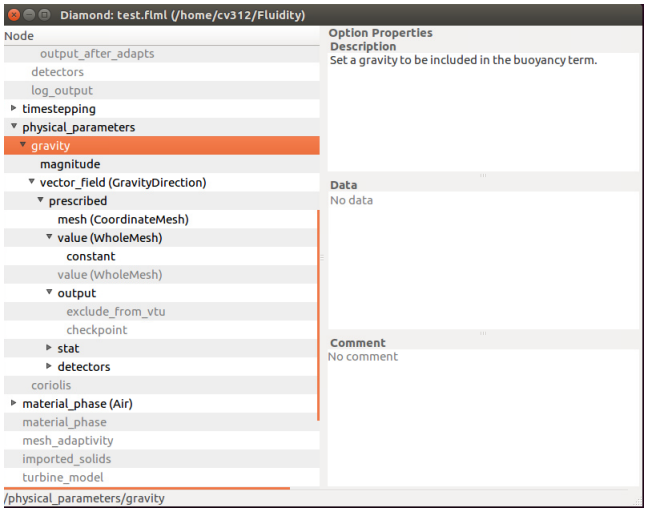


Figure 7.5: Physical parameters options in **Diamond**.

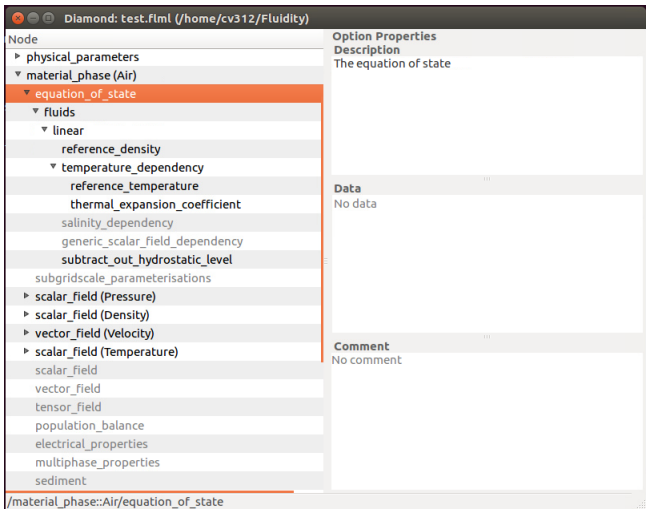


Figure 7.6: Equation of state options in **Diamond**.

7.5.2 Prognostic fields

The prognostic `scalar_field` and `vector_field` are used to define certain fields such as pressure and velocity as shown in Figure 7.7.
This is where boundary and initial conditions are defined as well as how each field is discretised and solved. Output options are also available. Finally `adaptivity_options` will allow to define the interpolation error bound used as a weight during the adaptivity process. The following options are chosen for the main prognostic fields.
For the pressure field:

- Spatial discretisation: `continuous_galerkin`.
- Scheme: `poisson_pressure_solution` with a `use_projection_method`.
- Solver: `iterative_method (cg)` with a `preconditioner (hypre)` and `hypre_type (boomeramg)`. Other options are `relative_error` and `max_iterations` with the suggested values as well as adding the `never_ignore_solver_failures`.

For the velocity field:

- Spatial discretisation: `continuous_galerkin`, including the options
  - `stabilisation/no_stabilisation`
  - `mass_terms/lump_mass_matrix`
  - `stress_terms/tensor_form`
  - `les_model/second_order` (with a Smagorinsky coefficient of 0.1 and a tensor `length_scale_type`)

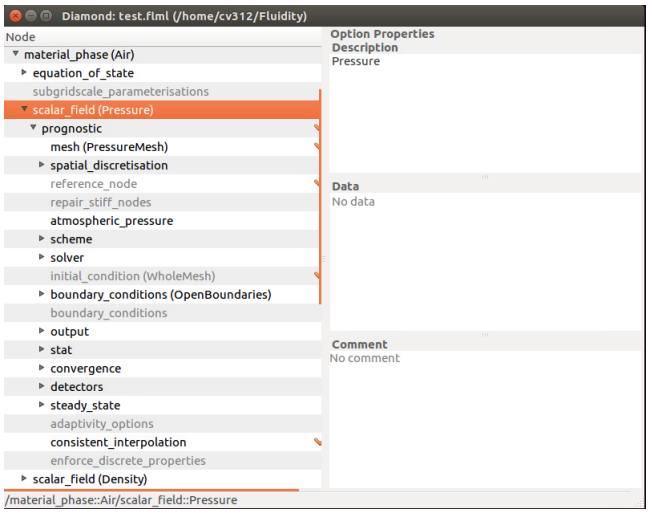


Figure 7.7: Prognostic field options in **Diamond**.

- Temporal discretisation: with a `theta` of 0.5 and `relaxation` of 0.5.
- Solver: `iterative_method(gmres)` and `preconditioner (sor)`. Other options are `relative_error` and `max_iterations` with the suggested values as well as adding the `never_ignore_solver_failures`.

For the temperature field:

- Spatial discretisation: `control_volumes` with a `face_value(FiniteElement)` of `limit_face_value` specified by a `limiter(Sweby)`. The `diffusion_scheme` is `ElementGradient` and the `conservative_advection` is set to 0.
- Temporal discretisation: `theta` is 0.5. The `control_volumes` option is selected with a `number_advection_iterations` set to 2.
- Solver: `iterative_method(gmres)` and `preconditioner (sor)`. Other options are `relative_error` and `max_iterations` with the suggested values as well as adding the `never_ignore_solver_failures`.

7.5.3 Diagnostic fields

The `material_phase` section also includes the calculated diagnostic fields as shown in Figure 7.8. See Section 6.3 for more details.

7.6 Mesh adaptivity

This section defines the adaptivity process and how it will be conducted. The available options are shown in Figure 7.9 for the chosen `hr_adaptivity` algorithm.

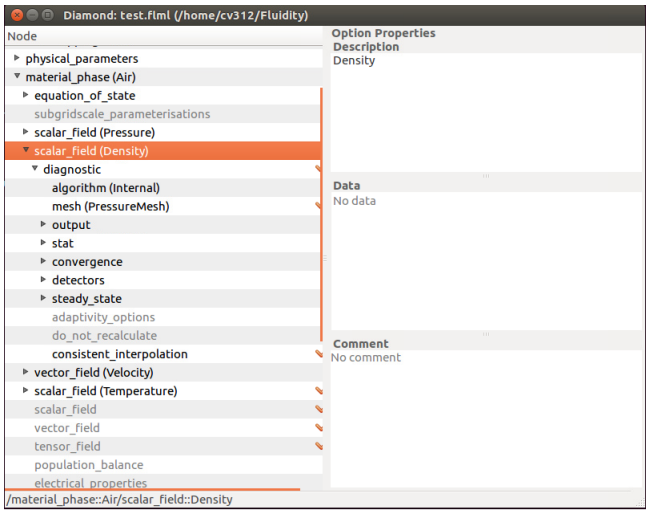


Figure 7.8: Diagnostic field options in **Diamond**.

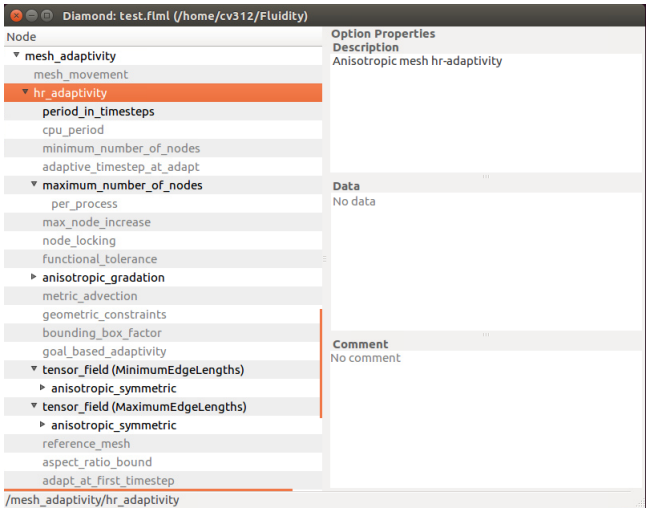


Figure 7.9: Mesh adaptivity options in **Diamond**.

In particular, `period_in_timesteps` allows to define how often adaptivity is to happen, `anistropic_gradation` how the mesh should be smoothed out, while `maximum_number_of_nodes` sets an upper bound on the number of nodes the mesh can be decomposed into. As a rule of thumb it is recommended to use at least 50,000 nodes per processor. Finally, the minimum and maximum edge lengths can also be defined in this section. In combination with the interpolation error bound they will define how the resolution of the mesh will vary with adaptation. Python scripts can be used to vary the specified lengths over the domain, allowing finer resolutions over areas of interest for instance. More details on the adaptivity process can be found in Chapter 5.

Chapter 8

Tricks

8.1 Size of the domain

8.1.1 Blockage ratio

The size of the computational domain has to be properly chosen and it is recommended for the user to read carefully [7] for a detailed method. The following summarises the principal rule of thumb and basically paraphrases [7]. First, let's define the blockage ratio r as expressed by equation 8.1:

$$r = \frac{A_{build}}{A_{inlet}} \tag{8.1}$$

where A_{build} is the projected area of the building in flow direction and A_{inlet} is the inlet area.
In the case of a single building: $A_{build} = lH$, where l is the width of the building and H its height. In the case of multiple buildings: $A_{build} = d_{area}H_{max}$, where d_{area} is the average diameter of the domain of interest and H_{max} is the height of the tallest building.

8.1.2 Height of the domain

To prevent artificial acceleration of the flow over the building, the height of the domain has to be chosen as follows.

- For a single building: the top of the computational domain should be at least $5H$ above the roof of the building. To eliminate errors due to the size of the computational domain, the blockage ratio is recommended to be lower than 3% in CFD simulations.
- For urban environment with more than one building: the top of the computational domain should be at least $5H_{max}$ above the tallest building.

Based on the blockage ratio, smaller and larger values can be used: $4H$ is sufficient for a small blockage, while $10H$ is recommended for a large blockage.
If the simulations are to be compared with wind tunnel experiments, it is recommended to use the wind tunnel's test section geometry for the computational domain. However, if the height of the wind tunnel is much larger than $6H_{max}$, then a lower height of the computational domain can be tested.

