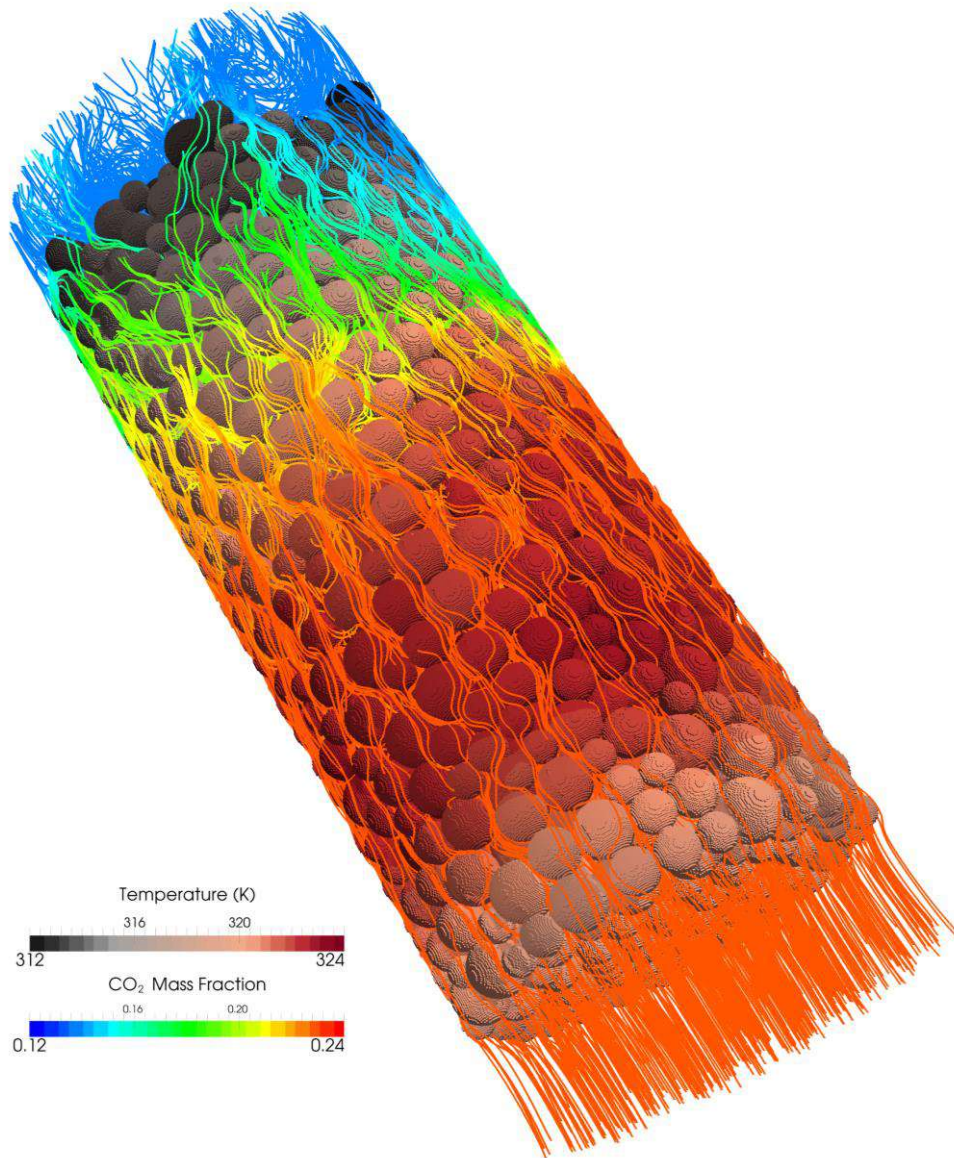


TU WIEN **WARDS** OpenFOAM®

OpenFOAM® Basic Training



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This book has been used as a basis for preparing a series of video lectures on youtube by Jozsef Nagy (JKU Linz):

www.youtube.com/channel/UCjdgpuXUAXH9BqheyE82Vvw
(Search for: Jozsef Nagy OpenFOAM at youtube.com)

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icoFoam – elbow (mesh)

Simulation

Using icoFoam solver, simulate 75 s of flow in an elbow for following GAMBIT meshes:

- Tri-mesh (comes with OpenFOAM® tutorial)
- Hex-mesh coarse (check GAMBIT “elbow 2D” tutorial)
- 2 times finer hex-mesh (refine previous step mesh)

Objectives

- Looking at the initial values for p and U.
- Ensuring proper boundary definitions (imported boundaries from GAMBIT, additional surfaces during conversion and boundaries definition in OpenFOAM®)

Post processing

Import your simulation to ParaView, extract data make two diagrams (using spreadsheet calculators) of pressure and velocity magnitude along a line between two tubes, do the same for all three simulations.

Step by step simulation

Setting system environment

Make sure your system environment is set correctly, check Appendix B.

Copying tutorial

Open a terminal and copy the elbow tutorial from the following path to your working directory (see Appendix A for using a terminal in Linux):

```
~/OpenFOAM/OpenFOAM-2.3.0/tutorials/incompressible/icoFoam/  
elbow
```

Converting mesh

The mesh which is produced by GAMBIT is not directly compatible with OpenFOAM®. First, the mesh needs to be converted to an OpenFOAM® mesh, using following tool:

```
>fluentMeshToFoam elbow.msh
```

If the mesh was created in mm and is converted using the mentioned command it will convert the mesh with wrong dimensions, since all the units in OpenFOAM® are SI¹ Units. There are different flags included with most of OpenFOAM® tools, for checking them use the flag `-help` after the command, e.g.:

```
>fluentMeshToFoam -help
```

The output gives an overview of available options of the tool and also a short description on how to use it:

```
Usage: fluentMeshToFoam [OPTIONS] <Fluent mesh file>  
options:  
  -case <dir>          specify alternate case directory, default is the cwd  
  -noFunctionObjects   do not execute functionObjects  
  -scale <factor>      geometry scaling factor - default is 1  
  -writeSets           write cell zones and patches as sets  
  -writeZones         write cell zones as zones  
  -srcDoc             display source code in browser  
  -doc               display application documentation in browser  
  -help              print the usage
```

```
Using: OpenFOAM-2.3.0 (see www.OpenFOAM.org)  
Build: 2.3.0-f5222ca19ce6
```

The `-scale` flag is used for converting the mesh dimensions from other units to SI units, e.g. if the mesh was created in mm it will be converted to meter by using `-scale 0.001` and if the flag is omitted, uses 1:

```
>fluentMeshToFoam elbow.msh -scale 1.0
```

Note: The mesh which is imported to OpenFOAM® should be a three dimensional mesh. For carrying out 2D (also 1D) simulations a three-dimensional mesh should be

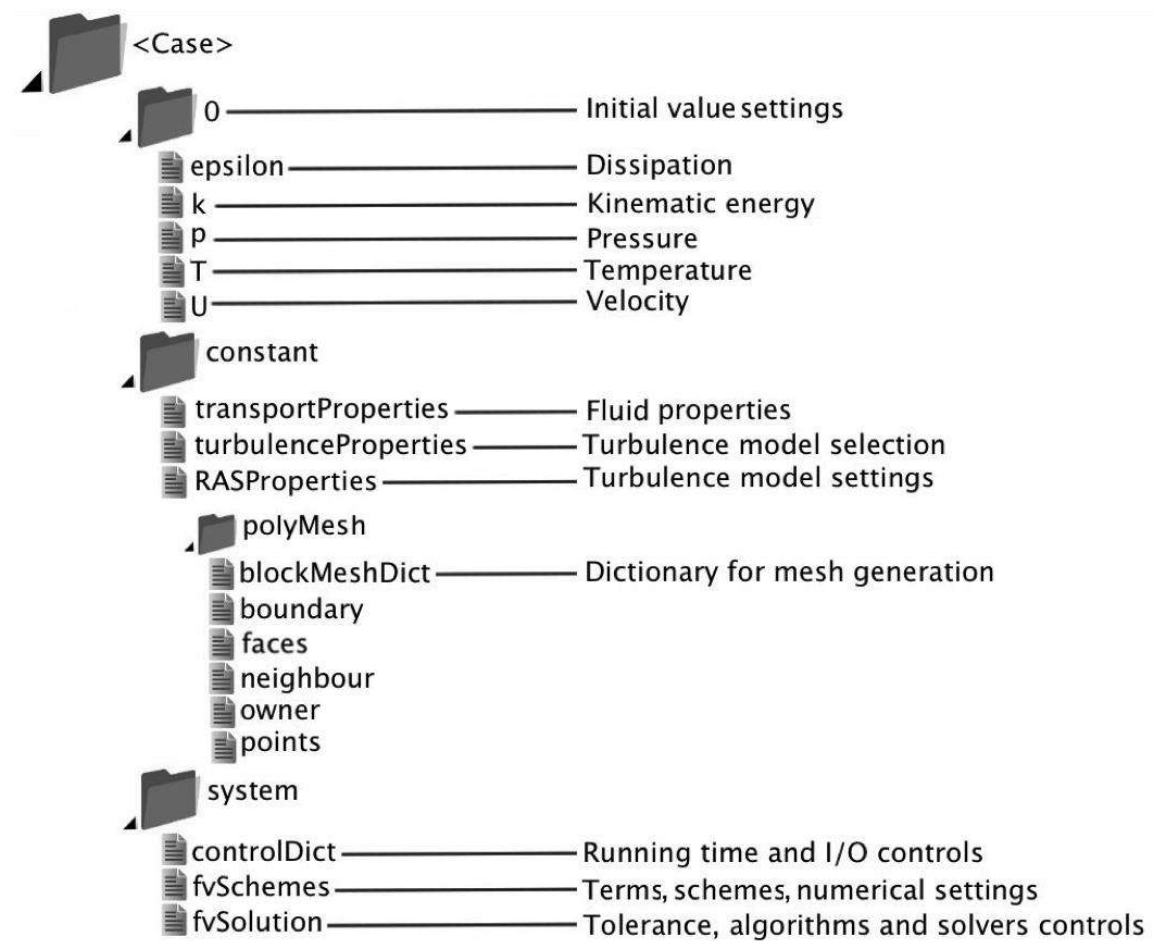
¹ International System of Units

created with just one cell in the third dimension (for 1D, one cell in the second and also one cell in the third direction).

Note: If there are internal boundaries in the mesh, there is another tool, *fluent3DMeshToFoam*. Using this tool, the internal boundaries will be kept during conversion.

Case structure

Most of the cases in OpenFOAM® have the following basic case structure (directory tree):



There are three main directories (0, constant, system) in each case folder:

0 directory

The 0 directory includes the initial conditions for running the simulation. In each file in this folder the initial conditions for one property can be set. The files are named after the property they are standing for, e.g. usually T file includes temperature initial conditions. In the elbow example there are only two files inside the 0 directory, p and U. p stands for pressure and U stands for velocity. Checking p:

>nano¹ p

It will be like this:

```

/*----- C++ -----*/
| ===== |
| \\      / F i e l d      | OpenFOAM: The Open Source CFD Toolbox |
| \\      / O p e r a t i o n | Version: 2.3.0 |
| \\      / A n d      | Web: www.OpenFOAM.com |
| \\      / M a n i p u l a t i o n | |
/*-----*/
FoamFile
{
    version      2.0;
    format       ascii;
    class        volScalarField;
    object       p;
}
// ***** //

dimensions      [0 2 -2 0 0 0 0];

internalField   uniform 0;

boundaryField
{
    wall-4
    {
        type      zeroGradient;
    }

    velocity-inlet-5
    {
        type      zeroGradient;
    }

    velocity-inlet-6
    {
        type      zeroGradient;
    }

    pressure-outlet-7
    {
        type      fixedValue;
        value     uniform 0;
    }

    wall-8
    {
        type      zeroGradient;
    }

    frontAndBackPlanes
    {
        type      empty;
    }
}
// ***** //

```

In the dimensions the physical dimension according to SI base units of the quantity is defined, for example here it shows that the p dimension is (m/s)².

¹ nano is a text editor used in Linux OS (for closing and saving: ctrl+x)

Note: As you can see the p unit is not the pressure unit (Pa). It is due to the fact that in incompressible solvers in OpenFOAM® p is defined as “reduced” pressure divided by density.

Note: In the dimension matrix the first number presents mass unit power, the second one the length, the third one time, the fourth one the temperature and the fifth one the quantity (mole).

The `internalField` sets the initial field of a specific quantity in the solution domain.

The type of each of our boundaries as well as the value of this quantity on the boundaries is defined in the `boundaryField`. There are different types of boundary conditions in OpenFOAM®:

- `zeroGradient`: Applies a zero gradient boundary type to this boundary (Neumann boundary condition).
- `fixedValue`: Applies a fixed value to this boundary (Dirichlet boundary condition).
- `empty`: It is for sides, which are vertical to the direction which is not going to be considered (e.g. in 2D simulations these boundaries are vertical to the third dimension). In this boundary type both of the sides vertical to one dimension should be selected together and named as one boundary.

Note: If a `fixedValue` boundary condition with `value` equals `$internalField` is used, it is equal to using `zeroGradient`, except `zeroGradient` applies the boundary condition implicitly, but `fixedValue` with `$internalField` value applies the boundary condition explicitly.

Note: In some mesh creation software like GAMBIT, empty boundary condition do not exist. All the faces perpendicular to the direction which is not going to be considered should be defined as a new boundary with type `wall`. After converting the mesh to OpenFOAM® mesh, modify that boundary in the file `constant/polyMesh/` `boundary`, and change its type from `wall` to `empty`, and also change `inGroups` from `wall` to `empty`.

The U file has to be defined via three components (since velocity is a vector): first one stands for the x component, second one for the y component, and the third one for the z component. For this case setup the z component is always zero because it is a 2D simulation and no calculations will be done in the z direction. The boundaries vertical to z direction have been already set to empty.

constant directory

The constant directory usually consists of a subdirectory and some files. The files (usually) include material properties, simulation physics and chemistry. In the directory “polyMesh” the mesh data are stored (in this case the data for converted mesh). The boundary file in this polyMesh directory includes the mesh boundary data,

Exporting simulation data

The data files created by OpenFOAM® should be exported (converted) by the appropriate tools, to the post processing tools data format. For ParaView:

```
>foamToVTK
```

where VTK is the ParaView data format. This command should be also executed in the case main directory, e.g. elbow. Here, ParaView is used as the post-processing tool, for running it

```
>paraview &
```

Note: There is also another option to open the OpenFOAM® simulation results with ParaView without converting them to VTK; Create an empty text file in the main case directory, name it <someName>.foam (e.g. foam.foam), and execute the following command. This method is good for fast evaluation of the data in the middle of the simulation or with a decomposed case in parallel simulations:

```
>paraview foam.foam &
```

Note: By putting & at the end of command, the command line will remain active and ready for further inputs while that program is running.

Examining different meshes

Do the same for the other two meshes. Just the mesh for the first simulation is included in the elbow example of OpenFOAM®. For the other two simulations the mesh should be provided by the user. For finding the tutorials on how to create the geometry and the mesh, search the internet for “GAMBIT elbow mesh 2D”. The dimensions and also the mesh info are provided in that tutorial. Try to create it by using GAMBIT. When you are done you have to convert it into a 3D mesh with 1 cell in the z-direction.

The comparisons of all three case results and charts are shown below.



Figure 1.1 The Hex Fine mesh created using GAMBIT

Note: As mentioned before after converting the mesh, change the boundaries perpendicular to the direction which is not going to be considered (the z direction) from wall to empty (just replace wall with empty for this boundary).

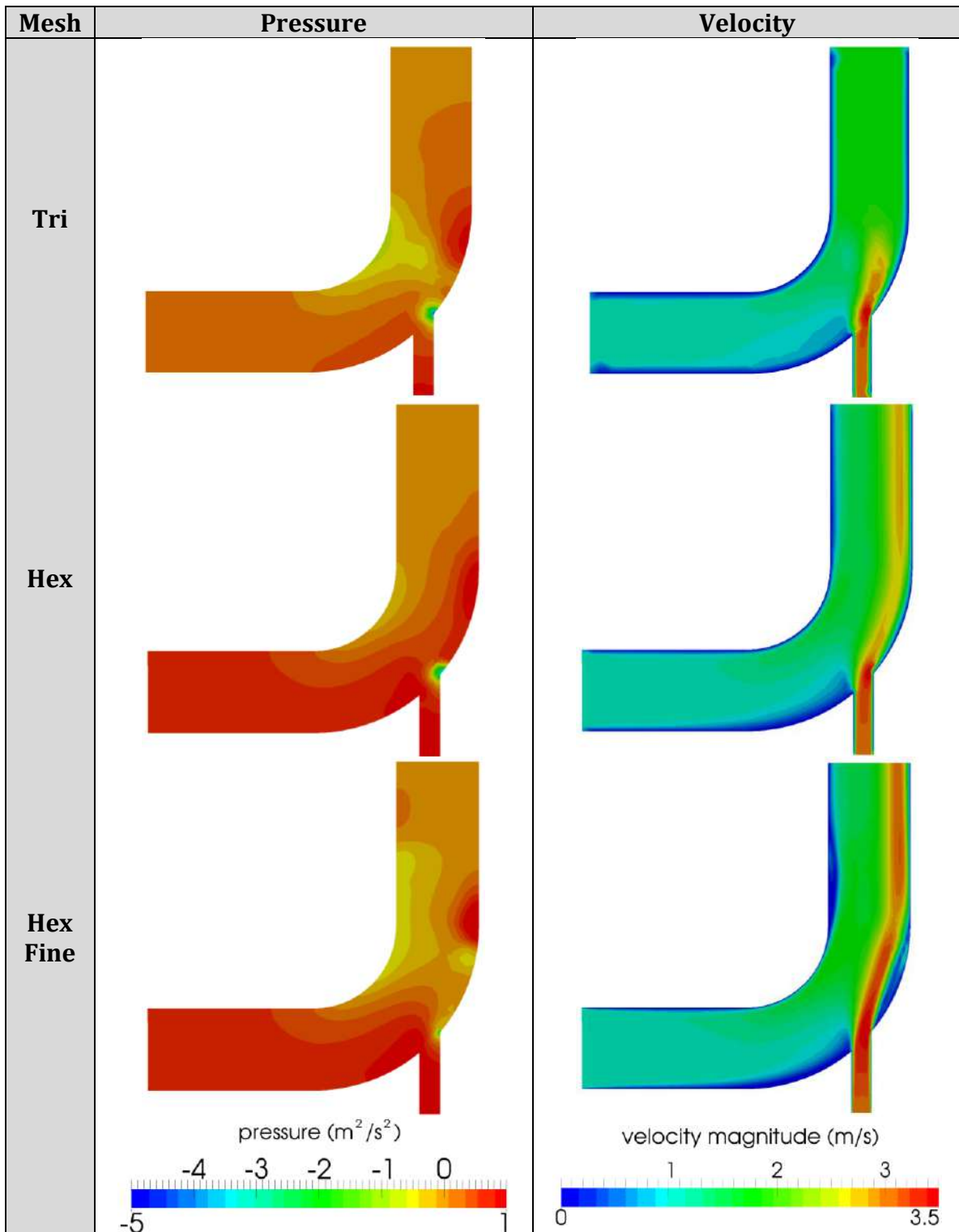


Figure 1.2 Comparison of different mesh type results at $t = 75$ s

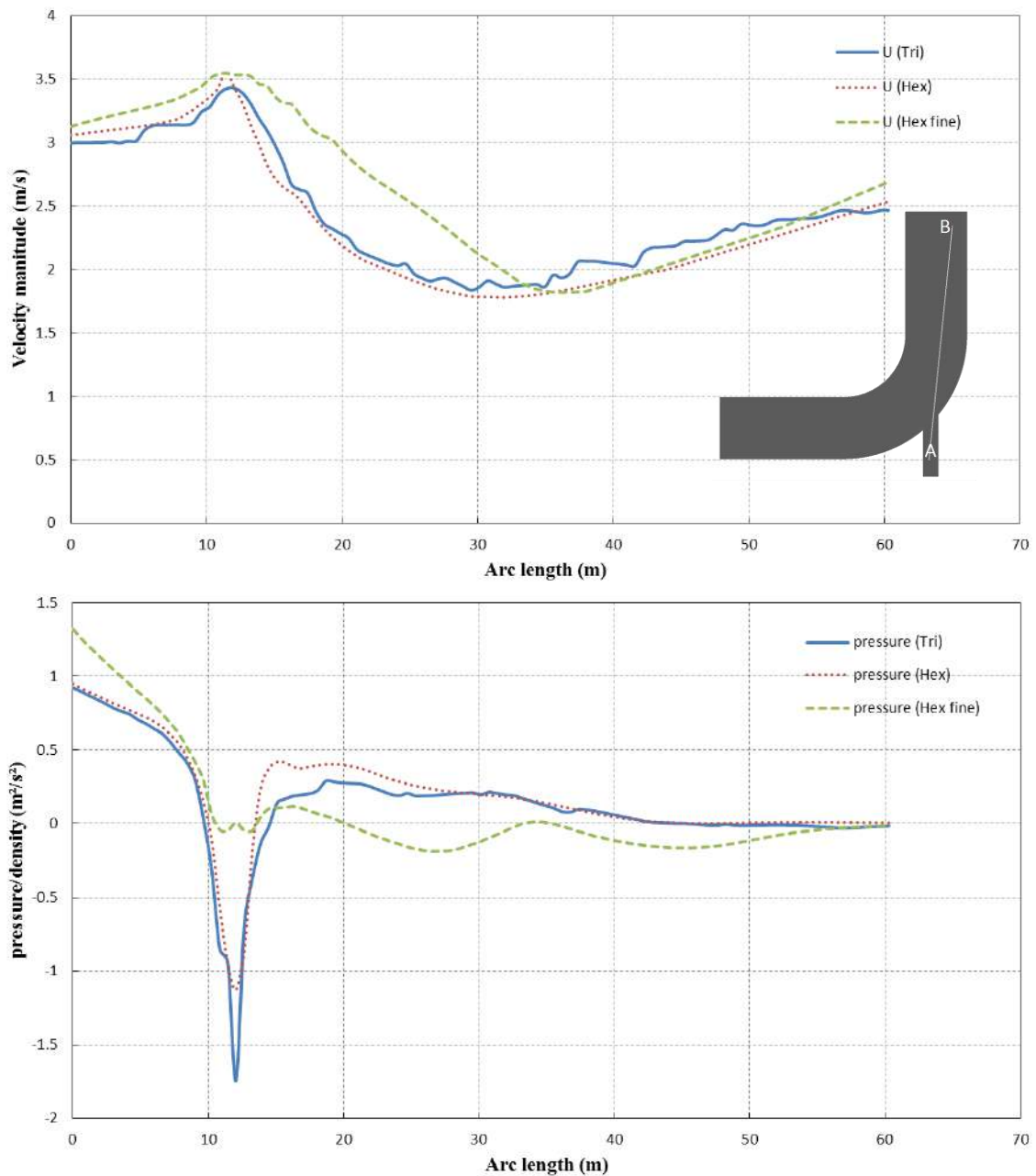


Figure 1.3 Pressure and velocity for different meshes at $t=75$ s, along the arc shown

The comparison plots are along the line between points A (54 0 0) at the small tube entrance and B (60 60 0) at the large tube exit part (length units are in meter) for Tri-mesh, for other two meshes created using GAMBIT the points are A (22 -33 0) and B (27 30 0).

Note: For extracting data over a line, the line should be defined in ParaView using “Plot Over Line”, then the data over this line can be exported by choosing Save Data from File menu in ParaView.

sonicFoam – forwardStep

Simulation

Using sonicFoam solver, simulate 10 s of flow over a forward step.

Objectives

- Understand blockMesh
- Define vertices via coordinates as well as surfaces and volumes via vertices.

Post processing

Import your simulation into ParaView, and examine the mesh and the results in detail.


```

edges
(
);
boundary
(
    inlet
    {
        type patch;
        faces
        (
            (0 8 10 2)
            (2 10 13 5)
        );
    }
    outlet
    {
        type patch;
        faces
        (
            (4 7 15 12)
        );
    }
    bottom
    {
        type symmetryPlane;
        faces
        (
            (0 1 9 8)
        );
    }
    top
    {
        type symmetryPlane;
        faces
        (
            (5 13 14 6)
            (6 14 15 7)
        );
    }
    obstacle
    {
        type patch;
        faces
        (
            (1 3 11 9)
            (3 4 12 11)
        );
    }
);

mergePatchPairs
(
);
// *****

```

As noted before units in OpenFOAM® are SI units. If the vertex coordinates differ from SI, they can be converted with the `convertToMeters` command. The number in the front of `convertToMeters` shows the constant, which should be multiplied with the dimensions to change them to meter (SI unit of length). For example:

```
convertToMeters    0.001
```

shows that the dimensions are in millimeter, and by multiplying them by 0.001 they are converted into meters.

In the `vertices` part, the coordinates of the geometry vertices are defined, the vertices are stored and numbered from zero, e.g. vertex `(0 0 -0.05)` is numbered zero, and vertex `(0.6 1 -0.05)` points to number 6.

In the `block` part, blocks are defined. The array of numbers in front each block shows the block building vertices, e.g. the first block is made of vertices `(0 1 3 2 8 9 11 10)`.

After each block the mesh is defined in every direction. e.g. `(25 10 1)` shows that this block is divided into:

- 25 parts in x direction
- 10 parts in y direction
- 1 part in z direction

As it was explained before, even for 2D simulations the mesh and geometry should be 3D, but with one cell in the direction, which is not going to be solved, e.g. here number of cells in z direction is one and it's because of that it's a 2D simulation in x-y plane.

The last part, `simpleGrading (1 1 1)` shows the size function.

In the `patches` part each boundary is defined by the vertices it is made of, and also its `type` and `name` are defined.

Note: For creating a face the vertices should be chosen clockwise when looking at the face from inside of the geometry.

Running simulation

Before running the simulation the mesh has to be created. In the previous step the mesh and the geometry data were set. For creating it the following command should be executed from case main directory (e.g. `forwardStep`):

```
>blockMesh
```

After that, the mesh is created in the `polyMesh` folder. For running the simulation, type the solver name from case directory and execute it:

```
>sonicFoam
```

Exporting simulation

The mesh is presented in the following way in ParaView, and you can easily see the three blocks, which were created.

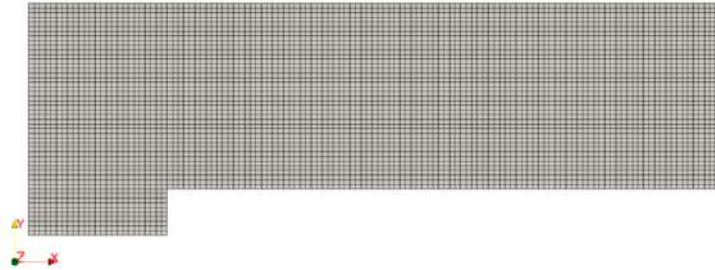


Figure 2.1 Mesh generated by blockMesh

Note: When a cut is created by default in ParaView, the program shows the mesh on that plane as a triangular mesh even if it is a hex mesh. In fact, ParaView changes the mesh to a triangular mesh for visualization, where every square is represented by two triangles. For avoiding this when creating a cut in ParaView in the Slice properties window, uncheck “Triangulate the Slice”.

The simulation results are as follows:

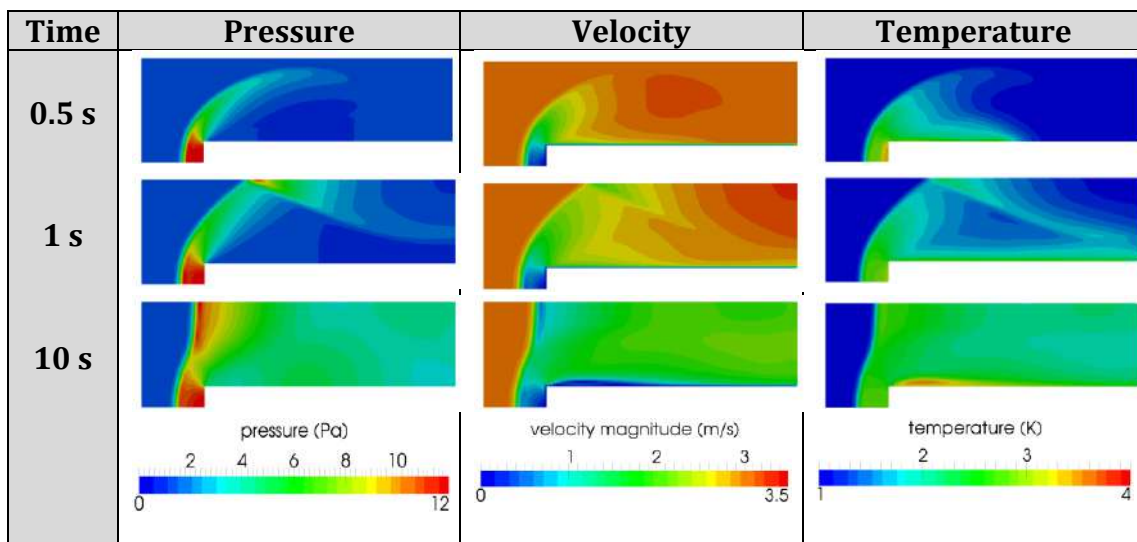


Figure 2.2 Pressure, velocity and temperature contours at different time steps

sonicFoam – shockTube

Simulation

Use the sonicFoam solver, simulate 0.007 s of flow inside a shock tube, with a mesh with 100, 1000 and 10000 cells in one dimension, for initial values 1 bar/0.1 bar and 10 bar/0.1 bar.

Objectives

- Understanding setFields
- Investigate effect of grid resolution

Post processing

Import your simulation into ParaView, and compare results.

Step by step simulation

Open tutorial

Copy the tutorial from the following directory to your working directory

```
~/OpenFOAM/OpenFOAM-2.3.0/tutorials/compressible/sonicFoam/
laminar/shockTube
```

constant directory

By checking the geometry and the mesh, it is obvious that it is a 1D mesh, because of the number of mesh cells in y and z directions is one, and also in the patches, plates vertical to these directions are defined as empty boundary condition. The mesh density can be set in the `blocks` part by changing x direction mesh size (e.g. change it from 1000 to 100 or 10000).

system directory

Checking system directory, there is a file “setFieldDict” which is used by the tool `setFields` for patching (assign an amount to a region) in the simulation. For example, here the pressure of 0.1 bar should be patched to half of the region (the geometry is from -5 to 5, so from 0 to 5 will be patched) and 10 bar to the other half.

```
// * * * * * //
defaultFieldValues ( volVectorFieldValue U ( 0 0 0 ) volScalarFieldValue T
348.432 volScalarFieldValue p 1000000 );

regions      ( boxToCell { box ( 0 -1 -1 ) ( 5 1 1 ) ; fieldValues (
volScalarFieldValue T 278.746 volScalarFieldValue p 10000 ) ; } );

// ***** //
```

In the `defaultFieldValues`, a value is assigned to the whole domain, for example here, the velocity has been set everywhere to zero, the temperature to 348.432 K, and the pressure to 1000000 Pa. In the `regions`, `boxToCell` defines the region to which a special amount must be patched. With `boxToCell` the region is chosen by a cube, and the cube is defined by giving the coordinates of one of its diagonals.

After choosing the region, the new values are assigned to the parameters (e.g. here temperature 278.746 K and pressure 10000 Pa).

Running simulation

In order to assign the values which were set in the `setFieldDict`:

```
>setFields
```

Then run:

```
>sonicFoam
```

Note: Checking `deltaT` in `controlDict` in the system directory, it is $1e-5$ s. The question is: What is the criteria for setting `deltaT`? If `deltaT` is bigger, the simulation will run faster, but a too big `deltaT` makes the simulation unstable and

sometimes physically meaningless. Therefore Δt should be selected in a way to have a fast and at the same time stable and also physically reasonable simulation. The Courant (Co) number is a dimensionless number, which is usually used as a necessary condition for having a convergent solution, for one dimension:

$$Co = \frac{u\Delta t}{\Delta x}$$

Where u is velocity magnitude in that direction, Δt is Δt and Δx is the mesh size in this direction. For having a convergent solution in most of the cases Co should be less than one in all the cells in the domain.

As it is obvious from the equation by decreasing the Δx or the mesh size Δt should be also adjusted (decreased) for having a stable and convergent solution.

In the OpenFOAM® simulations usually Co is calculated in a way to make sure maximum Courant number in the whole domain is less than 1. It is assumed $Co = 1$, and for Δx smallest cell size and for u maximum velocity magnitude in domain is selected. Then using these data, Δt is calculated. It is a rough estimation, but always helps to keep $Co < 1$!

Note: In the 10000 cell case with 10 bar and 0.1 bar, the simulation will crash with the default Δt ($1e-5$); After checking the same case with 1000 cells, you will find that the maximum Co is around 0.6:

```
Time = 0.001
```

```
Courant Number mean: 0.0508555 max: 0.589018
diagonal: Solving for rho, Initial residual = 0, Final residual = 0, No
Iterations 0
```

In the case with 10000 cells, the number of cells is increased by factor 10, so the cell size is reduced by factor 10. For keeping the Courant number in the same range (around 0.6), according to the above equation, Δt should be decreased by factor 10. After reducing it to $1e-6$ the simulation will run smoothly.

Note: After running `setFields` for the first time, the files in the 0 directory are overwritten. If the mesh will be changed these files are not compatible with the new mesh and the simulation will fail. To solve this problem replace the files in the 0 directory with the files in the 0.org. In the OpenFOAM® files or directories with suffix ".org" ("original") usually contain the backup files. If a command changes the original files these files can be replaced.