8.1.3 Width of the domain

Once the height of the domain is defined, the width of the domain can be determined using the blockage ratio formula.

- For a single building: assuming a domain height of $6H$ the requirement of 3% blockage leads to a distance of $2.3H$ between the building's side and the lateral boundaries of the computational domain. The published recommendations for this distance are however much larger and using $5H$, leading to a blockage of only 1.5%, is recommended.
- For urban environment with more than one building: the lateral boundaries of the computational domain can be placed closer than $5H_{max}$ from the built area.

If the simulations are to be compared with wind tunnel experiments, it is recommended to use the wind tunnel's test section geometry for the computational domain. However, if the lateral walls of the wind tunnel from the built area is much larger than $5H_{max}$, then a smaller width of the computational domain can be tested.

8.1.4 Length of the domain

The length of the domain has to be divided into two regions:

- The upstream region:
  - For a single building: a distance of $5H$ between the inflow boundary and the building is recommended.
  - For urban areas: a distance of $5H$ between the inflow boundary and the building is recommended.
- The downstream region:
  - For a single building: a distance of again $15H$ behind the building is recommended.
  - For urban areas: a smaller distance between the outflow boundary and the built area can be used.

Large values are recommended for the downstream region to avoid flow entering the domain through the outflow boundary. Indeed, this situation should be avoided as it can lead to the divergence of the solver and the crash of the simulation. However the recommended value of $15H$ can lead to too big domain that will increase considerably your computational time. Solutions to tackle this issue are discussed in the next Section 8.2.

8.2 Instabilities at the edges of the domain

Running example *3dBox_Case12a.fml* long enough, the user can observe that the simulation starts to behave weirdly around 74 seconds and finally crashes at 87 seconds. The user can test this example easily, it takes only 8 minutes to run until crashing. As shown in Figure 8.1, very high and unrealistic velocity magnitudes appear at the outlet of the domain: this is due to turbulent recirculation at the outlet which causes numerical instabilities until the divergence of the solver. This is a well-known numerical issue which unfortunately occurs often. There are two ways to avoid this issue:

- Extend the length of the domain as far as needed. This should be the first option to consider.
- Add a 'sponge' layer at the end of the domain to artificially dissipate the eddies.

To avoid any unwanted recirculation and/or instabilities occurring at the domain edges, the user can add a so-called 'sponge' layer which will stabilise the turbulent flow and suppress the eddies. When using this solution, it is recommended to the user to be sure that the results in the domain of interest are not affected by the 'sponge' layer, i.e to be sure that the killed turbulence does not have a direct impact and repercussion on the results. The 'sponge' layer is prescribed through a python script and there are two ways to define it:

- **Viscosity layer:** the value of the viscosity is linearly increased at the end of the domain as shown in Figure 8.2a. In the velocity field, the python script in Code 8.1 is used to prescribe the viscosity: the viscosity increases linearly from the typical value for air of 1.511×10^{-5} m^2/s to several orders of magnitude higher. The user can refer to example *3dBox_Case12b.fml*. This example runs properly and no instabilities occur anymore at the outlet as shown in Figure 8.2.

```
def val(X, t):
    # Function code
    # Viscosity values
    nu    = 1.5e-5    # Value of viscosity in the domain
    nuMax = 0.15      # Maximum value of the viscosity

    # Geometry variables
    xMax   = 21.0          # Length of the domain
    Llayer = 2.0           # Length of the layer - in meter
```

```
    xStart = xMax - Llayer # Where to start the sponge layer

    # Viscosity Ramp x-Direction ------ viscosity = a*x+b
    a = (nuMax - nu)/(xMax - xStart) # Slope
    b = nu - a * xStart

    val = nu
    # Assigning an increased value of viscosity near the outlet
    if (X[0] >= xStart):
      val = a * X[0] + b

    return val #Return value
```

Code 8.1: Python script to define an increasing viscosity at the outlet of the domain.

- **Absorption layer:** an absorption term is prescribe at the end of the domain as shown in Figure 8.3a. In the velocity field, the python script in Code 8.2 is used to prescribe an absorption term: the absorption is equal to zero in the domain and increases linearly to 0.25. The latest value will have to be adjusted by the user depending of the case used. The user can refer to example *3dBox_Case12c.fml*. This example runs properly and no instabilities occur anymore at the outlet as shown in Figure 8.3.

```
def val(X, t):
    # Function code
    # Absorption values
    AMin = 0.0  # Value of the absorption in the domain equal to
       zero.
    AMax = 0.25 # Maximum value of absorption

    # Geometry variables
    xMax   = 21.0          # Length of the domain
    Llayer = 2.0           # Length of the layer - in meter
    xStart = xMax - Llayer # Where to start the sponge layer

    # Absorption Ramp x-Direction ------ absorption = a*x+b
    a = (AMax - AMin)/(xMax - xStart) # Slope
    b = AMin - a * xStart

    val = [AMin, 0, 0]
    # Assigning an absorption term near the outlet
    if (X[0] >= xStart):
      val = [a * X[0] + b, 0, 0]

    return val #Return value
```

Code 8.2: Python script to define an absorption term at the outlet of the domain.

The difference of what is happening at the outlet of the domain when using a viscosity or an absorption layer can be seen in Figure 8.2 and Figure 8.3, and the authors leave the users to appreciate which one in the more suitable for their application.

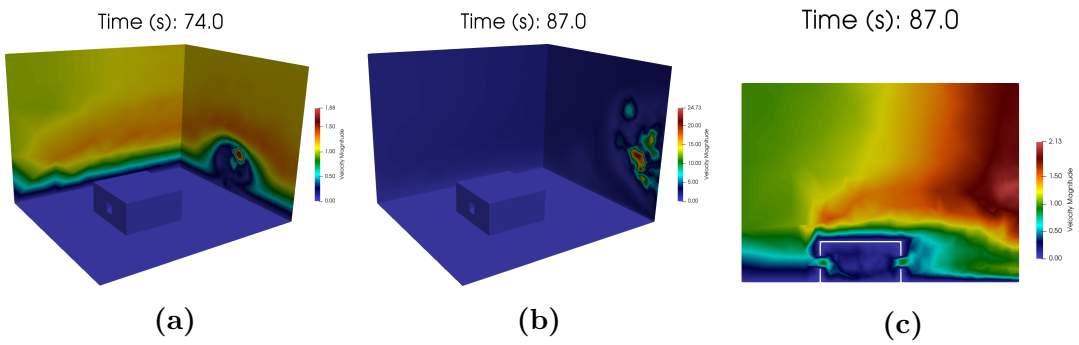


Figure 8.1: In example *3dBox_Case12a.fml*, instabilities occurs at the outlet of the domain. The instabilities are characterised by unrealistic high velocity magnitude at the outlet. Screenshots of the velocity magnitudes at (a) 74 seconds; (b) 87 seconds and (c) 87 seconds on a vertical plane.

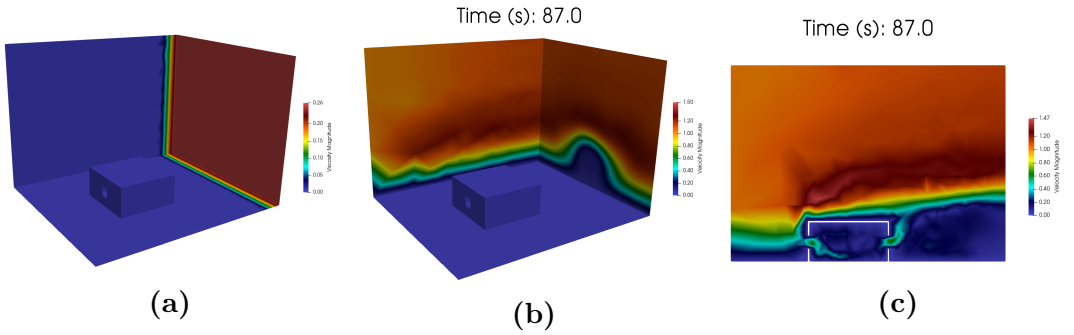


Figure 8.2: In example *3dBox_Case12b.fml* a viscosity layer is added at the outlet of the domain to avoid crash of the simulation. (a) Viscosity layer, (b) Velocity magnitude in the domain and (c) Velocity magnitude on a vertical plane.

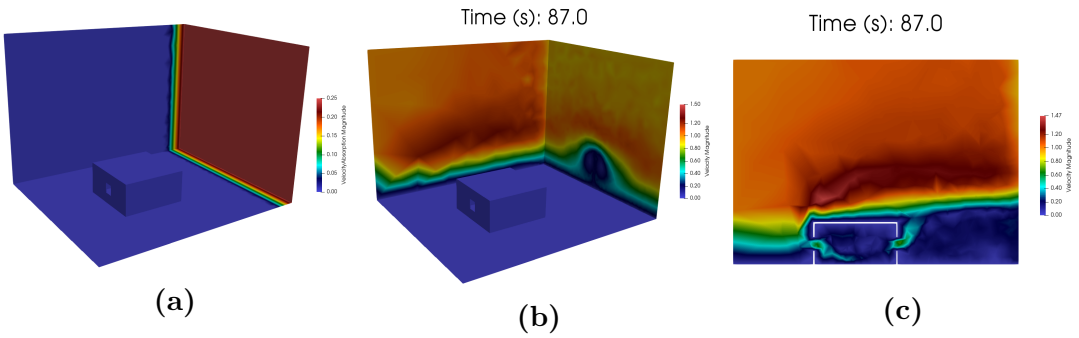
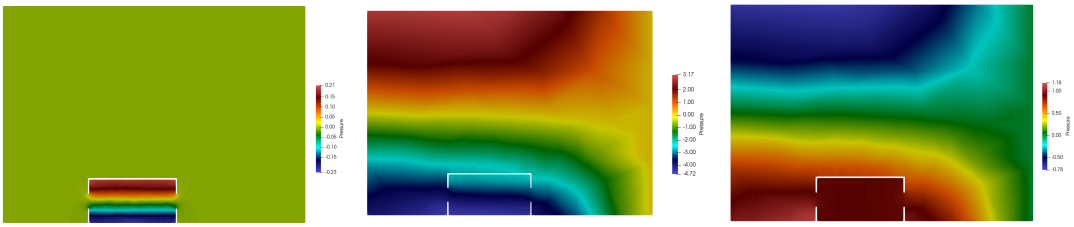


Figure 8.3: In example *3dBox_Case12c.fml* an absorption layer is added at the outlet of the domain to avoid crash of the simulation. (a) Absorption layer, (b) Velocity magnitude in the domain and (c) Velocity magnitude on a vertical plane.