Exporting simulation

The simulation results are as follows:

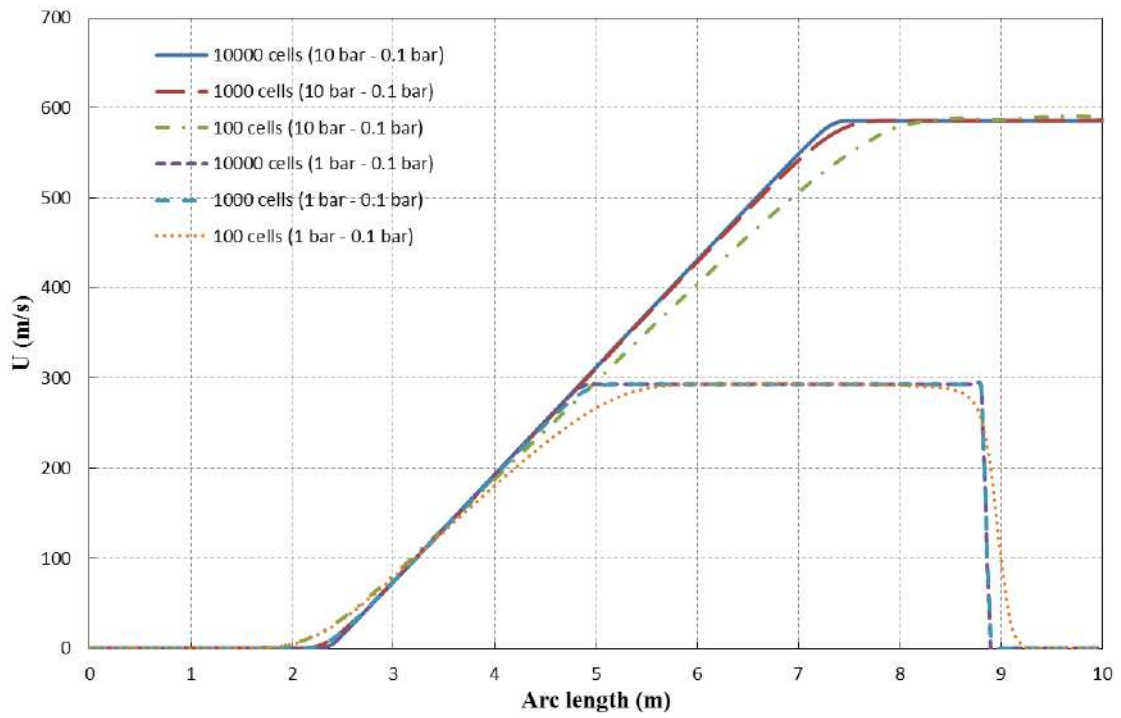


Figure 3.1 Velocities for different configurations along tube at $t = 0.007$ s

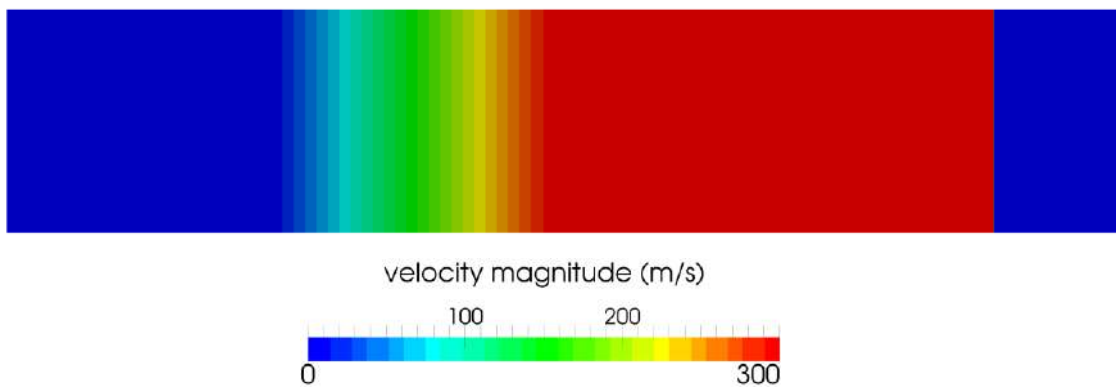


Figure 3.2 Velocity along tube axis for 10 bar/0.1 bar and 10000 cells case at $t = 0.007$ s

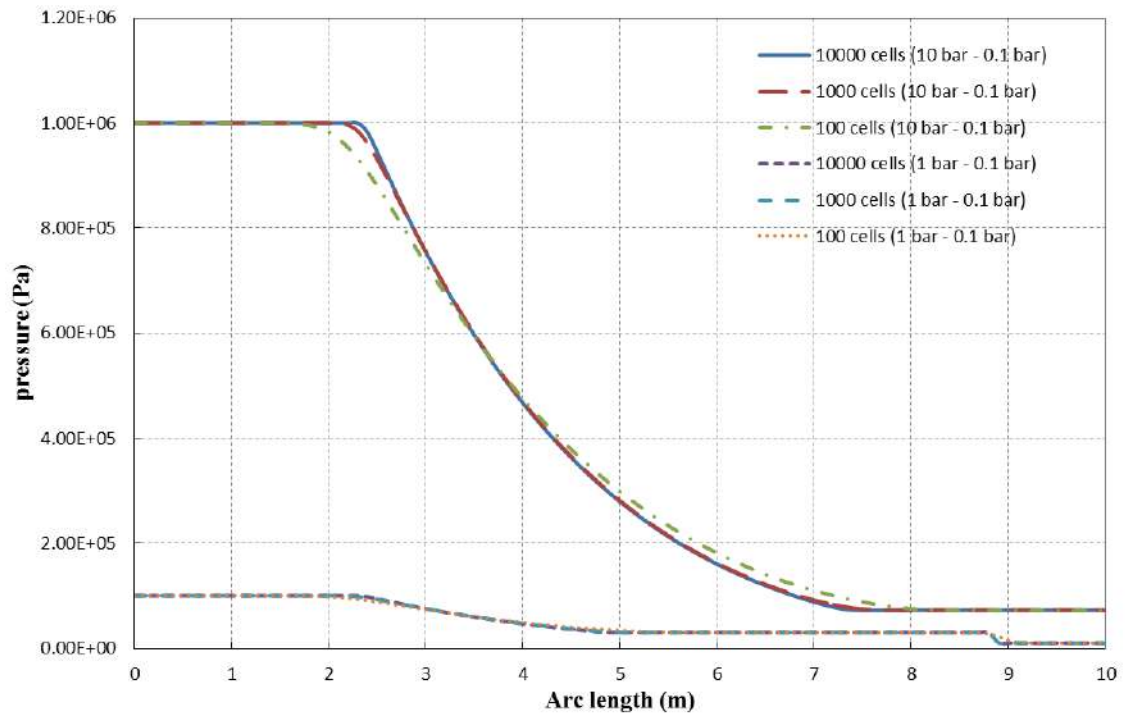


Figure 3.3 Pressures for different configurations along tube at $t = 0.007$ s

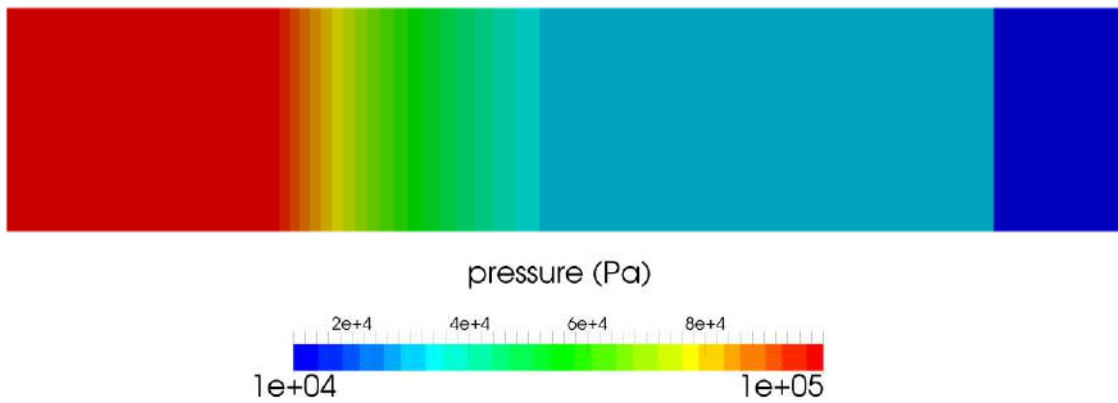


Figure 3.4 Pressure along tube axis for 10 bar/0.1bar and 10000 cells case at $t = 0.007$ s

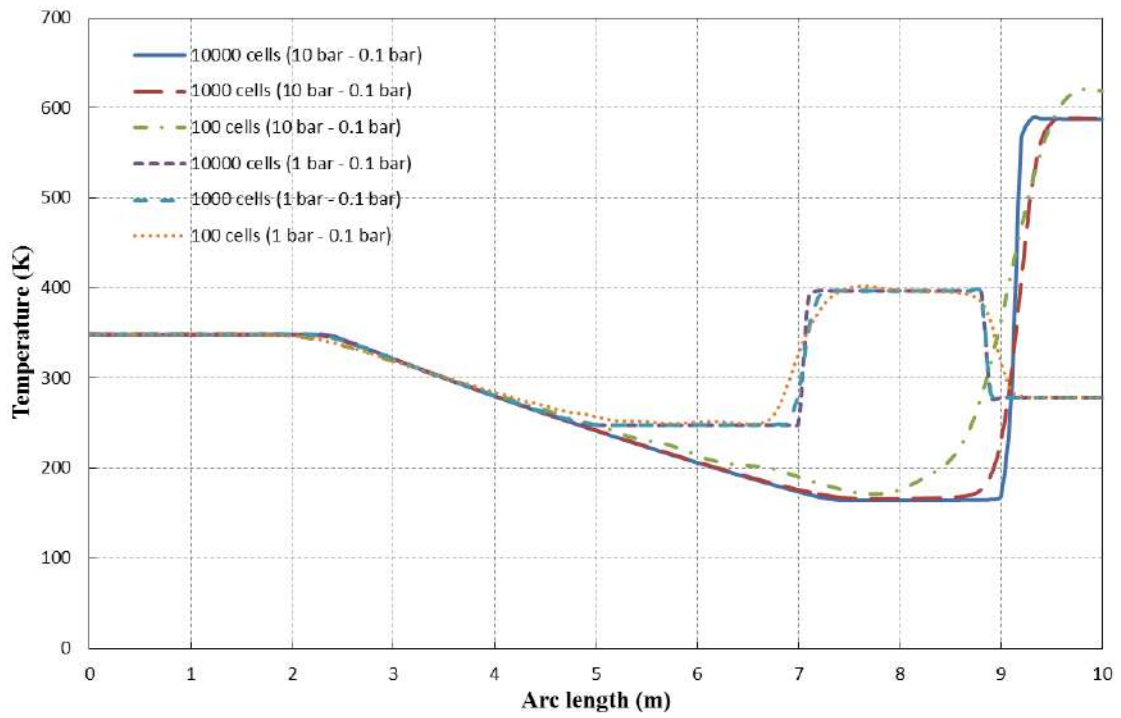


Figure 3.5 Temperature for different configurations along tube at $t = 0.007$ s

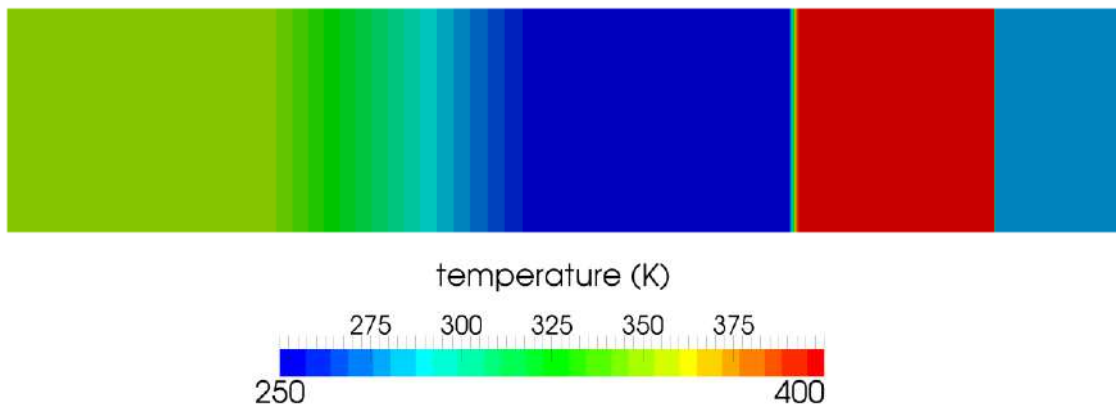


Figure 3.6 Temperature along tube axis for 10 bar/0.1 bar and 10000 cells case at $t = 0.007$ s

scalarTransportFoam – shockTube (discretization)

Simulation

Use the scalarTransportFoam solver, simulate 5 s of flow inside a shock tube, with 1D mesh of 1000 cells (10 m long geometry from -5 m to 5 m). Patch with a scalar of 1 from -0.5 to 0.5. Simulate following cases:

- Set U to uniform (0 0 0). Vary diffusion coefficient (low, medium and high value).
- Set the diffusion coefficient to zero and also U to (1 0 0) and run the simulation in the case of pure advection using following discretization schemes:
 - upwind
 - linear
 - linearUpwind
 - QUICK
 - cubic

Objectives

- Understanding different discretization schemes.

Post processing

Import your simulation into ParaView, and plot temperature along tube length.

As it was mentioned before, the discretization scheme for each operator of the governing equations can be set in `fvSchemes`.

```
// * * * * *
ddtSchemes
{
    default            Euler;
}

gradSchemes
{
    default            Gauss linear;
}

divSchemes
{
    default            none;
    div(phi,T)        Gauss linearUpwind grad(T);
}

laplacianSchemes
{
    default            none;
    laplacian(DT,T)    Gauss linear corrected;
}

interpolationSchemes
{
    default            linear;
}

snGradSchemes
{
    default            corrected;
}

fluxRequired
{
    default            no;
    T                  ;
}
// * * * * *
```

For each type of operation a default scheme can be set (e.g. for `divSchemes` is set to `none`, it means no default scheme is set). Also a special type of discretization for each element can be assigned (e.g. `div(phi,T)` it is set to `linearUpwind`). For each element, which a discretization method has not been set, the default method will be applied and if the default setting is `none` and no scheme is set for that element the simulation will crash.

Note: The general transport equation for property φ looks like the following:

$$\frac{\partial(\rho\varphi)}{\partial t} + \nabla \cdot (\rho\varphi\mathbf{u}) - \nabla \cdot (\Gamma\nabla\varphi) = S_\varphi$$

In this equation the first term shows the rate of change of property φ with time. The second term is responsible for the advection of property φ by the fluid flow and the third term shows the diffusion of property φ .

The right hand side of the equation also refers to the source terms. By setting the diffusion coefficient (Γ , in this simulation it is `DT`) to zero, the case will be switched to a pure advection simulation with no diffusion.

Note: In fvSchemes, the schemes for the time term of the general transport equation are set in ddtSchemes sub-dictionary. divSchemes are responsible for the advection term schemes and laplacianSchemes set the diffusion term schemes.

Note: divSchemes should be applied like this: Gauss + scheme. The Gauss keyword specifies the standard finite volume discretization of Gaussian integration which requires the interpolation of values from cell centers to face centers. Therefore, the Gauss entry must be followed by the choice of interpolation scheme (www.openfoam.org).

Running simulation

```
>blockMesh
>setFields
>scalarTransportFoam
```

Exporting simulation

The simulation results are as follows.

A) Case with zero velocity (pure diffusion):

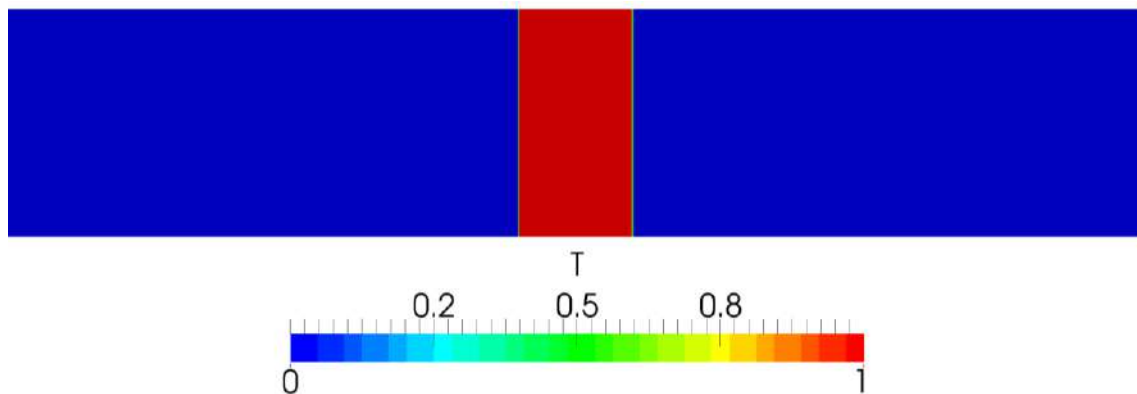


Figure 4.1 Pure diffusion with low diffusivity (0.00001) at $t = 5$ s

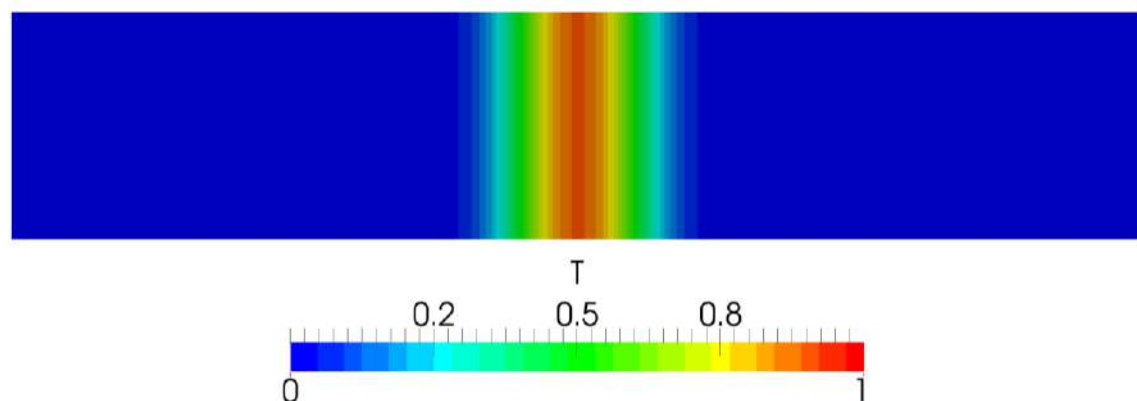


Figure 4.2 Pure diffusion with medium diffusivity (0.01) at $t = 5$ s

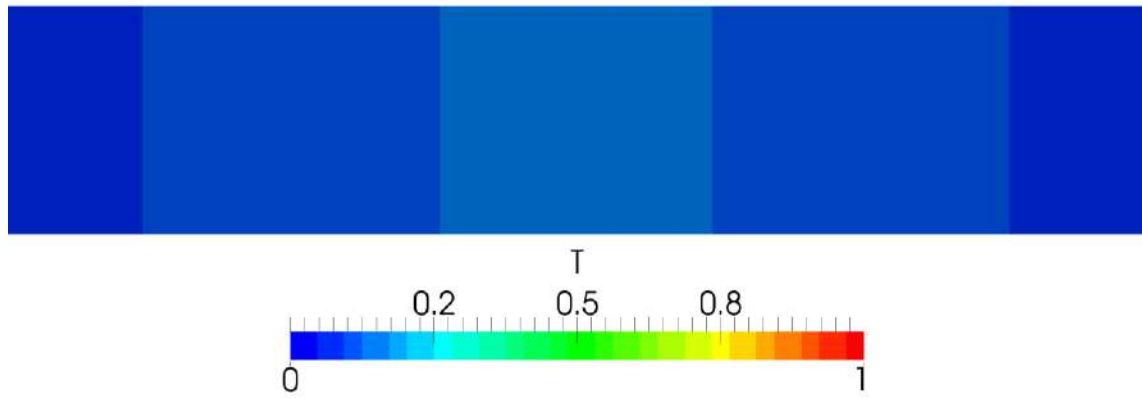


Figure 4.3 Pure diffusion with high diffusivity (1) at $t = 5$ s

B) Case with pure advection (diffusion coefficient = 0):