(a) 293 K **(b)** 273 K **(c)** 298 K

Figure 8.4: Pressure field obtained after the first time step for different reference temperature: (a) 293 K, (b) 273 K and (c) 298 K. The ambient and initial temperature is 293 K for the three cases. Results (a) are the one expected. Results (b) and (c) will generate fake recirculation at the outlet.

8.3 Reference temperature

In **Fluidity**, the option `subtract_out_hydrostatic_level` changes the buoyancy term. For the Boussinesq case, it changes to $g\rho' = g(\rho - \rho_0)/\rho_0$ and this option should always be used. Note that, using Boussinesq, the reference density does not influence any of the terms in the momentum equation. It may however influence the outcome of diagnostic fields depending on density. The **reference temperature**, used in the equation of state, needs to correspond to the **ambient temperature**. This will avoid unwanted re-circulation near the boundary where the pressure is defined, i.e. at the outlet boundary of the domain in the case presented here. Effect on the pressure field of not using the proper reference temperature is shown in Figure 8.4.

8.4 Walls boundary condition

See Section 4.5.3 for more details.
The velocity boundary conditions on solid surfaces can be applied either weakly or strongly and can represent a slip or a no-slip behaviour.

- It is to be noted that when boundary conditions are applying weakly, the discrete solution will not satisfy the boundary condition exactly. Instead the solution will converge to the correct boundary condition along with the solution in the interior as the mesh is refined. An alternative way of implementing boundary conditions, so called strongly imposed boundary conditions. Although this guarantees that the Dirichlet boundary condition will be satisfied exactly, it does not at all mean that the discrete solution converges to the exact continuous solution more quickly than it would with weakly imposed boundary conditions. Strongly imposed boundary conditions may sometimes be necessary if the boundary condition needs to be imposed strictly for physical reasons. Unlike the strong form of the Dirichlet conditions, weak Dirichlet conditions do not force the solution on the boundary to be point-wise equal to the boundary condition. If boundary

conditions are applied weakly, then the following options need to be turned on in **Diamond**:

  - Under Pressure field: `spatial_discretisation/continuous_galerkin/integrate_continuity_by_parts`
  - Under Velocity field: `spatial_discretisation/continuous_galerkin/advection_terms/integrate_advection_by_parts`

- A no-slip boundary condition is defined by the three components of the velocity being equal to zero, while a slip boundary condition corresponds to the normal component of the velocity only being equal to zero. Both are Dirichlet type.

There are two options available to apply a Dirichlet boundary condition in **Fluidity**:

- `align_bc_with_cartesian`: the three components of the velocity are assigned - Always work.
- `align_bc_with_surface`: the normal and the two tangential components of the velocity are assigned - Does not always work.

The option `align_bc_with_surface` in the Dirichlet type boundary condition is not well-implemented in **Fluidity** and not always work properly.

In summary:

- The option `align_bc_with_cartesian` should always be preferred if possible.
- Only one no-slip Dirichlet `align_bc_with_surface` applied strongly is allowed, while several can be used when applied weakly.
- For a slip boundary condition weakly applied, `align_bc_with_cartesian` type for simple geometry or `no_normal_flow` type for any geometry should be used. The Dirichlet `align_bc_with_surface` type does not work.
- A slip boundary condition is recommended instead of a no-slip one if the boundary layer is not going to be fully resolved with the chosen mesh, to avoid weird behaviour of the temperature field.

8.5 Consistent interpolation

This section is almost a copy-paste of the **Fluidity** manual [1], section 7.6 and the user can refer to it for more details. Unless you are running a simulation with discontinuous Galerkin fields, the option `consistent_interpolation` needs to be enabled in any prognostic and diagnostic field. Indeed, the application of adaptive re-meshing divides naturally into three sub-problems. The first is to decide what mesh is desired; the second is to actually generate that mesh. The third, discussed here, is how to interpolate any

necessary data from the previous mesh to the adapted one. For the third problem, the `consistent_interpolation` is almost universally used. This standard method consists of evaluating the previous solution at the locations of the nodes in the adapted mesh. The choice should be `consistent_interpolation`, unless any of the following conditions hold:

- The simulation has a discontinuous prognostic field which must be interpolated.
- Conservation of some field is crucial for the dynamics.

In such cases, `galerkin_projection` should be applied.

8.6 Comparing files

Files, like **.flml* files, can be compared using the Command 8.1:

```
user@mypc:~$ meld file1 file2
```

Command 8.1: Use of `meld` to compare two files.

`meld` is not a **Fluidity** tool and needs to be installed if not already using the command:

```
user@mypc:~$ sudo apt-get install meld
```

Command 8.2: `meld` installation.

8.7 Checkpointing

When running a **Fluidity** simulation, checkpoint files are outputted every n period, where n is specified by the user under `io_checkpointing` (see Figure 7.3). Checkpoints are useful if a simulation needs to be restarted from a particular point in time.
The files needed to checkpoint at a certain time step (`index`) are the following:

- The *flml* checkpoint file: `name_index_checkpoint.flml`
- The `CoordinateMesh` *msh* file: `name_CoordinateMesh_index_checkpoint.msh`
- The `PressureMesh` *vtu* file: `name_PressureMesh_index_checkpoint.vtu`
- The `VelocityMesh` *vtu* file: `name_VelocityMesh_index_checkpoint.vtu`

It must be noted that if the simulation is run on parallel on N processors there will be N `CoordinateMesh` *msh* and *halo* files as well as folders with the N `PressureMesh` and `VelocityMesh` *vtu* files on top of the *pvtu* files.
The new simulation will then be running using the command:

```
user@mypc:~$ <<FluiditySourcePath>>/bin/fluidity -l -v3
name_index_checkpoint.flml &
```

It should be repeated that there is currently a bug in **Fluidity** concerning the time-average field: when a simulation is run from a checkpoint the value of the previous time-average is not properly read from the checkpointed files implying that the average is then not correct. This will later be fixed but for now it is recommended to the user to specify a spin-up time higher than the checkpoint time to start a new time-average.

Chapter 9

Fluidity in parallel

9.1 When should Fluidity be run in parallel ?

As a rule of thumb, there should be 50,000 nodes per processor. If the number of nodes per processor is smaller than that, there will be no benefit in switching from serial to parallel, although the simulation should still run in parallel.

9.2 Running on a PC

In order for a simulation to run in parallel, the mesh first needs to be decomposed using `flredecomp` (more information on this tool is found in [1]). A mesh is decomposed (from 1 to 4 parts for example) using Command 9.1. It must be noted that the number of processors used to run the `mpiexec` command needs to be equal to the maximum number of parts in either the original or new mesh. If a mesh was to be recomposed from 4 parts to 1, the Command 9.2 is the one to use. Once the mesh is decomposed the simulation can be run in parallel, on 4 processors for example, using Command 9.3.

```
user@mypc:~$ mpiexec -n 4 <<FluiditySourcePath>>/bin/flredecomp -i 1 -o 4
foo foo_new
```

Command 9.1: Decomposition of the mesh from 1 processor to 4.

```
user@mypc:~$ mpiexec -n 4 <<FluiditySourcePath>>/bin/flredecomp -i 4 -o 1
foo foo_new
```

Command 9.2: Recomposition of the mesh from 4 processors to 1.

```
user@mypc:~$ mpiexec -n 4 <<FluiditySourcePath>>/bin/fluidity -l -v3
foo_new.flml &
```

Command 9.3: Running **Fluidity** in parallel.

Note: The tool `fldecomp` in **Fluidity** is obsolete and the tool `flredecomp` has always to be used.

9.3 Running on CX1

Fluidity can also be run on a computer cluster, and here the example of Imperial cluster CX1 is detailed. More information on CX1 in general is available online, particularly regarding job sizing:

- https://www.imperial.ac.uk/admin-services/ict/self-service/research-support/rcs/computing/high-throughput-computing/
- https://wiki.imperial.ac.uk/display/HPC/MPI+Jobs

The following `singlenode.pbs` script shown in Code 9.1 will run a simulation with the pre-installed **Fluidity** version on the chosen single node queue.

```
#!/bin/sh
# Job name
#PBS -N name
# Time required in hh:mm:ss
#PBS -l walltime=72:00:00
# Ressource requirements
#PBS -l select=1:ncpus=16:mem=30gb
# Files to contain standard error and standard output
#PBS -o stdout
#PBS -e stderr
echo Working Directory is $PBS_O_WORKDIR
cd $PBS_O_WORKDIR
rm -f stdout* stderr*
module load ese-software
module load ese-fluidity

cp -r $PBS_O_WORKDIR/* $EPHEMERAL
cd $EPHEMERAL
pbsexec mpiexec flredecomp -i 1 -o 16 foo foo_decomp
pbsexec mpiexec fluidity foo_decomp.flml -v1 -l
```

Code 9.1: Bash script to run a simulation with a single node on CX1.

Apart from the normal CX1 procedure, it is worth noting the loading of the pre-installed **Fluidity** modules with `module load ese-software` and `module load ese-fluidity`. During and after the simulation, the output can be visualised directly in the `ephemeral` directory. A maximum wall time in the *flml* can also be specified to match the one in the *pbs* file to ensure the simulation will be terminated on a checkpoint.
If a multinode queue is to be used, the mesh needs to be decomposed in the total number of processors used (i.e. for CX1: number of cpus $\times$ number of nodes).

Chapter 10

Post-processing data obtained with Fluidity

10.1 ParaView

Simulation's results can be viewed by loading the *vtu* files into **ParaView**. This software can be downloaded from `https://www.paraview.org/`, where a number of useful information can also be found, such as guides and tutorials. The interface is shown in Figure 10.1 and a number of useful features are described below:

- `Slice`: a type of view that allows the user to view an orthogonal slice of the simulation's results.
- `Glyph`: a type of filter that shows the data at specific points as markers with an orientation and size defined by the input. Typically, this tool is used to display velocity vectors.
- `Probe`: a type of filter that gives the values of the fields at a specific location.
- `Surface with edge`: a type of render that shows the values of a field as well as the mesh used during the simulation.
- `Follow cullback`: is found in `Backface styling` and allows the user to tune the rendering of the front and back faces (with regards to the camera), modifying the visualisation.

It is then recommended to play around with all **ParaView** features to become familiar with them.

10.2 Python scripts

The results can also be visualised and analysed using python scripts. The main python library used is the library **vtk**. In addition, the *vtktools.py* and *vtutools.py* python

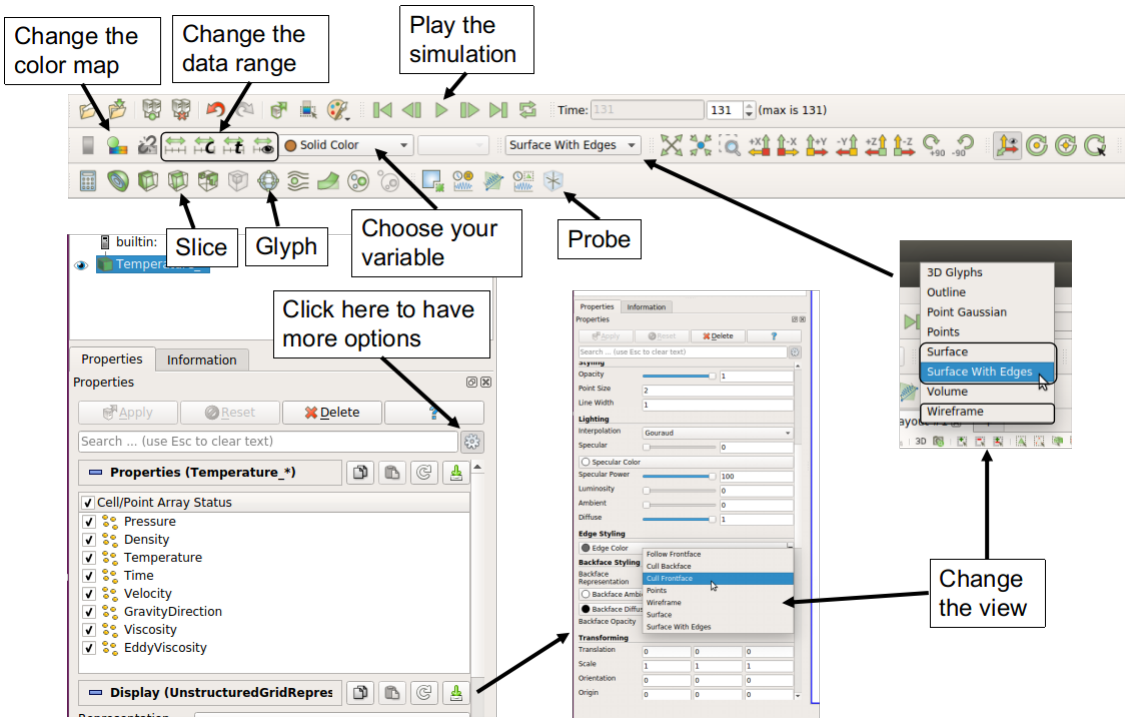


Figure 10.1: Options in **ParaView**.

modules can also be used and imported in every script. *vtktools.py* and *vtutools.py* can be found in `<<FluiditySourcePath>>` under `/python/` and `/python/fluidity/diagnostics/`, respectively. Both are including in the materials attached to this manual. Both scripts are really useful to work, manipulate and post-process **.vtu* or **.pvtu* data. Lots of example of python script using the **vtk** library can also be found online:

- https://www.vtk.org/doc/nightly/html/pages.html: the sections Class to Examples and Class to Tests are plenty of python and C++ script examples.
- https://lorensen.github.io/VTKExamples/site/Python/ is also full of script using vtk functions.

Documentations for **vtk** can also be found online:

- version 5.10 https://www.vtk.org/doc/release/5.10/html/index.html
- version 7.1 https://www.vtk.org/doc/release/7.1/html/

To take advantage of all the new **vtk** features, it is recommended to download one of the latest release available online: https://www.vtk.org/ and install it following https://www.vtk.org/Wiki/VTK/Configure_and_Build. During the installation, in the **Cmake** interface, use the 'advanced mode' (`t` keyboard) and make sure that `VTK WRAP PYTHON` is set to `ON`. Note that installing the **vtk** library is not trivial and a number of errors can occur. Please ask the help of an advanced user if needed. Once

the latest version is installed, the user should use the executable `vtkpython` located under `<<vtkPath>>/bin/`. Note that they are lots of major change between versions 5 and 6 of **vtk**. Please refer to the following for more details:

- https://www.vtk.org/Wiki/VTK/VTK_6_Migration_Guide
- https://www.vtk.org/Wiki/VTK/VTK_6_Migration/Overview

Note: the probe tool provided in the *vtktools.py* can behave weirdly when trying to probe data near/on solid walls due to inconsistent behaviour of the **vtk** library. This weird behaviour might also differ depending the version of **vtk** you are using. Have a look of the function in *vtktools.py* to know why and/or ask an advanced user to explain what is happening...
The library **matplotlib** is the one recommended to plot data. Following are two examples of python scripts using the module *vtktools.py*, the library **vtk** and that are inspired by some functions in *vtutools.py*. The following examples of python script will show how to:

- Compute the mass flow rate at openings: *MassFlowRate.py*
- Compute the radius of a thermal plume: *PlumeRadius.py*

10.3 Mass flow rate at the openings

10.3.1 Test case

The script *MassFlowRate.py* is located in `Scripts/MassFlowRate/`. The following results and discussions are based on data obtained with example *3dBox_Case11.ffml*.

10.3.2 Generality and method

Equation

The mass flow rate $\dot{m}$ (kg/s) through an opening is defined by equation 10.1:

$$\dot{m} = \rho v S \tag{10.1}$$

where ρ is the density of the fluid, v is the magnitude of the normal component of the velocity (normal to the surface considered) and S is the surface of the opening.

Method

When calculating the mass flow rate at openings, to compensate the possible lack of mesh resolution, it is recommended to do an average over several planes through the opening's thickness or (what we think to be less accurate) to compute the mass flow rate over a plane located at the middle of the opening's thickness, i.e thickness/2. In the

script *MassFlowRate.py* provided the first option is chosen. A Cartesian grid is defined through the opening, data are extracted for each points of this grid, then averaged to obtain the final mass flow rate through that particular plane. This procedure is repeated for several planes along the thickness of the opening. Finally, the final mass flow rate is computed averaging mass flow rates obtained for each planes.

Input variables

The user input variables are the followings:

- `path_simu` is the path where the simulation is located.
- `basename` is the name of the simulation.
- `vtu_start`, `vtu_end` and `vtu_step` are respectively the first *vtu* file, the last *vtu* file and the step between those *vtu* files that the user want to consider. This allows the user to have the evolution of the mass flow rate as a function of the time.
- `ni_start`, `ni_end` and `ni_step`, where `i` stands for the `x`, `y` and `z` direction, define the size of the grids that the user want consider. This allows the user to test different grid resolutions.

10.3.3 Results

The mass flow rate is evaluated at the two openings of the box. `Zone1` refers to the opening on the left, i.e. the one closer to the inlet of the domain where the velocity is prescribed, while `Zone2` refers to the opening on the right, i.e. closer to the outlet of the domain where the pressure is prescribed. In that particular case, the thickness of the openings is towards the x-direction, therefore the x-component of the velocity is used. The Cartesian grids where the data are extracted are aligned with (yOz). Figure 10.2 shows the computed mass flow rate at the inlet and at the outlet of the box as a function of time for a grid resolution $10 \times 10 \times 10$. Playing around with the script, the user will notice that for low grid resolution, the computed mass flow rate at the inlet is not equal to the one at the outlet. Increasing the resolution of the grid, the input and output mass flow rate tends to be more equal to each other, which is expected. Also, increasing the grid resolution tends to converge to the correct mass flow rate but at some point continuing increasing the grid resolution does not improve results. It is also to mention that the computed mass flow rate at the inlet and at the outlet are not strictly equal, due to lack of mesh resolution, and tends to be equal while refining the mesh at the openings.
The results are written in the text file *MassFlowRate.txt* where the 7 columns corresponds to:

1. Resolution used in the $x-$direction

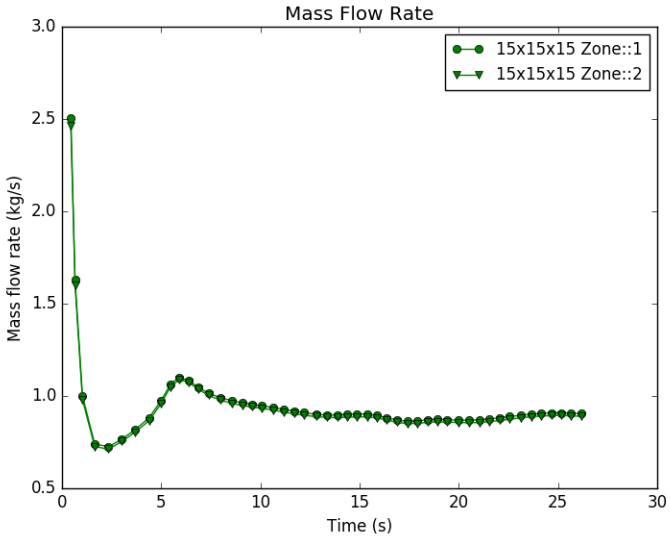


Figure 10.2: Mass flow rate at the inlet, i.e zone 1, and at the outlet, i.e. zone 2, of the box as a function of time and for a grid resolution $10 \times 10 \times 10$.