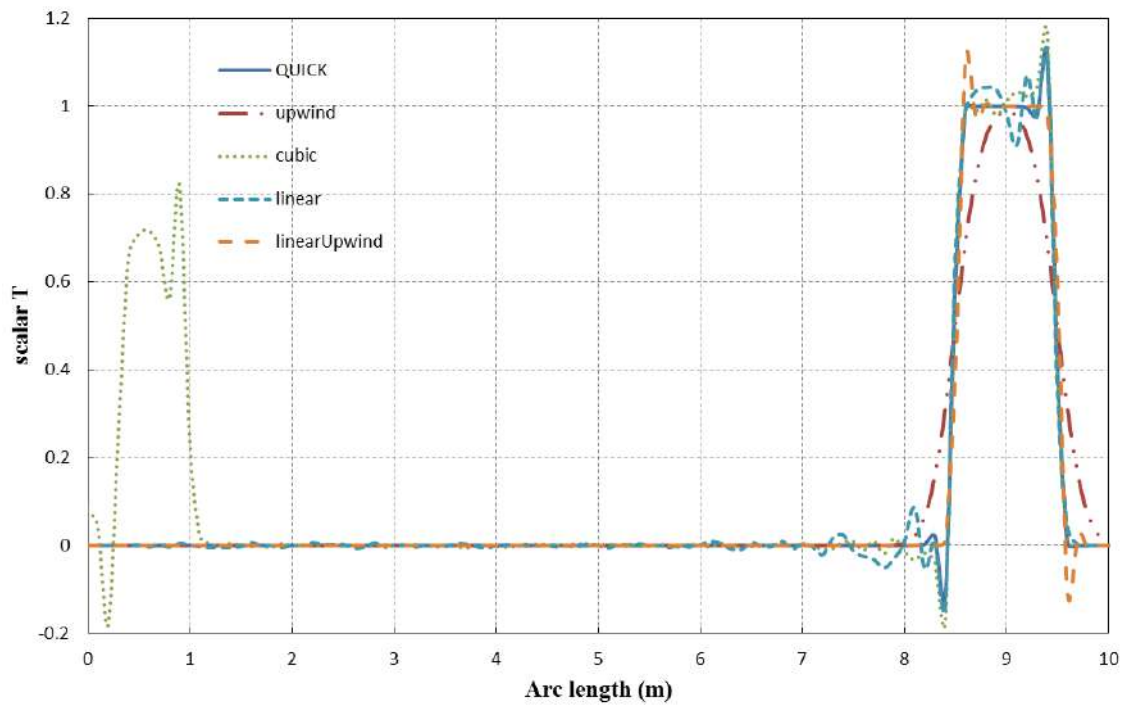


Figure 4.4 Scalar T along tube at $t = 4$ s

scalarTransportFoam – circle (discretization)

Simulation

Use the scalarTransportFoam solver, do simulate the movement of a circular scalar spot region (radius = 1 m) at the middle of a 100×100 cell mesh ($10 \text{ m} \times 10 \text{ m}$), then move it to the right, to the top and diagonally.

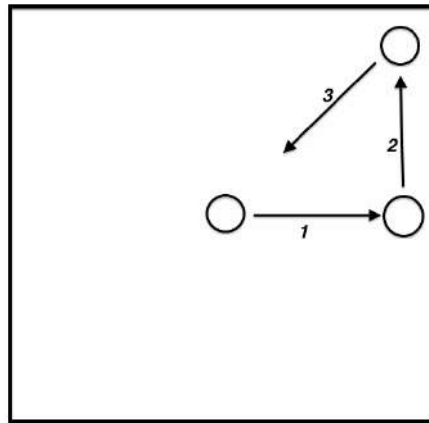


Figure 5.1 Schematic sketch of the problem

Objectives

- Choosing the best discretization scheme.

Post processing

Examine your simulation in ParaView.

Exporting simulation

The simulation results are as follows:

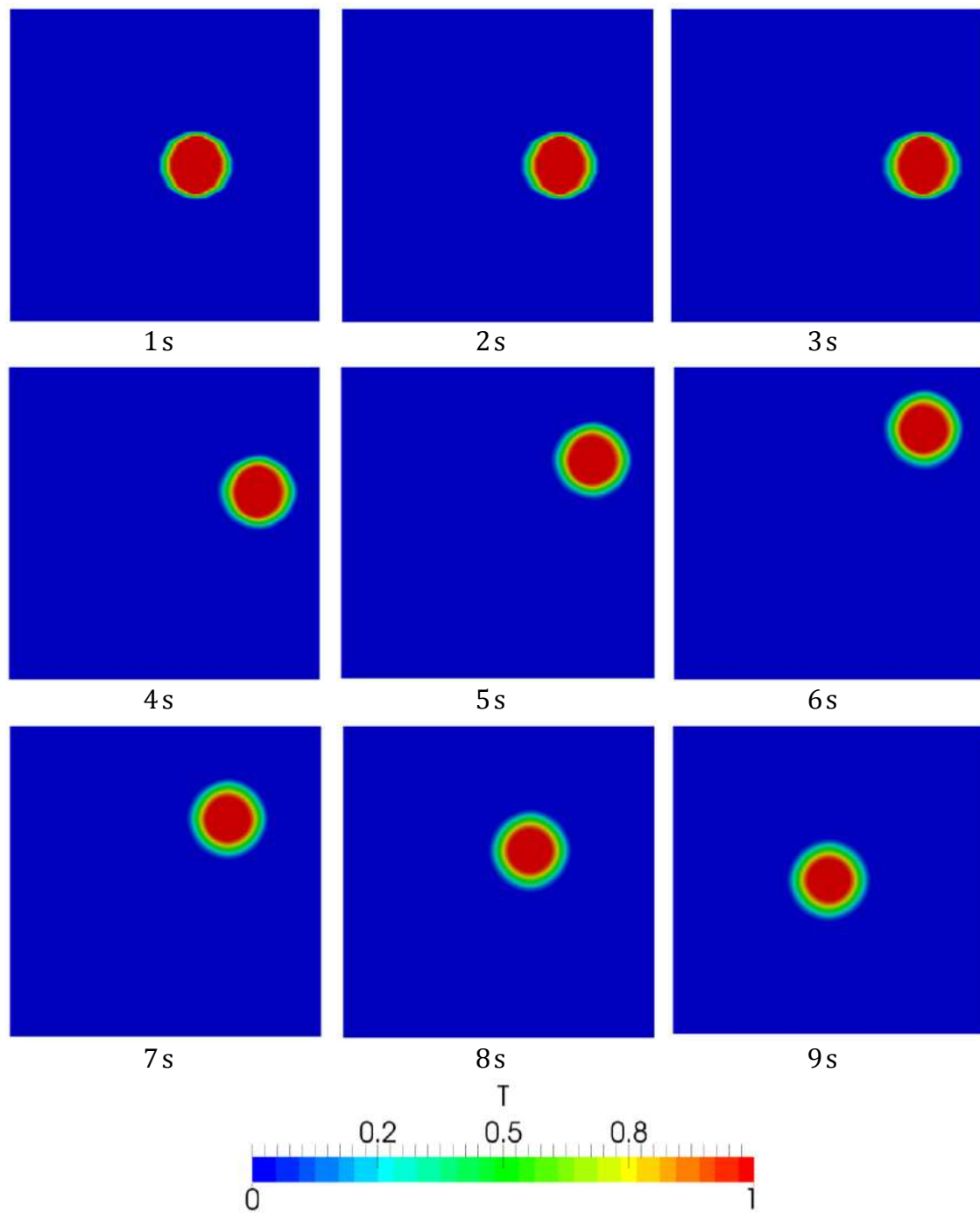


Figure 5.2 Position of the circle at different time steps

simpleFoam – pitzDaily (turbulence, steady state)

Simulation

Use simpleFoam solver, run a steady state simulation with following turbulence models:

- kEpsilon (RAS)
- kOmega (RAS)
- LRR (RAS)

Objectives

- Understanding turbulence modeling
- Understanding steady state simulation

Post processing

Show the results of U and the turbulent viscosity in two separate contour plots.

Step by step simulation

Copy tutorial

```
~/OpenFOAM/OpenFOAM-2.3.0/tutorials/incompressible/simpleFoam
/pitzDaily
```

0 directory

When a turbulent model is chosen, the value of its constants and its boundary values should be set in the appropriate files. For example in kEpsilon model the k and epsilon files should be edited, e.g. epsilon:

```
// * * * * * //
dimensions      [0 2 -3 0 0 0 0];
internalField   uniform 14.855;

boundaryField
{
    inlet
    {
        type          fixedValue;
        value          uniform 14.855;
    }
    outlet
    {
        type          zeroGradient;
    }
    upperWall
    {
        type          epsilonWallFunction;
        value          uniform 14.855;
    }
    lowerWall
    {
        type          epsilonWallFunction;
        value          uniform 14.855;
    }
    frontAndBack
    {
        type          empty;
    }
}
// ***** //
```

Note: Here is a list of files which should be available at 0 directory and need to be modified for each turbulence model:

- *laminar: no file*
- *kEpsilon (RAS): k and epsilon*
- *kOmega (RAS): k and omega*
- *LRR (RAS): k, epsilon and R*
- *Smagorinsky (LES): nuSgs*
- *oneEqEddy (LES): k and nuSgs*

- *SpalartAllmaras (LES): nuSgs and nuTilda*

Some files are available, e.g. epsilon, k and nuTilda, some files should be created by the user, e.g. R, omega. Templates for these files can be also found in the examples of older versions of OpenFOAM®, e.g. 1.7.1.

Note: A missing R file can be created by OpenFOAM®. In the constant directory in RASProperties file set the RASModel to kEpsilon. The turbulenceProperties file is also needed. Copy it from another tutorial and set simulationType to RASModel in the file. Run the command “R” from terminal, it will create the R file in the 0 directory.

constant directory

The type of simulation turbulence model is set in turbulenceProperties file, e.g. it is a RASModel or LESModel (this file is not available in this tutorial, but can be copied from other tutorials). For choosing a specific turbulence model the RASProperties file should be checked (e.g. here kEpsilon).

```
// * * * * *
RASModel          kEpsilon;

turbulence        on;

printCoeffs       on;

// *****
```

Note: For the laminar model both turbulenceProperties and RASProperties should be set to laminar. In the RASProperties set turbulence and also printCoeffs to off.

system directory

Note: Since it is a steady state simulation in controlDict endTime shows the number of iterations instead of time and deltaT should be 1, because it is the amount of increase in the iteration number.

Running simulation

```
>blockMesh
>simpleFoam
```

Note: When the solution converges, “SIMPLE solution converged in ... iterations” message will be displayed in the Shell window. If nothing happens and you do not see a message after a while (this is not the case in here, it converges after a short time), then you should check the residuals which are displayed in the Shell window manually (you should check initial residual values, it shows the difference between this iteration and the last one), if all of the Initial residual (see below) values are close to amounts you have set in the fvSolution then you can stop simulation (ctrl+c).

Time = 817

```
smoothSolver: Solving for Ux, Initial residual = 0.00013826, Final residual =
9.87886e-06, No Iterations 2
smoothSolver: Solving for Uy, Initial residual = 0.000994709, Final residual =
7.317e-05, No Iterations 2
GAMG: Solving for p, Initial residual = 0.00192871, Final residual =
0.000174838, No Iterations 7
time step continuity errors : sum local = 0.000840075, global = 6.13868e-05,
cumulative = -0.193739
smoothSolver: Solving for epsilon, Initial residual = 0.000175322, Final
residual = 1.138e-05, No Iterations 2
smoothSolver: Solving for k, Initial residual = 0.000404928, Final residual =
2.99083e-05, No Iterations 2
ExecutionTime = 20.11 s ClockTime = 20 s
```

SIMPLE solution converged in 817 iterations

Exporting simulation

The simulation results are as follows (all simulations scaled to the same range):

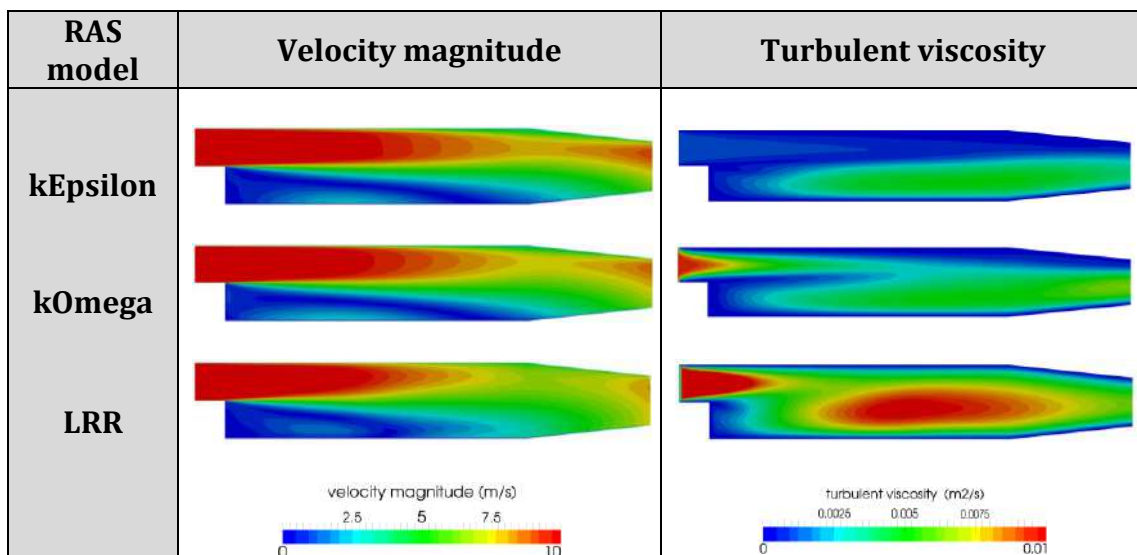


Figure 6.1 Comparison of different turbulent models at steady state

pisoFoam – pitzDaily (turbulence, transient)

Simulation

Use the pisoFoam solver, run a backward facing step case for 0.2 s with different turbulence models:

- Smagorinsky (LES)
- oneEqEddy (LES)
- kEpsilon (RAS)

Objectives

- Understanding turbulence models
- Understanding the difference between transient and steady state simulation
- Finding appropriate turbulence model

Post processing

Display the results of U and the turbulent viscosity in two separate contour plots at three different time steps. Compare with steady state simulation (example 6).

Step by step simulation

Copy tutorial

Copy the tutorial from the following directory to your working directory:

```
~/OpenFOAM/OpenFOAM-2.3.0/tutorials/incompressible/pisoFoam
/les/pitzDaily
```

0 directory

Set the turbulence model initial and boundary values.

Note: For different turbulent models, different constant files should be modified (check example 6).

constant directory

As mentioned in example 6, in turbulenceProperties the turbulent model type has to be set.

```
// * * * * * //
simulationType  LESModel;
// ***** //
```

For setting a turbulence model, if RAS models are being used, in the constant directory there is the RASProperties file and we should modify it, but if LES models are used the LESProperties file should be found and modified.

```
// * * * * * //
LESMoDel      oneEqEddy;
delta         cubeRootVol;
printCoeffs   on;
cubeRootVolCoeffs
{
    deltaCoeff  1;
}
PrandtlCoeffs
{
    delta         cubeRootVol;
    cubeRootVolCoeffs
    {
        deltaCoeff  1;
    }
    smoothCoeffs
    {
        delta         cubeRootVol;
        cubeRootVolCoeffs
        {
            deltaCoeff  1;
        }
        maxDeltaRatio  1.1;
    }
}
Cdelta        0.158;
```

```

}

vanDriestCoeffs
{
    delta            cubeRootVol;
    cubeRootVolCoeffs
    {
        deltaCoeff    1;
    }

    smoothCoeffs
    {
        delta            cubeRootVol;
        cubeRootVolCoeffs
        {
            deltaCoeff    1;
        }

        maxDeltaRatio    1.1;
    }

    Aplus            26;
    Cdelta            0.158;
}

smoothCoeffs
{
    delta            cubeRootVol;
    cubeRootVolCoeffs
    {
        deltaCoeff    1;
    }

    maxDeltaRatio    1.1;
}

// ***** //

```

Running simulation

```

>blockMesh
> pisoFoam

```

Exporting simulation

The simulation results are as follows:

For the kEpsilon model after 0.2 s the results are similar to the steady state simulation. Therefore, it can be assumed it has reached the steady state. Other models do not have a steady situation and are fluctuating all the time, so they require averaging for obtaining steady state results.

kEpsilon and other RAS models use averaging to obtain the turbulence values, but LES does not include any averaging by default. Therefore, LES simulations should use a higher grid resolution (smaller cells) and smaller time steps (for reasonable Co number). Contour plots or other LES results should be presented time averaged over reasonable number of time steps (not done in this example).