2. Resolution used in the $y-$direction
3. Resolution used in the $z-$direction
4. Time in seconds
5. Mass flow rate at the inlet of the box in kg/s
6. Mass flow rate at the outlet of the box in kg/s
7. Error in percentage (%) between the inlet and outlet mass flow rates

10.3.4 Numerical implementation

The results described above are implemented in a python script and the main libraries used are the followings:

- **vtk** is used to read the data obtained with **Fluidity** and extract data at specific points (Code 10.1).
- **matplolib** is used to plot the data (Figure 10.2).

```
20 #-----------------------------------------------#
21 #-- Function to probe data at specific locations -#
22 #-----------------------------------------------#
23 def ExtractData(coordinates):
24
```

```
    v    = []
    t    = []
    rho  = []
    r    = 0

    for fileID in range(vtu_start,vtu_end+1,vtu_step):
        filename = path_simu+basename+'_'+str(fileID)+'.vtu'
        print '␣␣␣␣␣␣␣␣File::', basename+'_'+str(fileID)+'.vtu'
        # Read the vtu files
        data = vtktools.vtu(filename)
        v.append([])
        rho.append([])
        for j in range(len(coordinates)):
            coord_temp = vtktools.arr([coordinates[j]])
            v[r].append(data.ProbeData(coord_temp, 'Velocity')[0][0])
                # X component of the velocity
            rho[r].append(data.ProbeData(coord_temp, 'Density')[0][0])

        r = r+1
        t.append(data.ProbeData(coord_temp, 'Time')[0][0])

    return v, t, rho
```

Code 10.1: Function to extract data at specific coordinates using the **vtk** library.

10.4 Plume radius

10.4.1 Test case

The script *PlumeRadius.py* is located in the folder `Scripts/PlumeRadius`. The script can be tested using the file *Case9b_Box_300.vtu* (obtained from *3dBox_Case9b.fml*) located in the same folder. However, in the following, pictures and plots showing results were obtained using another set of more complicated simulations not provided with this manual. Indeed, in the case presented below, the box is in the middle of the big domain with two openings at the bottom, two openings at the top and a heat source at the bottom of the box. Moreover, if the user wants to use that script then the `path` (path of where the data are stored), the `name` (name of the simulation) and the `vtu_start` (the number of the vtu) need to be changed in the script according to the user's requirements. Also note that the data presented below is obtained from instantaneous data. In practice, the user should have included the time average of the velocity (and of any other interesting quantities) in the simulation and those quantities should be used to compute the time average radius of the plume. In that case, the line `Vz=up.GetField('Velocity')[:,2]` should be replaced by `Vz=up.GetField('VelocityAverage')[:,2]`, assuming that `VelocityAverage` is the name of the time average velocity field chosen by the user in **Diamond**.

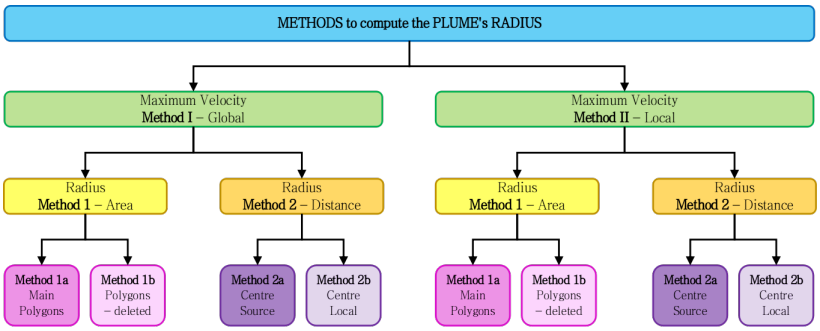


Figure 10.3: Summary of the different methods tested to compute the radius of the plume as a function of the height.

10.4.2 Generality

The radius r of the plume is usually defined by equation 10.2:

$$r = \alpha V_{max} \tag{10.2}$$

where V_{max} is the time-averaged maximum velocity and α is a threshold usually equal to 0.02. In the following, it is assumed that the z-axis is pointing up. Therefore, the maximum velocity is given by the z-component of the velocity, i.e v_z.
The Figure 10.3 summarises the different methods tested to compute the radius of the plume as a function of the height. All these methods are described in detail in the following sections.

10.4.3 Description of the methods

a) Algorithms

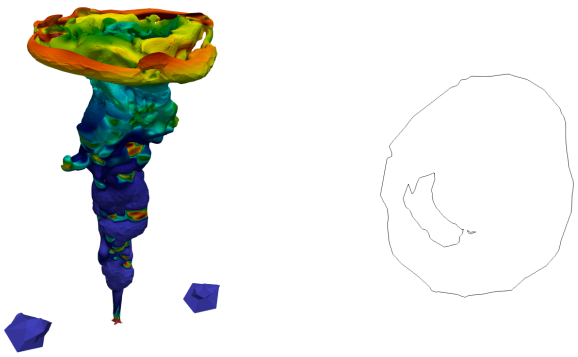
The general idea is to get the geometry of the plume at different height and deduce the radius of the plume based on the geometry. Based on equation 10.2, two methods are tested and described in the following sections:

- Method I: Based on the global maximum velocity: $V_{z,max,global}$
- Method II: Based on the local maximum velocity: $V_{z,max,local}(z)$

Method I based on the global velocity
This method consists of generating a contour based on the global maximum velocity and then creating slice cuts at every height.
Method II based on the local velocity
This method consists of generating slices at every height, then determining the local maximum velocity and finally generating the contour of the plume.
Comparison of the two methods
Figure 10.6 shows the plumes contour at different height generated by Algorithm 1 and Algorithm 2. The red lines are the results obtained for Algorithm 1, while black lines

Algorithm 1 Method I

1: Find $V_{z,max,global}$
2: Extract the 3D contour of value $\alpha V_{z,max,global}$ (Figure 10.4a). This contour is saved in the file *VelocityZ_Contour_Global.vtu*
3: **for** every height z: **do**
4: Do a slice which gives the 2D geometry of the plume at z (Figure 10.4b).
5: Contours are saved in *VelocityZSliceContour_Global_n.vtu* where n is the height index.
6: Get all the polygons which define the plume geometry
7: Clean the geometry
8: Compute the different radii
9: **end for**

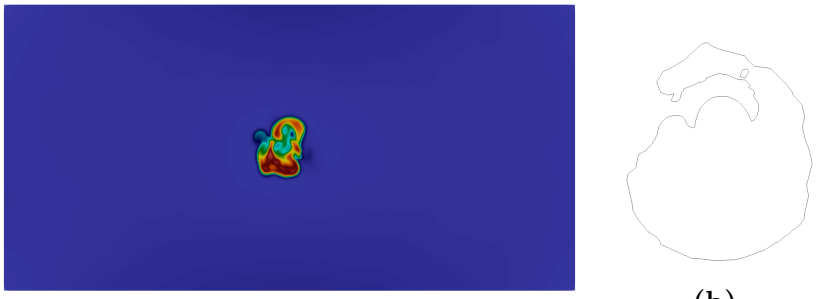


(a) **(b)**

Figure 10.4: (a) 3D contour obtained for the value $\alpha V_{z,max,global}$ (Step 2 of Algorithm 1) and (b) 2D contour obtained at height z (Step 5 of Algorithm 1).

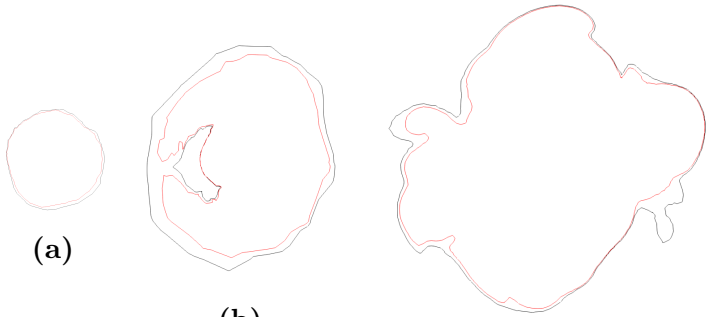
Algorithm 2 Method II

1: **for** every height z: **do**
2: Do a slice at the height z (Figure 10.5a). Slice is saved in *VelocityZSlice_Local_n.vtu* where n is the height index
3: Find $V_{z,max,local}(z)$
4: Extract the 2D contour of value $\alpha V_{z,max,local}(z)$ (Figure 10.5b). This contour is saved in *VelocityZ_ContourSlice_Local_n.vtu* where n is the height index.
5: Get all the polygons which define the plume geometry
6: Clean the geometry
7: Compute the different radii
8: **end for**



(a) (b)

Figure 10.5: (a) 2D slice at height z (Step 2 of Algorithm 2) and (b) 2D contour obtained for the value $\alpha V_{z,max,local}(z)$ (Step 4 of Algorithm 2).



(a) (b) (c)

Figure 10.6: Contour of the plume at different heights generated by Algorithm 1 (red lines) and Algorithm 2 (black lines) before the geometry cleaning.

are the results obtained using Algorithm 2. It can be noted that Algorithm 1 generally predicts a geometry of smaller area than the one found with Algorithm 2 (as also shown in Figure 10.6).

b) Cleaning the geometry - Step 6 of the algorithms

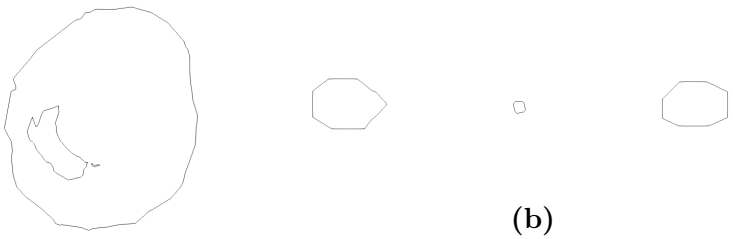
The process of cleaning the geometry is explained below:

- The polygons within the main plume geometry are deleted. In Figure 10.7a, for example, the polygons within the main polygon are not taken into account in the later computation of the radius. However, the area of these polygons is kept (see section 2.3.1 - method 1b to know why and have more details).