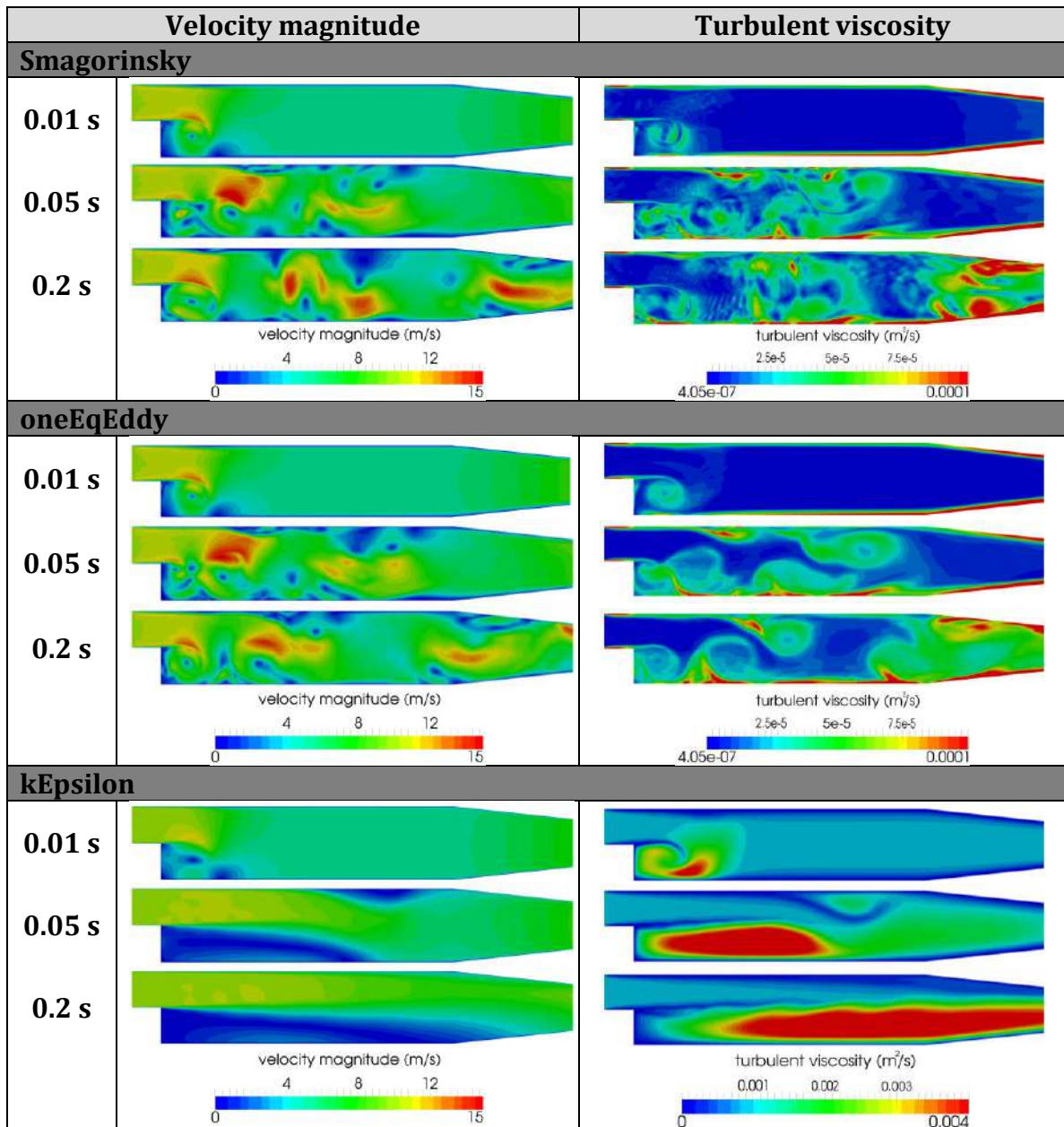


Figure 7.1 Comparison of different turbulent models for transient simulation.

interFoam – damBreak (multiphase)

Simulation

Use the interFoam solver to simulate breaking of a dam for 2s.

Objectives

- Understanding how to set viscosity, surface tension and density for two phases

Post processing

See the results in ParaView.

Step by step simulation

Copy tutorial

Copy tutorial from the following folder to your working directory:

```
~/OpenFOAM/OpenFOAM-2.3.0/tutorials/multiphase/interFoam
/laminar/damBreak
```

0 directory

In the 0 directory following files exist:

```
alpha.water.org  p_rgh  U
```

In the `alpha.water.org` and `p_rgh` files the initial values and also boundary conditions for phase water and also pressure are set. Copy `alpha.water.org` to `alpha.water` (remember: the `*.org` files are back up files, and solvers do not use them). E.g. `alpha.water`:

```
// * * * * * //
dimensions      [0 0 0 0 0 0 0];
internalField   uniform 0;
boundaryField
{
    leftWall
    {
        type            zeroGradient;
    }
    rightWall
    {
        type            zeroGradient;
    }
    lowerWall
    {
        type            zeroGradient;
    }
    atmosphere
    {
        type            inletOutlet;
        inletValue      uniform 0;
        value            uniform 0;
    }
    defaultFaces
    {
        type            empty;
    }
}
// ***** //
```

Note: *The inletOutlet and the outletInlet boundary conditions are used when the flow direction is not known. In fact, these are derived types and are a combination of two different boundary types.*

- inletOutlet: *When the flux direction is toward the outside of the domain, it works like a zeroGradient boundary condition and when the flux is toward inside the domain it is like a fixedValue boundary condition.*
- outletInlet: *This is the other way around, if the flux direction is toward outside the domain, it works like a fixedValue boundary condition and when the flux is toward inside the domain, it is like a zeroGradient boundary condition.*

E.g. if the velocity field outlet is set as inletOutlet and the inletValue is set to (0 0 0), it avoids backflow at the outlet! The “inletValue” or “outletValue” are values for fixedValue type of these boundary conditions and “value” is a dummy entry for OpenFOAM® for finding the variable type. Using (0 0 0), OpenFOAM® understands that the variable is a vector.

constant directory

In the transportProperties file the properties of two phases can be set under each phase sub-dictionary, e.g. water or air:

```
// * * * * *
phases (water air);

water
{
    transportModel    Newtonian;
    nu                nu [ 0 2 -1 0 0 0 0 ] 1e-06;
    rho              rho [ 1 -3 0 0 0 0 0 ] 1000;
    CrossPowerLawCoeffs
    {
        nu0          nu0 [ 0 2 -1 0 0 0 0 ] 1e-06;
        nuInf        nuInf [ 0 2 -1 0 0 0 0 ] 1e-06;
        m            m [ 0 0 1 0 0 0 0 ] 1;
        n            n [ 0 0 0 0 0 0 0 ] 0;
    }

    BirdCarreauCoeffs
    {
        nu0          nu0 [ 0 2 -1 0 0 0 0 ] 0.0142515;
        nuInf        nuInf [ 0 2 -1 0 0 0 0 ] 1e-06;
        k            k [ 0 0 1 0 0 0 0 ] 99.6;
        n            n [ 0 0 0 0 0 0 0 ] 0.1003;
    }
}

air
{
    transportModel    Newtonian;
    nu                nu [ 0 2 -1 0 0 0 0 ] 1.48e-05;
    rho              rho [ 1 -3 0 0 0 0 0 ] 1;
    CrossPowerLawCoeffs
    {
        nu0          nu0 [ 0 2 -1 0 0 0 0 ] 1e-06;
        nuInf        nuInf [ 0 2 -1 0 0 0 0 ] 1e-06;
        m            m [ 0 0 1 0 0 0 0 ] 1;
        n            n [ 0 0 0 0 0 0 0 ] 0;
    }

    BirdCarreauCoeffs
    {
        nu0          nu0 [ 0 2 -1 0 0 0 0 ] 0.0142515;
        nuInf        nuInf [ 0 2 -1 0 0 0 0 ] 1e-06;
    }
}
```

```

        k          k [ 0 0 1 0 0 0 0 ] 99.6;
        n          n [ 0 0 0 0 0 0 0 ] 0.1003;
    }
}

sigma          sigma [ 1 0 -2 0 0 0 0 ] 0.07;

// ***** //

```

In both phases the coefficients for different models of viscosity are given, e.g. `nu`, `CrossPowerLawCoeffs` and `BirdCarreauCoeffs`.

Depending on which model is selected, the coefficients from the corresponding sub-dictionary are read. The selected model is `Newtonian`, only the `nu` coefficient is used and the others remain unused (`CrossPowerLawCoeffs` and `BirdCarreauCoeffs`).

`sigma` is the surface tension between two phases, in this example it is the surface tension between air and water.

Checking the `g` file, the gravitational field and also its direction are defined, it is 9.81 m/s^2 in the negative `y` direction.

```

// * * * * * //

dimensions      [0 1 -2 0 0 0 0];
value          ( 0 -9.81 0 );

// ***** //

```

Running simulation

```

>blockMesh
>setFields
>interFoam

```

Exporting simulation

The simulation results are as follows (these are not the results for the original mesh, but a 2x refined finer mesh):

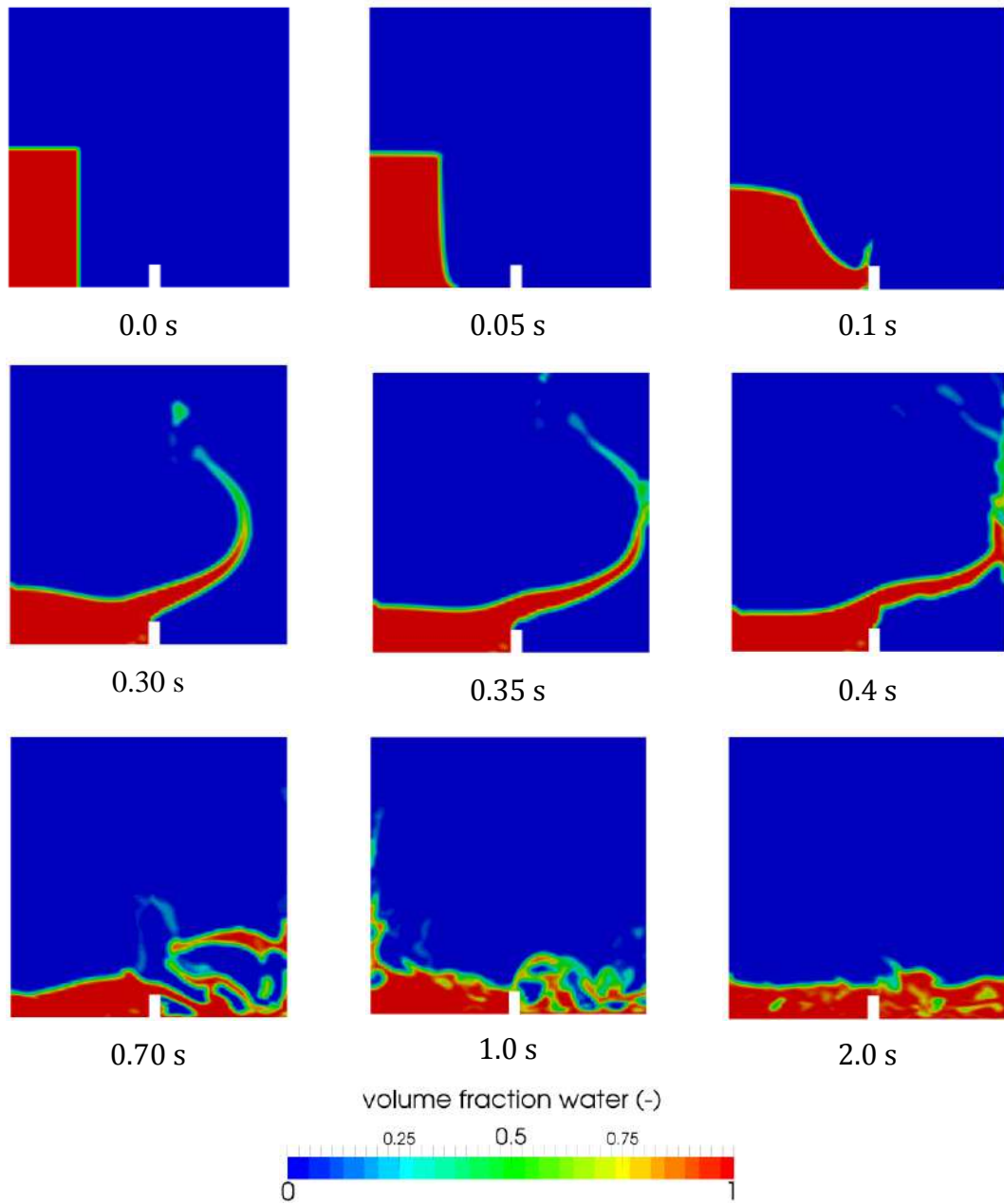


Figure 8.1 Contours of the water volume fraction at different time steps

compressibleInterFoam – depthCharge3D

Simulation

Use the compressibleInterFoam solver, simulate the example case for 0.5 s.

Objectives

- Understanding the difference between incompressible and compressible solvers
- Understanding parallel processing and different discretization methods

Post processing

Investigate the results in ParaView.

Step by step simulation

Copy tutorial

Copy the tutorial from following directory to your working directory:

```
~/OpenFOAM/OpenFOAM-2.3.0/tutorials/multiphase/
compressibleInterFoam/laminar/depthCharge3D
```

0 directory

Copy alpha.water.org, p_rgh.org, p.org and T.org to alpha.water, p_rgh, p and T files.

constant directory

Phases and common physical properties of the two phases are set in the thermophysicalProperties file. Individual phase properties are set in thermophysicalProperties.phase files, e.g. thermophysicalProperties.air.

```
// * * * * * //
phases (water air);
pMin          pMin [ 1 -1 -2 0 0 0 0 ] 10000;
sigma         sigma [ 1 0 -2 0 0 0 0 ] 0.07;
// ***** //
```

system directory

The decomposeParDict file includes the parallel settings, such as the number of domains (partitions) and also how the domain is going to be divided into these subdomains for parallel processing.

```
// * * * * * //
numberOfSubdomains 4;

method          hierarchical;

simpleCoeffs
{
    n              ( 1 4 1 );
    delta          0.001;
}

hierarchicalCoeffs
{
    n              ( 1 4 1 );
    delta          0.001;
    order          xyz;
}

manualCoeffs
{
    dataFile       "";
}

distributed     no;

roots           ( );
// ***** //
```

`numberOfSubdomains` should equal the number of cores used. `method` should show the method to be used. In the above example, the case is simulated with the `hierarchical` method and 4 processors.

If the `simple` method is being used, the parameter `n` must be changed accordingly. The three numbers (1 4 1) indicate the number of pieces the mesh is split into in the x, y and z directions, respectively. Their multiplication result should be equal to `numberOfSubdomains`.

If the `hierarchical` method is being used, these parameters and also the order in which the mesh should be split up in each direction should be provided.

If the `scotch` method is being used, then no user-supplied parameters are necessary except for the number of subdomains.

There is also a parameter `delta`, known as the cell skew factor. This factor is set to a default value of 0.001, and measures to what extent skewed cells should be accounted for.

Note: In order to check the quality of the mesh, the `checkMesh` tool can be used (run it from main case directory). If the message “Mesh OK” is displayed – the mesh is fine and no corrections need to be done.

If the mesh fails in one or more tests, try to recreate or refine the mesh for a better mesh quality (less non-orthogonally and skewness). If the error exists after correcting the mesh then a possible course of action is to increase the `delta` parameter (for example: to 0.01) and then rerun the `blockMesh` and `checkMesh` tools.

If non-orthogonal cells exist in a mesh, another option is using non-orthogonal corrections in the `fvSolution` file in the algorithm sub-dictionary (e.g. PIMPLE or PISO). Usually using 1 or 2 as `nNonOrthogonalCorrectors` is enough.

Running simulation

```
>blockMesh  
>setFields
```

For running the simulation in parallel mode the computing domain needs to be divided into subdomains and a core should be assigned to each subdomain. This is done by following command:

```
>decomposePar
```

This decomposes the mesh according to the supplied instructions. One possible source of error is the product of the parameters in `n` does not match up to the number of the subdomains. This appears for the `simple` and `hierarchical` methods.

After executing this command four new directories will be made in the simulation directory (`processor0`, `processor1`, `processor2` `processor3`), and each subdomain calculation will be saved in the respective processor directory.