- When z is low, the contour obtained shows the influence of the inlets. Figure 10.7b and Figure 10.4a are good examples showing the influence of the inlets: indeed the right and the left polygons do not define the main plume geometry. Therefore, these polygons need to be detected and deleted.

c) Radius of the plume - Step 7 of the algorithms

The computation of the radius is performed based on two different methods described



(b)

(a)

Figure 10.7: (a) Two polygons are within the main polygon defining the plume. These two polygons need to be detected and ignored. (b) Contour of $\alpha V_{z,max}$ at a low height showing that the right and left polygons are the consequence of the inlets. These two polygons do not belong to the plume and need to be detected and ignored.

in the following sections:

- Method 1: the radius is computed based on the area of the polygons.
- Method 2: the radius is computed based on the distance between the center and the exterior boundary of the polygons.

Method 1 based on the area
This method consists of computing the radius r of the plume assuming an ideal circle, such that:

$$r = \sqrt{\frac{\mathcal{A}}{\pi}} \tag{10.3}$$

where $\mathcal{A}$ is the total area of the plume. The aim of this method is to compute $\mathcal{A}$ and then determine the radius of the plume based on equation 10.3. This method is explained based on Figure 10.8 geometry. Figure 10.8 shows the 2D geometry of the plume at a certain height z. The geometry is composed by 3 main polygons (labelled 1, 2 and 3). The polygon 1 has also another polygon (labelled 4) within. Based on the cleaning process described in the previous paragraph, the small polygon 4 is detected. The total area $\mathcal{A}$ is therefore computed in two different ways as follows:

- **Method 1a** - polygon 4 is ignored.

$$\mathcal{A} = \mathcal{A}_1 + \mathcal{A}_2 + \mathcal{A}_3 \tag{10.4}$$

- **Method 1b** - polygon 4 is taken into account and subtracted to the total area.

$$\mathcal{A} = \mathcal{A}_1 + \mathcal{A}_2 + \mathcal{A}_3 - \mathcal{A}_4 \tag{10.5}$$

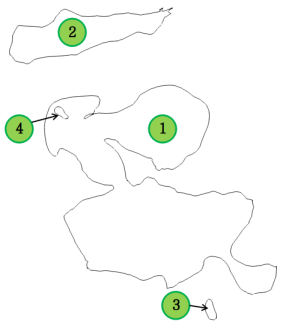


Figure 10.8: 2D geometry of the plume at height z composed of 3 main polygons (labelled 1, 2 and 3). Polygon 1 has another polygon (labelled 4) within.

Method 2 based on the distance

In this section, the radius is computed based on the distance between a centre point of the plume and the nodes defining the exterior boundaries of the polygons (themselves defining the plume geometry) and denoted by pink dots in Figure 10.9. A simple arithmetic mean is performed:

$$r = \frac{\sum d_i}{N} \tag{10.6}$$

where d_i is the distance between the node i and the centre of the plume and N is the total number of nodes defining the polygons.

Now the main question consists of determining the centre of the plume. For this, two approaches are tested:

- **Method 2a:** the centre of the plume is assumed to be the centre of the source.
- **Method 2b:** the centre of the plume is taken locally at each height. For this, the centroid of the polygons defining the plume geometry is used as the local centre.

It has to be noted that this method is somehow not really accurate for the following reason:

- Even if the method is acceptable in the case shown in Figure 10.9a, it is not the case for the case shown in Figure 10.9b. Indeed, the nodes of the small polygon will artificially weigh the mean radius towards the distance between this polygon and the centre of the plume.
- For both case shown in Figure 10.9, it can be observed that certain region has lot of point defining the boundary (it happens where there is sharp change in the geometry) while other regions have less nodes. Once again, the computed radius will be artificially weighted by the region where there are lots of nodes, which is not desirable.

However, comparing this method with the one using the area, the mean radii generated are quite close.

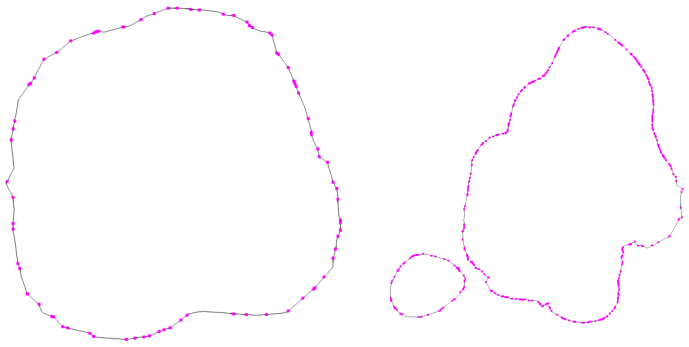


Figure 10.9: 2D geometry of the plume at two different heights. The pink dots show the locations of the nodes defining the boundary of the polygon. (a) Case of a single polygon and (b) case of multiple polygons.

10.4.4 Outputs and plots

Summary of the methods

In summary, these methods give as output:

- **Method I.1.a** r based on the global velocity using the area of the polygons.
- **Method I.1.b** r based on the global velocity using the area of the polygons minus the area of the polygons deleted.
- **Method I.2.a** r based on the global velocity using the distance between the centre of the source and the boundaries of the polygons.
- **Method I.2.b** r based on the global velocity using the distance between the local centre and the boundaries of the polygons.
- **Method II.1.a** r based on the local velocity using the area of the polygons.
- **Method II.1.b** r based on the local velocity using the area of the polygons minus the area of the polygons deleted.
- **Method II.2.a** r based on the local velocity using the distance between the centre of the source and the boundaries of the polygons.
- **Method II.2.b** r based on the local velocity using the distance between the local centre and the boundaries of the polygons.

Text files with data

The data are written in text files and each files are explained below.

- **Radius_Global.txt**
  Radii computed by method I - Global Velocity - 5 columns

  1. The height z in meters
  2. r computed by method I.2.a
  3. r computed by method I.2.b
  4. r computed by method I.1.a
  5. r computed by method I.1.b

- **Radius_Local.txt**
  Radii computed by method II - Local Velocity - 5 columns

  1. The height z in meters
  2. r computed by method II.2.a
  3. r computed by method II.2.b
  4. r computed by method II.1.a
  5. r computed by method II.1.b

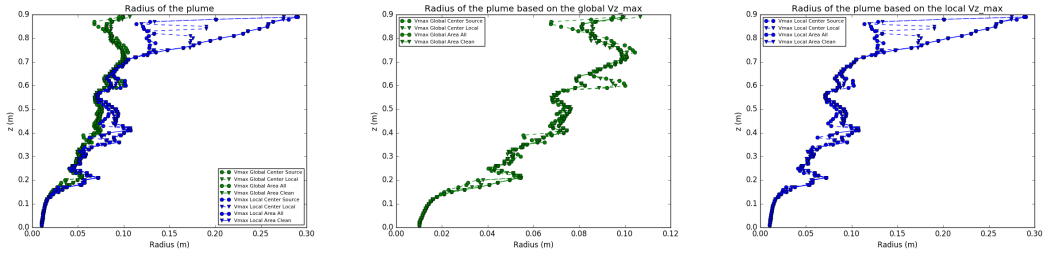
- **Centre_Global.txt**
  Centre of the plume computed by method I - Global Velocity - 5 columns

  1. The height z in meters
  2. x coordinate of the local centre computed by method I.2.b
  3. y coordinate of the local centre computed by method I.2.b
  4. x coordinate of the source
  5. y coordinate of the source

  Note that columns 4 and 5 have constant values.

- **Centre_Local.txt**
  Centre of the plume computed by method II - Local Velocity - 5 columns

  1. The height z in meters
  2. x coordinate of the local centre computed by method II.2.b
  3. y coordinate of the local centre computed by method II.2.b
  4. x coordinate of the source
  5. y coordinate of the source



(a) **(b)** **(c)**

Figure 10.10: Variation of the plumes radius as a function of the height. (a) Using all the methods presented, (b) using method I and (c) using method II.

Note that columns 4 and 5 have constant values.

- **Location_VelocityZ_max.txt**
  Location of the velocity max in the domain - 6 columns

  1. x coordinate of the location of the maximum velocity for method II
  2. y coordinate of the location of the maximum velocity for method II
  3. z coordinate of the location of the maximum velocity for method II
  4. x coordinate of the location of the maximum velocity for method I
  5. y coordinate of the location of the maximum velocity for method I
  6. z coordinate of the location of the maximum velocity for method I

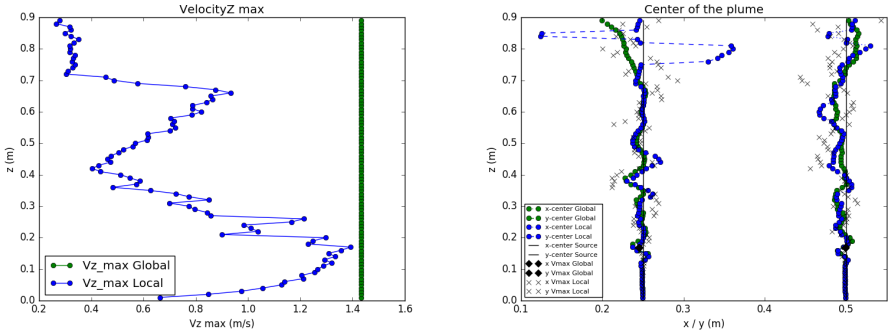
  Note that columns 4, 5 and 6 have constant values.

Plots

This section shows examples of plots that can be obtained. Figure 10.10 shows the variation of the plumes radius as a function of the height for all the methods presented above. Figure 10.11a shows the variation of the maximum velocity as a function of the height for methods I and II. Figure 10.11b shows the location of the plume centre as a function of the height for methods I and II. The green lines are for method I, while the blue lines are for method II. In Figure 10.11b, the black crosses depicts the location of the maximum velocity while using method II. The global maximum velocity is depicted by black diamonds. Figure 10.12 to Figure 10.15 show the x and y locations of the plume centre as a function of the height for the method I.2 and II.2. The error bars depicts the radius computed by the associated method centred on the source location (Figure 10.12 and Figure 10.13) and the local plumes centre (Figure 10.14 and Figure 10.15).

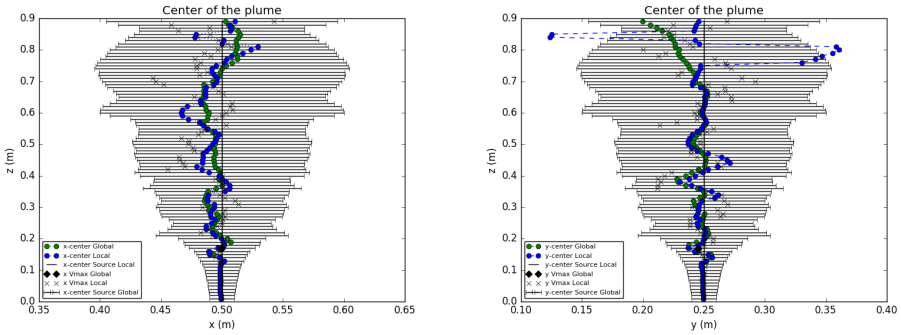
10.4.5 Numerical implementation

All the methods described above are implemented in a python script and the main libraries used are:



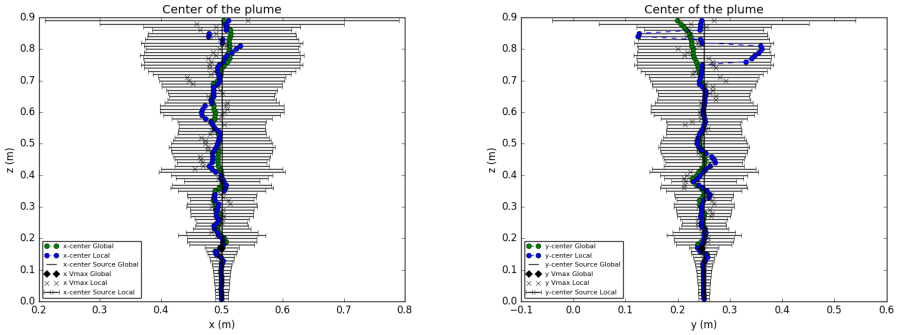
(a) **(b)**

Figure 10.11: (a) Variation of the maximum velocity as a function of the height for methods I and II. (b) Location of the plumes centre as a function of the height for methods I.2 and II.2.



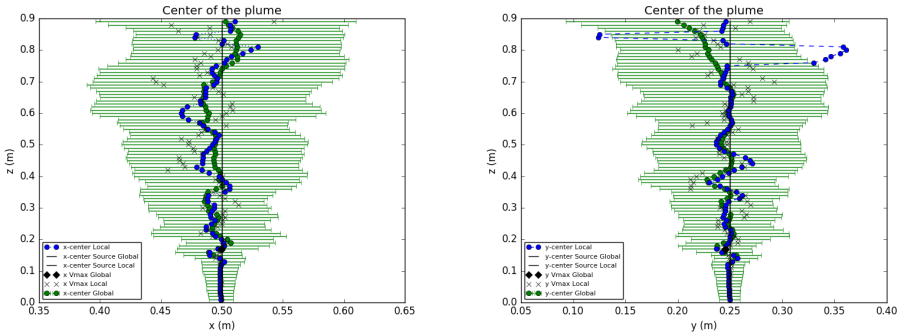
(a) **(b)**

Figure 10.12: (a) x and (b) y location of the plumes centre. The error bars depict the computed radius at each height using the method I.2.a.



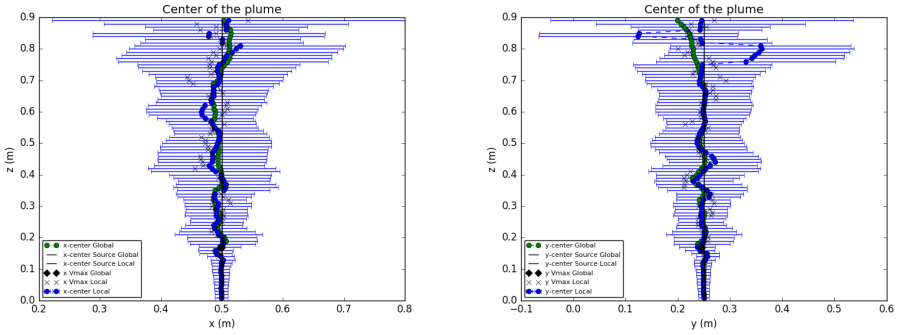
(a) **(b)**

Figure 10.13: (a) x and (b) y location of the plumes centre. The error bars depict the computed radius at each height using method II.2.a.



(a) **(b)**

Figure 10.14: (a) x and (b) y location of the plumes centre. The error bars depict the computed radius at each height using method I.2.b.



(a) **(b)**

Figure 10.15: (a) x and (b) y location of the plumes centre. The error bars depict the computed radius at each height using method II.2.b.

- **vtk** is used to read the data obtained with **Fluidity**, to obtain the contours (Code 10.2), the slices (Code 10.3) and to write data into *vtu* files (Code 10.4).
- **shapely** is used to play around with the geometry. For example, the centroid of the polygons and the detection of polygons within others are done using this library.
- **matplotlib** is used to plot all the data (Figure 10.10 to Figure 10.15).

Codes 10.5 and 10.6 show the functions used to compute the radius.

```
27 #-------------------------------------------------------------#
28 #-- Function to generate the contour based on a given value -#
29 #-------------------------------------------------------------#
30 def Contour(ugrid, value):
31     filter = vtk.vtkContourFilter()
32     if vtk.vtkVersion.GetVTKMajorVersion() <= 5:
33         filter.SetInput(ugrid)
34     else:
35         filter.SetInputData(ugrid)
36 
37     filter.SetNumberOfContours(1)
38     filter.SetValue(0, value)
39     filter.Update()
40     cutContour = filter.GetOutput()
41 
42     return cutContour
```

Code 10.2: Function to generate a contour using the **vtk** library.

```
81 #---------------------------#
82 #-- Function to do a slice -#
83 #---------------------------#
84 def Plane(origin, normal, ugrid):
85 
86     plane = vtk.vtkPlane()
87     plane.SetNormal(normal[0], normal[1], normal[2])
88     plane.SetOrigin(origin[0], origin[1], origin[2])
89 
90     cutter = vtk.vtkCutter()
91     cutter.SetCutFunction(plane)
92     if vtk.vtkVersion.GetVTKMajorVersion() <= 5:
93         cutter.SetInput(ugrid)
94     else:
95         cutter.SetInputData(ugrid)
96 
97     # Cut
98     cutter.Update()
99     cutPlane = cutter.GetOutput()
100 
101     # Write the data in a new grid
102     uugrid = vtk.vtkUnstructuredGrid()
```

```
103     # Add the points
104     uugrid.SetPoints(cutPlane.GetPoints())
105 
106     return uugrid, cutPlane
```

Code 10.3: Function to generate a plane using the **vtk** library.

```
44 #-------------------------------------------#
45 #-- Function to write the data in a vtu file -#
46 #-------------------------------------------#
47 def WriteData(cutContour, filename):
48 
49     ugrid = vtk.vtkUnstructuredGrid()
50 
51     # Add the points
52     ugrid.SetPoints(cutContour.GetPoints())
53 
54     # Add the cells
55     for i in range(cutContour.GetNumberOfCells()):
56         cellType = cutContour.GetCellType(i)
57         cell = cutContour.GetCell(i)
58         ugrid.InsertNextCell(cellType, cell.GetPointIds())
59 
60     # Add the point data
61     for i in range(cutContour.GetPointData().GetNumberOfArrays()):
62         ugrid.GetPointData().AddArray(cutContour.GetPointData().
               GetArray(i))
63 
64     # Add the cell data
65     for i in range(cutContour.GetCellData().GetNumberOfArrays()):
66         ugrid.GetCellData().AddArray(cutContour.GetCellData().GetArray
               (i))
67 
68     # Write the contour in a new vtu file
69     gridwriter=vtk.vtkXMLUnstructuredGridWriter()
70     gridwriter.SetFileName(filename)
71 
72     if vtk.vtkVersion.GetVTKMajorVersion() <= 5:
73         gridwriter.SetInput(ugrid)
74     else:
75         gridwriter.SetInputData(ugrid)
76 
77     gridwriter.Write()
78 
79     return ugrid
```

Code 10.4: Function to write data in a *vtu* file using **vtk** library.

```
254 #-------------------------------------------------------------------#
255 #-- Function to find the mean radius based on the area of polygons -#
256 #-------------------------------------------------------------------#
257 #---------------------------------#
```

```
# Method 1 Area                    #
#--------------------------------#
def RadiusArea(poly,area_del):
    sum_area = 0.0
    for polyID in range(len(poly)):
        poly1 = poly[polyID]
        area = poly1.area
        sum_area = sum_area + area

    sum_area = sum_area - area_del
    mean_radius = np.sqrt((sum_area/np.pi))

    return mean_radius
```

Code 10.5: Function to get the radius using Method 1.

```
#-------------------------------------------------------------------#
#-- Function to find the mean radius after cleaning the geometry -#
#-------------------------------------------------------------------#
#--------------------------------#
# Method 2 Distance              #
#--------------------------------#
def RadiusPoly(coordinates, x0, y0):
    sum_dist = 0.0
    tot_pts = 0
    for nodeID in range(len(coordinates)-1):
        x, y = coordinates[nodeID][0], coordinates[nodeID][1]
        distance = np.sqrt(np.power(x-x0,2)+np.power(y-y0,2))
        sum_dist = sum_dist + distance
        tot_pts += 1

    mean_radius = sum_dist/tot_pts

    return mean_radius
```

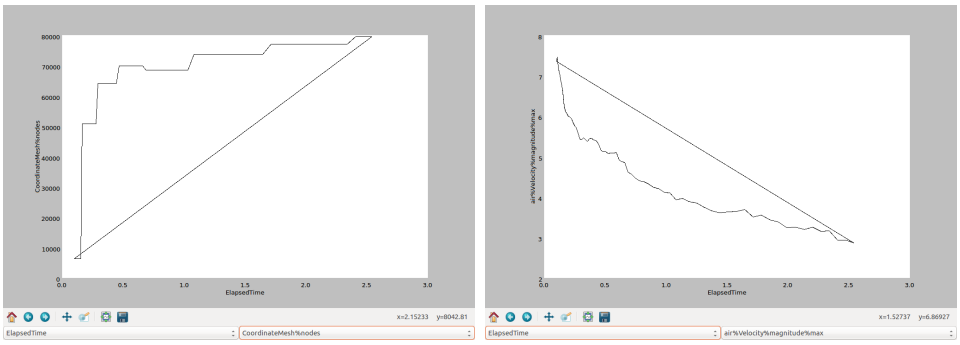
Code 10.6: Function to get the radius using Method 2.