Note: When the domain is divided to subdomains in parallel processing new boundaries are defined. The data should be exchanged with the neighbor boundary, which it is connected to in the main domain.

```
>mpirun -np <No of cores> solver -parallel > log
```

<No of cores> is the number of cores being used. solver is the solver for this simulation. For example, if 4 cores are desired, and the solver is compressibleInterFoam following command is used:

```
>mpirun -np 4 compressibleInterFoam -parallel > log
```

> log is the filename for saving the simulation status data, instead of printing them to the screen. For checking the last information which is written to this file the following command can be used during the simulation running:

```
>tail -f log
```

Note: Before running any simulation, it is important to run the top command (type the top command in the terminal), to check the number of cores currently used on the machine. Check the load average. This is on the first line and shows the average number of cores being used. There are three numbers displayed, showing the load averages across three different time scales (one, five and 15 minute respectively).

Add the number of cores you plan to use to this number – and you will get the expected load average during your simulation. This number should be less than the total number of cores in the machine – or the simulation will be slowed or the machine will crash (if you run out of memory). If you do run on a multi user server it is recommended to leave at least a few cores free, to allow for any fluctuations in the machine load.

Note: top command execution can be interrupted by typing q (or ctrl+c)

The simulation can take several hours, depending on the size of the mesh and time step size.

Exporting simulation

For exporting data for post processing, at first all the processors data should be put together and a single combined directory for each time step was created. By executing the following command all the cores data will be combined and new directories for each time step will be created in the simulation main directory:

```
>reconstructPar
```

Convert the data to ParaView format:

```
>foamToVTK
```

Note: To do the reconstruction or foamToVTK conversion from a start time until an end time the following flags can be used:

```
>reconstructPar -time [start time name, e.g. 016]:[end time name, e.g. 020]
```

```
>foamToVTK -time [start time name, e.g. 016]:[end time name, e.g. 020]
```

Using above commands without entering end time will do the reconstruction or conversion from start time to the end of available data:

```
>reconstructPar -time [start time name, e.g. 016]:
```

```
>foamToVTK -time [start time name, e.g. 016]:
```

For reconstructing or converting only one time step the commands should be used without end time and “:”:

```
>reconstructPar -time [start time name, e.g. 016]
```

```
>foamToVTK -time [start time name, e.g. 016]
```

The simulation results are as follows:

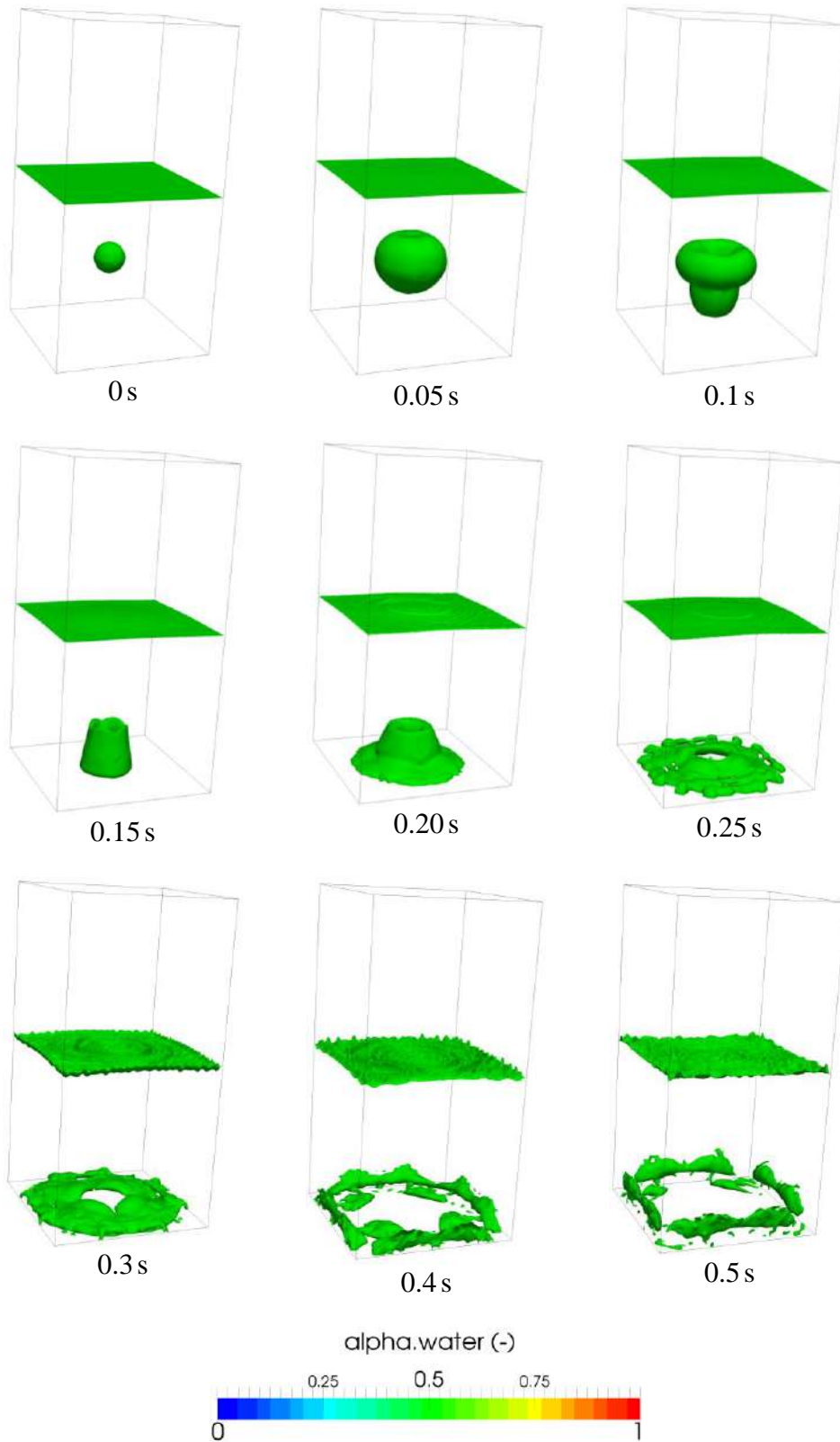


Figure 9.1 3D depth charge, alpha = 0.5 iso-surfaces, parallel simulation


```
>paraview &
```

For each of the processor directories, perform the following steps:

- Open the VTK files in the relevant processor directory
- Double click them to open them and click on “Apply”
- The part of the mesh decomposed by that core will appear, in grey.
- Change the color in the drop-down menus in the toolbar. This is to ensure that each individual part can be easily seen.

Once this is done for all processors, the entire mesh will appear. However, the processor regions can now easily be seen in a different color.

In order to save this, there are two options. The first option is to take a screenshot:

File > Save a screenshot

The second option is to save the settings and modifications as a ParaView state file.

File > Save State

The current settings and modifications can then be easily recovered by:

File > Load State

Saving the state allows changes to be made afterwards. Saving a screenshot keeps only a picture, while losing the ability to make changes after exiting ParaView. Doing both is recommended.

simpleFoam & scalarTransportFoam – TJunction (Residence Time Distribution)

Simulation

Use the simpleFoam and scalarTransportFoam to simulate the flow through a square cross section T pipe and calculate RTD (Residence Time Distribution) for both inlets using a step function injection:

- Inlet and outlet cross sections: $1 \times 1 \text{ m}^2$
- Gas in the system: air at ambient conditions
- Operating pressure: 10^5 Pa
- Inlet 1: 0.1 m/s
- Inlet 2: 0.2 m/s

Objectives

- Understanding RTD calculation using OpenFOAM[®]
- Using multiple solver for a simulation

Post processing

Plot the step response function and the RTD curve.

Step by step simulation

Copy tutorial

Copy the following tutorial to your working directory as a base case:

```
~/OpenFOAM/OpenFOAM-2.3.0/tutorials/incompressible/simpleFoam
/pitzDaily
```

0 directory

Update p, U, nut, nuTilda, k and epsilon files with the new boundary conditions, e.g. U:

```
// * * * * * //
dimensions      [0 1 -1 0 0 0 0];
internalField   uniform (0 0 0);

boundaryField
{
    inlet_one
    {
        type          fixedValue;
        value          uniform (0.1 0 0)
    }
    inlet_two
    {
        type          fixedValue;
        value          uniform (-0.2 0 0)
    }
    outlet
    {
        type          zeroGradient;
    }
    walls
    {
        type          fixedValue;
        value          uniform (0 0 0)
    }
}
// ***** //
```

constant directory

Edit the blockMeshDict in the polyMesh directory as following for creating an appropriate geometry.

```
// * * * * * //
convertToMeters 1.0;

vertices
(
    (0 4 0) // 0
    (0 3 0) // 1
    (3 3 0) // 2
    (3 0 0) // 3
    (4 0 0) // 4
    (4 3 0) // 5
    (7 3 0) // 6
    (7 4 0) // 7
    (4 4 0) // 8
    (3 4 0) // 9
    (0 4 1) // 10
)
```

```

(0 3 1) // 11
(3 3 1) // 12
(3 0 1) // 13
(4 0 1) // 14
(4 3 1) // 15
(7 3 1) // 16
(7 4 1) // 17
(4 4 1) // 18
(3 4 1) // 19

);
blocks
(
    hex (0 1 2 9 10 11 12 19) (10 30 10) simpleGrading (1 1 1)
    hex (9 2 5 8 19 12 15 18) (10 10 10) simpleGrading (1 1 1)
    hex (8 5 6 7 18 15 16 17) (10 30 10) simpleGrading (1 1 1)
    hex (2 3 4 5 12 13 14 15) (30 10 10) simpleGrading (1 1 1)
);
edges
(
);
patches
(
    patch inlet_one
    (
        (0 10 11 1)
    )
    patch inlet_two
    (
        (7 6 16 17)
    )
    patch outlet
    (
        (4 3 13 14)
    )
    wall walls
    (
        (0 1 2 9)
        (2 5 8 9)
        (5 6 7 8)
        (2 3 4 5)
        (10 19 12 11)
        (19 18 15 12)
        (18 17 16 15)
        (15 14 13 12)
        (0 9 19 10)
        (9 8 18 19)
        (8 7 17 18)
        (2 1 11 12)
        (3 2 12 13)
        (5 4 14 15)
        (6 5 15 16)
    )
);

mergePatchPairs
(
);
// ***** //

Check RASProperties file for the turbulence model (kEpsilon).

// * * * * * //
RASModel          kEpsilon;

turbulence        on;

printCoeffs       on;
// ***** //

```

Running simulation

```
>blockMesh
```

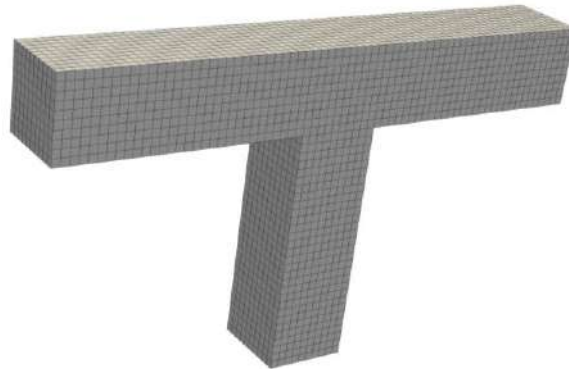


Figure 10.1 mesh created using blockMesh

```
>simpleFoam
```

Wait for simulation to converge. After convergence check the results to be sure the solution is converged (?).

```
>foamToVTK
```

The simulation results are as follows (results are on the cut plane in the middle):

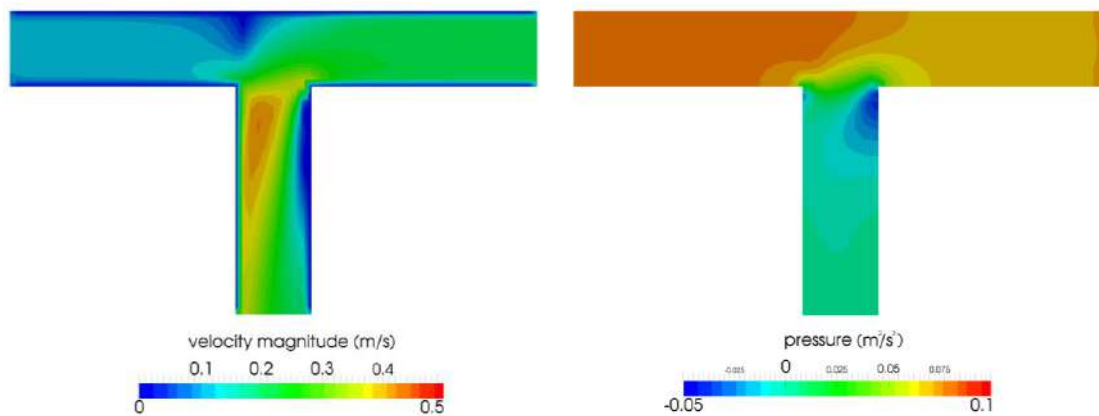


Figure 10.2 Simulation results after convergence (114 iterations)

RTD calculation

Copy tutorial

Copy following tutorial to your working directory:

```
~/OpenFOAM/OpenFOAM-2.3.0/tutorials/basic/scalarTransportFoam  
/pitzDaily
```

0 directory

Delete the U file and replace it with the calculated velocity field from the first part of the tutorial (use the latest time step velocity field from previous part of simulation to

calculate RTD for this geometry). There is no need to modify or change it. The solver will use this field to calculate the scalar transportation.

Update T (T will be used as an inert scalar in this simulation) file boundary conditions to match new simulation boundaries, to calculate RTD of the `inlet_one` set the `internalField` value to 0, T value for `inlet_one` to 1.0 and T value for `inlet_two` to 0.

constant directory

Replace the `blockMeshDict` file with the one from the first part of tutorial.

system directory

In the `controlDict` file change the `endTime` from 0.1 to 120 (approximately two times ideal residence time) and also `deltaT` from 0.0001 to 0.1 (Courant number approximately 0.4).

Running simulation

```
>blockMesh
>scalarTransportFoam
>foamToVTK
```

Simulation results

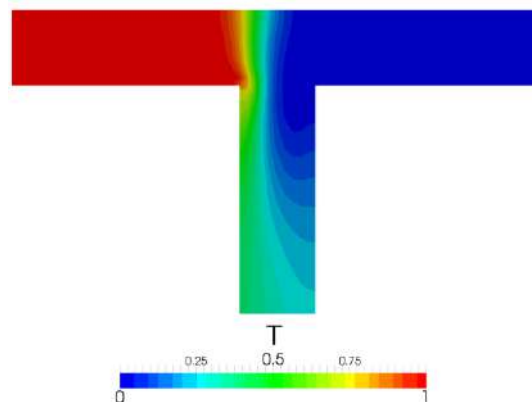


Figure 10.3 Contour plots scalar T at 120 s for inlet 1

Calculating RTD

To calculate RTD the average T value at the outlets should be calculated first. The “integrate variables function” of ParaView can be used for this purpose.

```
>foamToVTK
```

Load the outlet VTK file into paraview using following path:

File > Open > VTK > outlet > outlet_..vtk > OK > Apply

Select T from variables menu, and then integrate the variables on the outlet:

Filters > Data Analysis > Integrate Variables > Apply

The values given in the opened window are integrated values in this specific time step. By changing the time step values for different time steps are displayed. As mentioned before, the average value of the property is needed. Therefore, these values should be divided by outlet area to get average values (1m × 1m).

The same procedure should be followed for calculating RTD of `inlet_two`, except T value for `inlet_one` should be 0 and for `inlet_two` it should be 1.0.