10.5 **.stat* file

While a **Fluidity** simulation is running, a **.stat* file is generated, which is basically a text file that can be viewed with any text editor. This file records a number of interesting information such as the number of nodes, the maximum and minimum values of each fields... As shown in Figure 10.16, information in the **.stat* file can also be viewed directly using the graphical interface **statplot** launched by typing in a terminal:

```
user@mypc:~$ statplot simu_name.stat
```

Command 10.1: Visualising a *stat* file using **statplot**.



(a) **(b)**

Figure 10.16: (a) Number of nodes and (b) maximum velocity magnitude as a function of the time visualised with the tool **statplot**.

The data can also be read easily using a python script: an example of python script, *StatReader.py*, can be found in the folder `Scripts/StatReader/`. As shown in Code 10.7, Line 10, the `fluidity_tools` library is required. The **.stat* file needs to be imported (Line 25 in Code 10.7), then the data can be extracted (see Lines 32 to 38 in Code 10.7). This allows the manipulation of the data and some plots are shown in Figure 10.17

```
3  from numpy import *
4  from math  import *
5
6  import sys, os
7  import numpy as np
8  from termcolor import colored
9
10 import fluidity_tools
11
12 import matplotlib.pyplot as plt
13
14 os.system('rm -r *txt *png')
15
16 #---------------------------------#
17 # User Input variables            #
18 #---------------------------------#
19 path_simu = '../../Examples/Case11_T0.1_All/' # Path of the simu
20 basename  = 'Case11_Box'                      # Name of the simu
21
22 #---------------------------------#
23 # Read stat file                  #
24 #---------------------------------#
25 stat = fluidity_tools.stat_parser(path_simu+basename+'.stat')
26 print colored('The variables in the stat file are ::', 'red')
27 print stat['air'].keys()
28
29 #---------------------------------#
30 # Extract data from stat file     #
31 #---------------------------------#
```

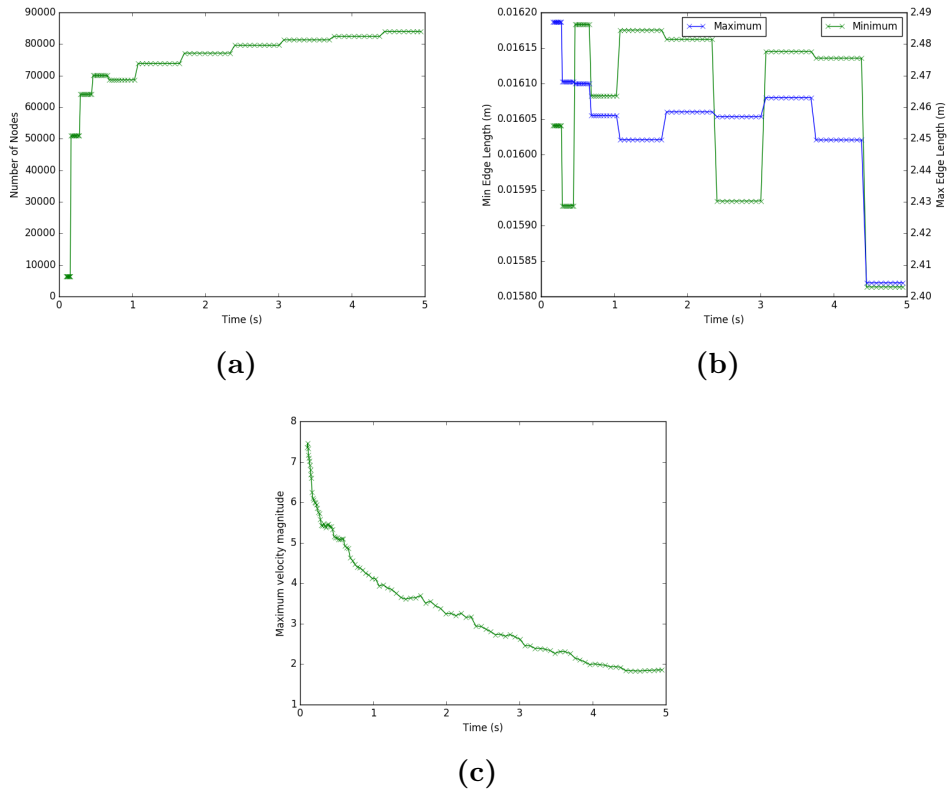


Figure 10.17: (a) Number of nodes, (b) minimum and maximum edge length and (c) maximum velocity magnitude as a function of the time. Data were extracted from the **.stat* file using the python script *StatReader.py*.

```
Time      = stat['ElapsedTime']['value']
NbrNodes  = stat['CoordinateMesh']['nodes']

EdgeLength_min   = stat['air']['EdgeLength']['min']
EdgeLength_max   = stat['air']['EdgeLength']['max']
Velocity_max     = stat['air']['Velocity%magnitude']['max']
Reynolds_uu_max  = stat['air']['uuAverage']['max']
```

Code 10.7: Extract data from the **.stat* file using a python script.

10.6 fltools

A number of **Fluidity** tools exist and are detailed in the manual. Here are described the more useful ones. For information, the executable of these tools are located under the directory: `<<FluiditySourcePath>>/bin/`.

10.6.1 rename_checkpoint

When running a simulation from a checkpoint, the new simulation will have the name of the simulation following by `_checkpoint` and the files' numbering will re-start at 0. Therefore, it can be useful to rename these files afterwards to visualise them as continuous files in **ParaView** for example. Hence, the tool `rename_checkpoint` allows to rename the **ParaView** files (**.vtu* or **.pvtu*) of a simulation that has been checkpointed. It is run typing in a terminal Command 10.2, where `base_filename` is the original name of the simulation before it was checkpointed and `index` is the index at which it was checkpointed. For example, if simulations were run from a file called `Case11_Box_10_checkpoint.flml` the resulting checkpointed files would have to be renamed with the command `rename_checkpoint Case11_Box 10`.

```
user@mypc:~$ rename_checkpoint base_filename index
```

Command 10.2: Use of `rename_checkpoint` to rename checkpointed simulations.

10.6.2 pvtu2vtu

When running a simulation in parallel, **.pvtu* files are generated. When visualising these files in **ParaView** and particularly when using the `cull frontface` visualisation style, the overlapping region used during parallelisation (due to the domain decomposition) are visible, making difficult to view the results. One easy way to avoid this is to convert the **.pvtu* files into **.vtu* files using the tool `pvtu2vtu` which combines the **.pvtu* obtained in parallel into **.vtu* files. This tool is run typing in a terminal Command 10.3, where `base_filename` is the name of the simulation, `index` and `last index` are the first and the last index of the files to convert.

```
user@mypc:~$ pvtu2vtu base_filename index [last index]
```

Command 10.3: Use of `pvtu2vtu` to convert **pvtu* files into **.vtu* files.

10.6.3 genpvd

Finally, `genpvd` can be used to generate a **.pvd* file from the list of **.vtu* or **.pvtu* files. This will notably allow the user to have access to the simulation real time. It can be run using Command 10.4, where `base_filename` is the name of the simulation. It must be noted that checkpointed files will have to be renamed before this can be done.

```
user@mypc:~$ genpvd base_filename
```

Command 10.4: Use of `genpvd` to generate a **.pvd* file.

Chapter 11

Others

11.1 Past and present people using Fluidity

Following are past and present people working with **Fluidity** to perform outdoor simulations and/or indoor-outdoor exchange simulations. This manual was initiated by Dr Laetitia Mottet, post-doc in the Earth Science and Engineering department, Imperial College London and in the Architecture department, University of Cambridge; and Carolanne Vouriot, PhD student in the Civil Engineering department, Imperial College London. It is also important to mention that **Fluidity** was initially developed by Prof. Christopher Pain c.pain@imperial.ac.uk, department of Earth Science and Engineering, Imperial College London.
Contacts: prioritise people in red if you have any questions or amendment to this manual to suggest.

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- Huw Woodward - h.woodward@imperial.ac.uk
- Carolanne Vouriot - carolanne.vouriot12@imperial.ac.uk

Complex outdoor simulations			
Since 2000	E. Aristodemou	Senior Lecturer	London South Bank University
Since 2016	L. Mottet	Post-doc	Imperial / Cambridge
Since 2017	H. Woordward	Post-doc	Imperial

Table 11.1: People who worked or are currently working with **Fluidity** on simulations in urban environment.

Box simulations of indoor - outdoor exchanges				
Summer 2017	Faron Hesse	MRes	ICL	*H. Burridge*
Summer 2017	Jean-Etienne Debay	Intern	Cam	*M. Davies Wykes*
Since 2018	Carolanne Vouriot	PhD Student	ICL	*H. Burridge*
Summer 2018	Nouhaila Fadhi	Intern	Cam	*M. Davies Wykes*
Summer 2018	Theresa Bischof	MSc	ICL	*H. Burridge*
Summer 2018	Sam Charlwood	UROP	Cam	*M. Davies Wykes*

Table 11.2: People who worked or are currently working with **Fluidity** on indoor - outdoor simulations. ICL stands for Imperial College London and Cam for the University of Cambridge, names in italic are the *supervisors*.

11.2 Online open-source data set

Following is a non-exhaustive list of open-source experimental and/or numerical data available for indoor-outdoor exchange and urban environment simulations.

- **Urban environment simulations**
  - https://www.windforschung.de/CODASC.htm
  - http://mi-pub.cen.uni-hamburg.de/index.php?id=432
  - https://mi-pub.cen.uni-hamburg.de/index.php?id=6339
  - https://www.aij.or.jp/jpn/publish/cfdguide/index_e.htm
  - http://www.dapple.org.uk/
- **Indoor-outdoor exchanges**
  - Please contact Laetitia Mottet and/or Carolanne Vouriot if you are aware of open-source data available online, either numerical or experimental, on indoor-outdoor exchanges.

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