Calculating RTD

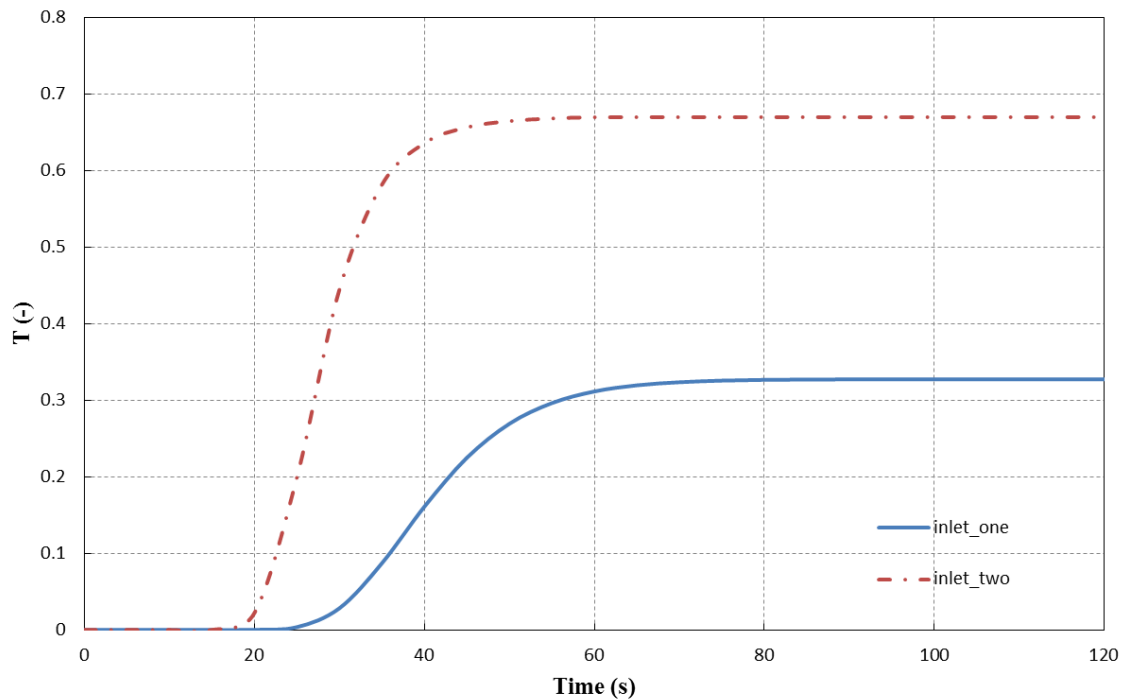


Figure 10.4 Average value of T on the outlet for two inlets versus time

The average value of T for each outlet approaches a certain constant value, which is the ratio of that scalar mass inlet to the whole mass inlet. For plotting data over time “Plot Selection Over Time” option in ParaView can be used, in the opened SpreadSheetView window (IntegrateVariables) select the set of data which you want to plot over time and then:

Filters > Data Analysis > Plot Selection Over Time > Apply

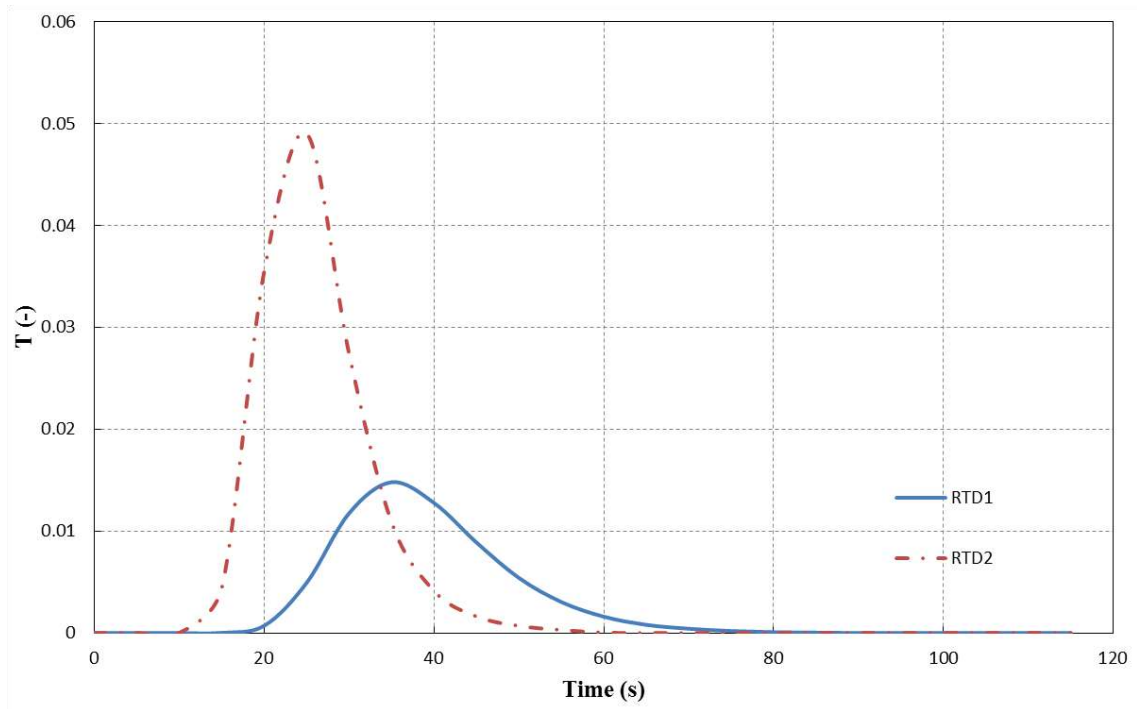


Figure 10.5 RTD of two inlets

reactingFoam – reactingElbow

Simulation

Use the reactingFoam solver, simulate combustion of CH₄ and O₂ in a mixing elbow:

- Use the two times finer Hex mesh from Example One
- Domain initially filled with N₂
- velocity-inlet-5:
 - Velocity: 1 m/s
 - Mass fractions: 23 % O₂, 77 % N₂
 - Temperature: 800 K
- velocity-inlet-6:
 - Velocity: 3 m/s
 - Mass fractions: 50 % CH₄, 50 % N₂
 - Temperature: 293 K
- Operating pressure: 10⁵ Pa
- Operating temperature: 298 K
- Isolated walls

Objective

- Understanding multi-species and reaction modeling in OpenFOAM®

Post processing

Evaluate your results in ParaView.

Step by step simulation

Copy tutorial

Copy the following tutorial to your working directory:

```
~/OpenFOAM/OpenFOAM-2.3.0/tutorials/combustion/reactingFoam
/ras/counterFlowFlame2D
```

Copy the GAMBIT mesh from example one (two times finer mesh) to the case main directory.

0 directory

Update all the files in 0 directory with new boundary conditions, e.g. U:

```
// * * * * * //
dimensions      [0 1 -1 0 0 0 0];
internalField   uniform (0 0 0);
boundaryField
{
    wall-4
    {
        type          fixedValue;
        value          uniform (0 0 0);
    }

    velocity-inlet-5
    {
        type          fixedValue;
        value          uniform (1 0 0);
    }

    velocity-inlet-6
    {
        type          fixedValue;
        value          uniform (0 3 0);
    }

    pressure-outlet-7
    {
        type          zeroGradient;
    }

    wall-8
    {
        type          fixedValue;
        value          uniform (0 0 0);
    }

    frontAndBackPlanes
    {
        type          empty;
    }
}

// ***** //
```

The reaction taking place in this simulation CH₄ combusting with O₂ creating CO₂ and H₂O. N₂ is the non-reacting species. The boundary condition and initial value of all species should be defined in the 0 directory. These values are mass fractions (between 0 and 1) and dimension less, e.g. CH₄:

```
// * * * * *
dimensions      [0 0 0 0 0 0];
internalField   uniform 0.0;

boundaryField
{
    wall-4
    {
        type      zeroGradient;
    }

    velocity-inlet-5
    {
        type      fixedValue;
        value     uniform 0; //no CH4 at this inlet
    }

    velocity-inlet-6
    {
        type      fixedValue;
        value     uniform 0.5; //50% CH4 mass fraction at this inlet
    }

    pressure-outlet-7
    {
        type      zeroGradient;
    }

    wall-8
    {
        type      zeroGradient;
    }

    frontAndBackPlanes
    {
        type      empty;
    }
}

// *****
```

Note: If the file for a species does not exist in the 0 directory, the values from Ydefault will be used for that species.

constant directory

In the thermophysicalProperties file the physical properties of the species can be set:

```
// * * * * *
thermoType
{
    type          hePsiThermo;
    mixture       reactingMixture;
    transport     sutherland;
    thermo        janaf;
    energy        sensibleEnthalpy;
    equationOfState perfectGas;
    specie        specie;
}

inertSpecie N2;

chemistryReader foamChemistryReader;

foamChemistryFile "$FOAM_CASE/constant/reactions";
```

```
foamChemistryThermoFile "$FOAM_CASE/constant/thermo.compressibleGas";
// ***** //
```

The mixture type is set to a reacting mixture for calculating the mixture properties and the heat capacities are calculated using “janaf polynomials”.

N₂ is defines as `inertSpecie`. In reaction solvers in OpenFOAM® the inert specie is calculated explicitly using the mass balance equation (to satisfy mass conservation):

$$\text{mass fraction of inert specie} = 1 - \sum \text{mass fraction of all other species}$$

The species and the reactions are addressed using `foamChemistryFile`. In this simulation reactions and species are read from reactions file in the constant directory:

```
species
(
  O2
  H2O
  CH4
  CO2
  N2
);

reactions
{
  methaneReaction
  {
    type      irreversibleArrheniusReaction;
    reaction  "CH4 + 2O2 = CO2 + 2H2O";
    A         5.2e16;
    beta      0;
    Ta        14906;
  }
}
```

The species in this simulation are O₂, H₂O, CH₄, CO₂ and N₂. They are defined in the species sub-dictionary. In the reactions sub-dictionary, reactions are specified. The reaction of methane combustion is defined and it is of type irreversible Arrhenius reaction, `irreversibleArrheniusReaction`.

In the Example Two it was explained the coefficients for calculating gas mixture properties are defined in the `mixture` sub-dictionary because it was a homogeneous mixture. But in this example the mixture is not homogenous so coefficients for calculating properties of each species are needed separately to calculate mixture properties based on each cell composition. The coefficients of each species are defined in the `foamChemistryThermoFile`, which reads the file `thermo.compressibleGas` from the constant directory, e.g. for O₂ coefficients for each model is mentioned bellow:

```
// ***** //

O2
{
  specie
  {
    nMoles      1;
    molWeight    31.9988;
  }
  thermodynamics
```

```

    {
      Tlow          200;
      Thigh         5000;
      Tcommon       1000;
      highCpCoeffs ( 3.69758 0.00061352 -1.25884e-07 1.77528e-11 -
                    1.13644e-15 -1233.93 3.18917 );
      lowCpCoeffs  ( 3.21294 0.00112749 -5.75615e-07 1.31388e-09 -
                    8.76855e-13 -1005.25 6.03474 );
    }
    transport
    {
      As          1.67212e-06;
      Ts          170.672;
    }
  }
  ...
// ***** //

```

In the `thermodynamics` sub-dictionary the janaf polynomial model coefficients for calculating the heat capacity can be found and in `transport` the sutherland model coefficients for viscosity are stored.

system directory

By setting the `adjustTimeStep` to `yes` in the `controlDict`, the solver automatically ignores `deltaT`, and calculates the `deltaT` based on the maximum Courant number `maxCo` defined for it. Change the `endTime` to 120 (approximately one time the volumetric residence time based on velocity-inlet-5) and `writeTimeInterval` to 10, to write every 10 s to case directory.

```

// * * * * * //
application      reactingFoam;

startFrom        startTime;

startTime        0;

stopAt           endTime;

endTime          120;

deltaT           1e-6;

writeControl     adjustableRunTime;

writeInterval    10;

purgeWrite       0;

writeFormat      ascii;

writePrecision   6;

writeCompression off;

timeFormat       general;

timePrecision    6;

runTimeModifiable true;

adjustTimeStep   yes;

maxCo            0.4;

```

// ***** //

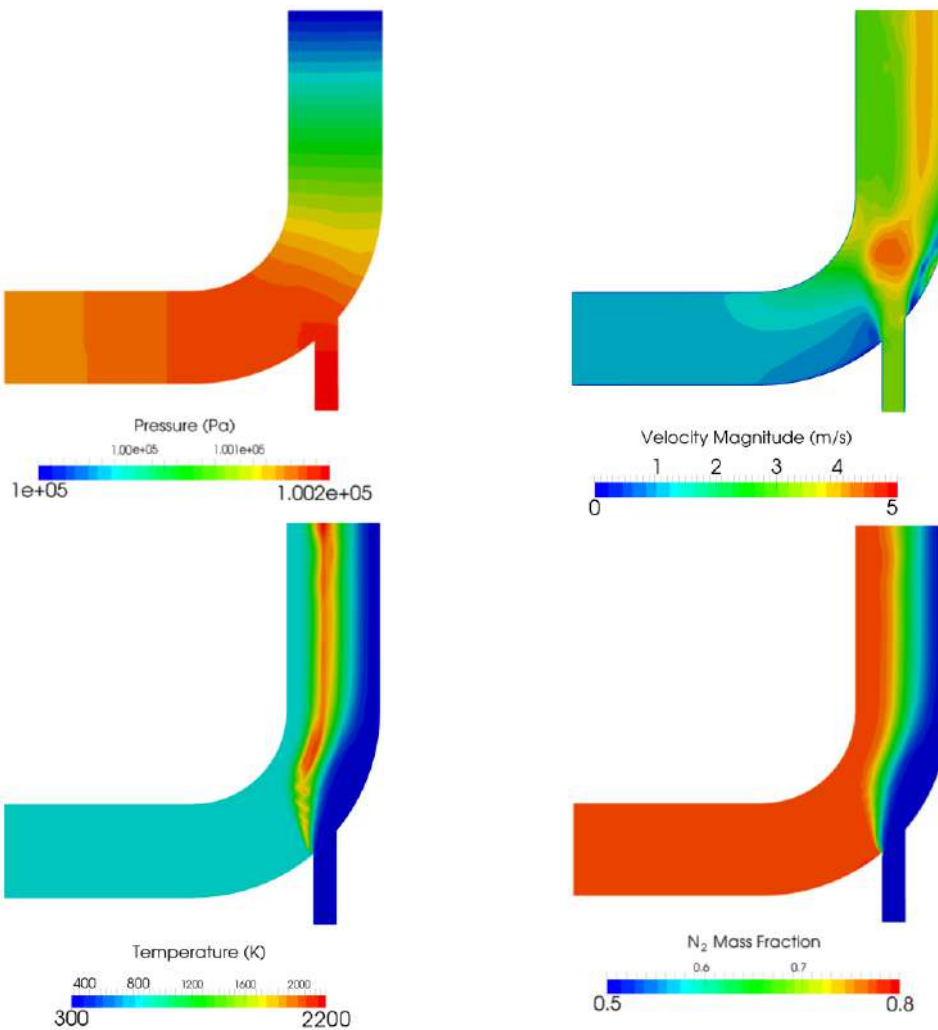
Running simulation

```
>fluentMeshToFoam fineHex.msh
```

After converting the mesh, check the boundary file in the constant/polyMesh directory and change the type and inGroups of boundary frontAndBackPlanes from wall to empty (it is a 2D simulation).

```
>reactingFoam
>foamToVTK
```

The simulation results are as follows:



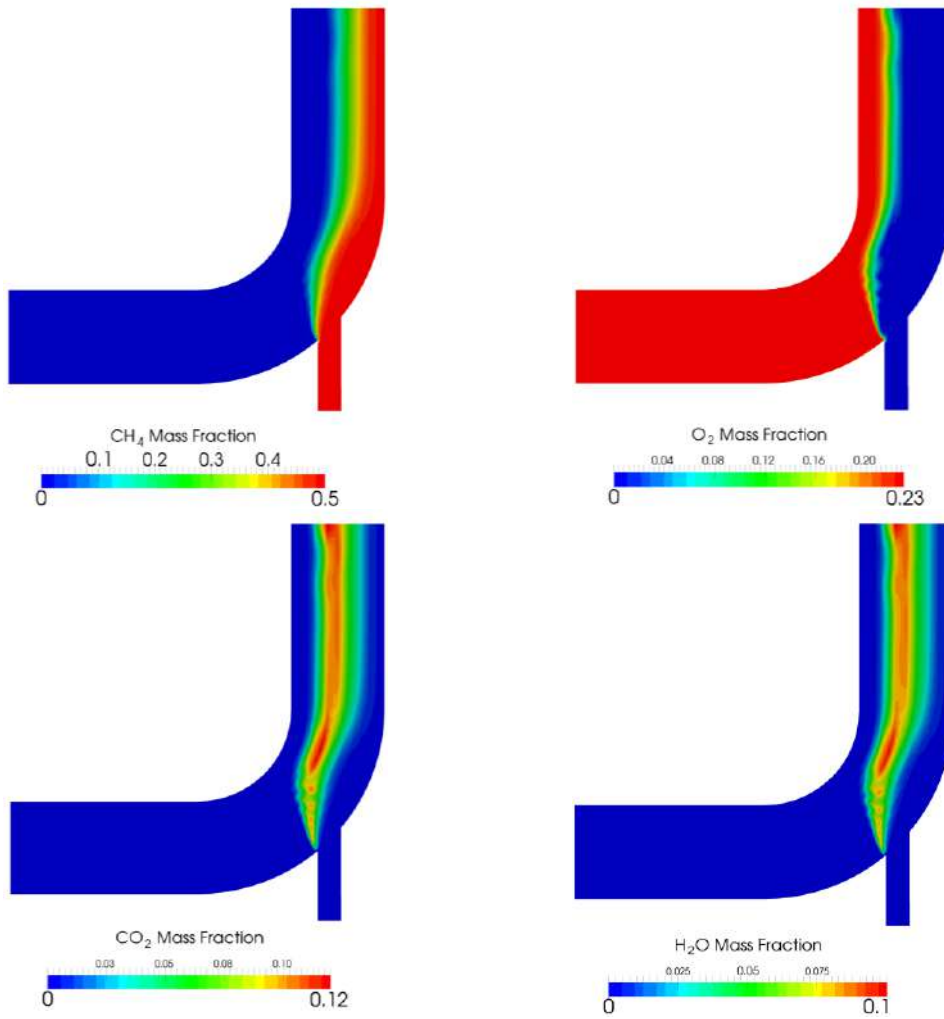


Figure 11.1 Simulation results after 120 s

Appendix A

Important commands in Linux Terminals (Mostly on Unix [IRIX, Alpha Unix... usable])

cat, more, less	File viewer with pure read function - in order of ease of operation. In <i>less</i> with <i>pagedown/pageup</i> you can navigate within the file, with / and ? can forward / backward search for strings, <i>q</i> can be used for closing <i>less</i> . <i>cat</i> is universally available on Unix.
cd, cd ..	Changing the directory, <i>cd ..</i> goes one directory up and <i>cd ~</i> moves to home directory. Important to note is the space between <i>cd</i> and .. as opposed to DOS!
cp, cp -r	Copying files or entire directory trees (with <i>-r</i> option). Caution: There is no warning or prompt when overwriting existing files! The important thing is that a target has to be always given, at least one . which means, copy to the current directory.
ctrl+r	Reverse command line search, for searching an already typed command in a terminal window.
du, du -s, du -k	Calculates the amount of space consumed in a directory. For safety reasons you should use the <i>-k</i> option (output in kilobytes), since some systems provide the space in blocks that include only 512 bytes ...
exit	Closing connection (terminal window).
gedit	Text editor with graphical user interface. When working with <i>gedit</i> some temporary files (originalFileName~) are created, they can be deleted after saving.
grep	Search command for plain-text data sets for lines matching a regular expression.
gzip, gunzip	Compression/decompression program for individual files (as opposed to <i>zip/unzip</i> , this can also work on directories or file lists). The great advantage of <i>gzip</i> : Fluent® and OpenFOAM® are able to read and write <i>gz</i> files directly, which saves about 30-90% space.
kill, kill -9	Stopping processes. For this the process ID is required, which can be

	found with <i>top</i> or <i>ps</i> . The <i>Exit</i> is irrevocable course - but you cannot shoot processes, if you are not the "owner".
ls, ls -la	Lists the contents of a directory, with option <i>-la</i> also hidden files are displayed, as well as the file size and characteristics.
mc	Program that enables navigation in the text window, esc-keys, may be necessary: <i>mc -c</i> , for navigating through mc use function keys or <i>esc+[number]</i> combination, e.g. <i>F9</i> or <i>esc+9</i> for moving to the menus at the top.
mkdir	Creates a new directory.
mv	Moving or renaming files and directories. Caution: There is no prompt when overwriting existing files!
nano, pico	The command to run the <i>nano</i> text editor, a terminal based text editor.
passwd	The command to change the login password.
	It is known as pipe and is used for merging two commands, redirecting one command as input to another, e.g. <i>less/grep</i> searches a specified word in the output of file opened with less.
ps, ps -A ps waux	Lists all the processes that were started in the respective command window with the options are all running processes on the system display.
pwd	Shows the current working directory.
rm, CAUTION: rm -fr	Deletes files. The option <i>-r</i> will also remove directories and files recursively and delete directories, <i>f</i> (force) prevents any further inquiry. - <i>Incorrectly applied, this command can lead to irreversible loss of all (private) data. There is no undelete or undo!</i>
rmdir	Deletes an empty directory.
scp	The copy command over the network - as secure FTP replacement. Also dominates the <i>-r</i> (recursive) option. Usage: <i>scp</i> source file destination file with source and the destination format can be USERNAME@

COMPUTER.DOMAIN:PATH/TO/FILE. Source or target can of course also be created locally, then (your) user name and computer are not required.

- ssh Telnet replacement with encryption used to connect to remote machines. On Windows, for example, implemented with putty.
- tail, tail -f File viewer, the default outputs the last 10 lines of a file. With option *-n XX* can spend the last XX lines, with the *-f* option, the command is running from those lines, which are attached to a file. The command is therefore perfect for watching log files.
- top Displays a constantly updated list of all running processes, with process ID, memory and CPU usage. For processes of one user *top [username]* should be used, and for quitting *q* or *ctrl+c* should be applied.
- vi, vim File editor. For forward searching use */*, for backward searching use *?*. For exiting *esc+:*. *nano* or *pico* are recommended for beginners, which are easier to handle.

Appendix B

Running OpenFOAM®

Part A) Running OpenFOAM® on a Local Linux PC (or virtual machine):

- Open a terminal
- Go to the OpenFOAM® installation directory (e.g. /opt/openfoam230) in the opened terminal
- Change to the etc directory in the OpenFOAM® installation directory
- Run the following command:

`>. ./bashrc`
- If a new terminal is opened, the same procedure should be repeated in that in order to activate OpenFOAM® in here.

Part B) Running OpenFOAM® on Remote Computers via SSH (e.g. server):

B-1) Windows:

- Run PuTTY (search for: PuTTY windows).
- Set the following:

Category>Session

Host name: openhost.university.edu

Connection type: SSH

Category>Connection>SSH>Tunnels

Source port: 5901

Destination: localhost:59**¹

- Do not forget to press *Add!*

Please make sure that this display is not used by others.

Category>Connection>Data

Auto-login username: openFoamUser

Category>Session

¹ Display number

Saved Sessions: openFoamUser

- Press *Save*.
- Now choose from “saved sessions” your session (*openFoamUser*) and press *Open*. In the opened Command (Prompt) window, it prompts for your password. The password is not echoed to the screen and the passwords are case sensitive.
- Immediately after entering your password, your computer will attempt to establish a connection to your server. If it is your first time connecting to that server, you will see a message asking you to confirm the identity of the machine. Make sure you entered the address properly, and type *yes*, followed by the *return* key, to proceed.
- To log out use whatever command is used to logout from the server you are logged into (typically `exit` / `ctrl + d`).

B-2) Mac OS X and Linux:

- Open your Terminal application. You will see a window with a \$ or > symbol and a blinking cursor. From here, you may issue the following command to establish the SSH connection to your server (be careful about upper case ‘L’ in the -gL).

```
>ssh -gL 5901:localhost:59** openFoamUser@university.edu
```

- Immediately after issuing this command, your computer will attempt to establish a connection to your server. If it is your first time connecting to that server, you will see a message asking you to confirm the identity of the machine. Make sure you have entered the address properly, and type *yes*, followed by the return key, to proceed.
- You will then be prompted to enter your password. Type or copy/paste your SSH user password into the Terminal. You will not see the cursor moving while entering your password. This is normal. Once you are finished inputting your password, press return on your keyboard. At this point, you will be connected to your server remotely through SSH.

Part C) Running OpenFOAM® in Graphical Interface (VNC):

- Connect to remote machine via SSH connection using part B.
- Make sure [VNC Server](#) is installed on the remote machine and it is started (ask administrator for display number, port and other information, for starting VNC Server check FAQ)
- Install the appropriate [VNC Viewer](#) and run it (search for: vnc viewer):

VNC Server: localhost:01

- Press *Connect*
- Press *Continue*
- Enter your password
- Press *Ok*
- On VNC desktop open a terminal
- Change to etc directory in OpenFOAM® installation directory
- Execute the following command:

```
> . ./bashrc
```
- If a new terminal in the VNC desktop is opened, the last two steps should be done in that to activate OpenFOAM® in there (or add to bashrc).

Appendix C

Frequently Asked Questions (FAQ)

Q - What should I do in case of a GAMBIT failure?

A - e.g. Program stops responding:

- Type "ps" in the command window, search for the GAMBIT process number.
- "kill -9 PROCESS NUMBER" Enter

GAMBIT creates lock files, which must also be deleted, otherwise it is not possible to open of the affected files:

- "rm *.lok" Enter

Furthermore, "junk" (temporary files from GAMBIT) should be disposed of:

- "rm -fr GAMBIT.xxx" erases the complete directory, xxx again is the process number.
- If you have forgotten to save before the crash, you should copy the file "jou" (it contains all the commands that have been executed and can be processed automatically in GAMBIT) from the directory, to resume its status before the crash.

Q - How can I prevent typing long commands in the terminal for couple of times?

A - Using cursor keys to navigate line by line.

Type beginning of the command and use Tab (auto completion).

By using reverse search, use ctrl+r to search for previous commands typed in the terminal, e.g. typing a part of command show the suggestions and you can navigate through them.

Q - My VNC is not responding from server side?

A - First you should kill your VNC server:

```
>vncserver -kill :[YOUR DISPLAY NUMBER]
```

Restart your VNC server (according to SSH forward):

```
>vncserver:[YOUR DISPLAY NUMBER] -geometry 1600x800 -depth 24
```

Q - I have deleted some of my files accidentally. What should I do?

A - Sorry, no recycling or undelete in Linux

Q - Why can I not connect to the server?

A - Check to see if you have an IP address for your network card.

Q - How can I start VNC Viewer from my Linux computer terminal?

A - Use command:

```
>vncviewer :[NUMBER OF LOCAL PORT, e.g. 1 or 2]
```

Q - Error “command not found”?

A - Make sure OpenFOAM® and ParaView are installed correctly. Check Appendix B for starting OpenFOAM®.

Q - Does foamToVTK command not work for chtMultiRegionFoam?

A - Use command:

```
>foamToVTK -region[REGION NAME]
```

Q - Is it possible to export animations from ParaView?

A - Yes, by choosing .ogv file format from “file/save animation” menu. The output will be a video file with .ogv format. In the new ParaView versions (4.3.0) the animation can also be saved using .avi format.

Q - Is there any tool in Linux to convert series of ParaView pictures to video?

A - Yes, command line tool ffmpeg:

```
>ffmpeg -r [FRAME PER SECOND RATE] -f image2 -i [images names, e.g. rho.%4d.jpg] [OUTPUT FILE NAME].[OUTPUT FILE FORMAT, e.g avi]
```

Q - How can complex geometries be patched?

A - During creating the geometry in the preprocessing software, e.g. GAMBIT, create volume zones, which you will need to patch later (see software user manual for creating regions in each software). For converting the mesh to the OpenFOAM® mesh use the appropriate tool with “-writeZones” flag to import zones to OpenFOAM®, e.g.:

```
>fluentMeshToFoam -writeZones <your mesh>
```

then in the setFieldDict change it like this:

```
regions
(
  zoneToCell
  {
    name air; // region name which you assigned in gambit
    fieldValues
    (
      volScalarFieldValue alpha.water 0 // the value of property
                                         //which you want to patch
    );
  }
);
```

Then after running setFields tool, it will assign the values to that region.

Q - How can I create a bash scripting file for executing couple of command in series?

A - Instead of typing command sequences one by one after each other and executing

them. It is possible to put all those commands in a file and execute that file to run them. This is known as “bash scripting”.

Bash scripting is typically used in the cases when the same simulation should be run with identical settings a couple of times, but with a few changes. For bash scripting create an empty file (e.g. using nano editor creating text file “go”):

```
> nano go
```

Add the commands to this file (e.g. commands for running blockMesh, setFields, decomposePar, compressibleInterFoam in parallel mode and reconstructPar):

```
blockMesh
setFields
decomposePar
mpirun -np 4 compressibleInterFoam -parallel >log
reconstructPar
```

Exit the editor and save the file (ctrl+x , y, enter for nano editor).

For changing this file to an executable file, file permissions should be set. By using this command file permissions are displayed:

```
>ls -la go
```

```
-rw-r--r-- 1 e166**** E020D166 73 Aug 23 9:15 go
```

The first ‘r’ shows that this text file can be read by user, the ‘w’ shows that user has the permission to write this file, but the ‘-’ sign shows that this file is not executable by the user. To change this permissions execute following command:

```
>chmod u+x go
```

Now this file is executable:

```
>ls -la go
```

```
-rwxr--r-- 1 e166**** E020D166 73 Aug 23 9:15 go
```

Now you can run the simulation by this executable text file:

```
>./go
```

After executing the file, the commands added to the file will be executed one by one. In most of the OpenFOAM® tutorials there are **Allrun** and **Allclean** files, which are bash scripts for running the case and cleaning a case, respectively.

Appendix D

ParaView

The visualization application, which is usually used with OpenFOAM® is ParaView (Figure D-1) which is a free, open source program. The OpenFOAM® command `foamToVTK` converts OpenFOAM® files to readable formats for ParaView.

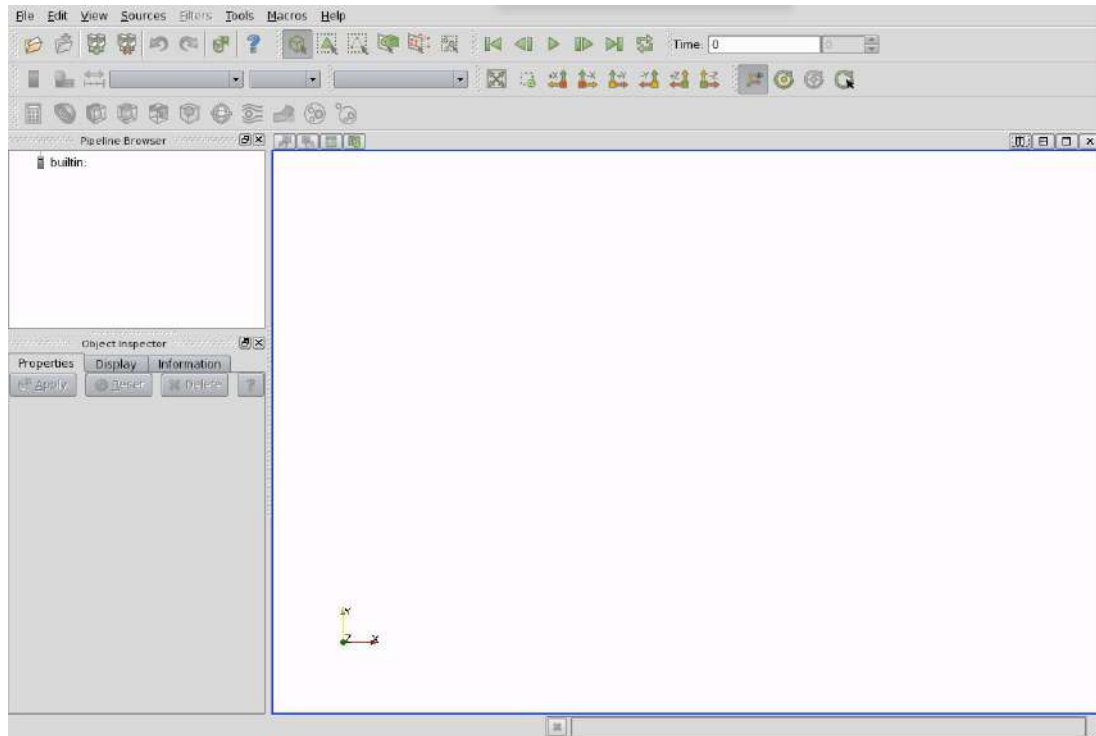


Figure D-1 The paraView window

The tree structure (“pipeline”) of ParaView helps the user to easily choose and display suitable sub-models for creating the desired image or animation. Adding a mesh or velocity vectors to a contour plot of pressure is an example of this functionality.

For general operations a selection should be made and then the green *Apply* button should be pressed. The reset button is used for resetting the window and delete deletes the selected operation.

Properties panel (Figure D-2)

Setting for time step, regions and fields can be done in the Properties panel.

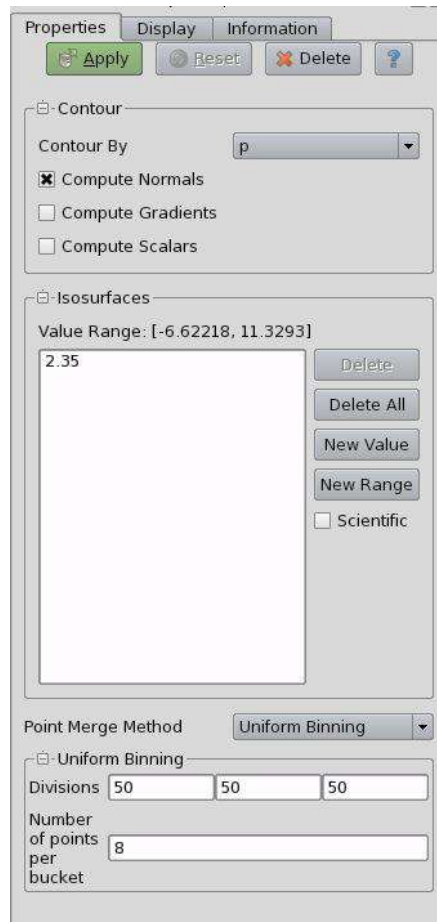


Figure D-2 The Properties panel for contour plots

Display panel (Figure D-3)

For a given case settings for visualizing the data are in the Display panel.

Some important notes:

- The max/min data range might not be updated automatically, so check and if needed, rescale the data range after appropriate intervals (e.g. after loading the case).
- Two panels can be accessed by clicking the Edit Color Map button:
 1. Color Scale panel: scale colors can be chosen, for resetting the color to standard blue to red, click choose preset, and select from opened window, Blue to Red HSV.
 2. Color Legend panel: the legend layout (e.g. the font) can be set in this panel.
- For displaying the mesh select Wireframe from Representation menu of the Style panel.
- Single color can be used for visualizing the geometry, e.g. a mesh (if Wireframe is selected), by selecting Solid Color from the “Color by” menu and specifying the color in the Set Ambient Color window.

- The opacity of the image can be set (1 = solid, 0 = invisible) in the *Opacity* in the Style panel.

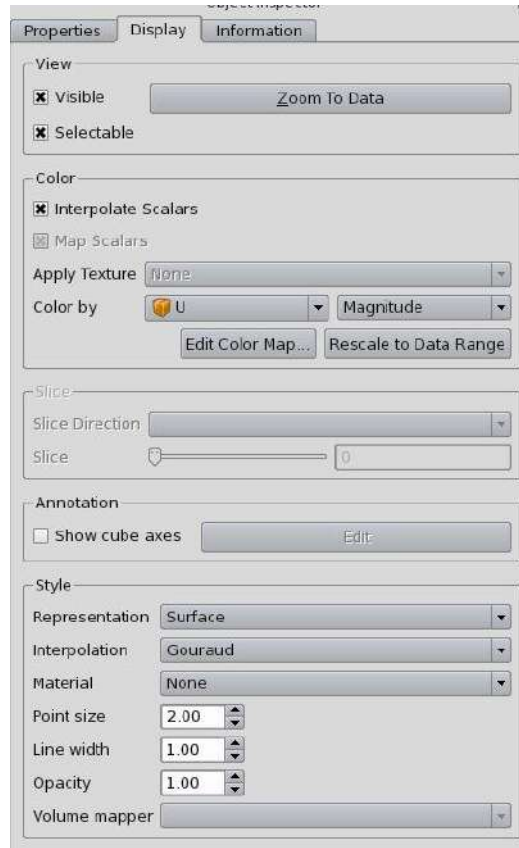


Figure D-3 The Display panel

Button toolbars

Pull-down menus at the top of the main window and the major panels, in the toolbars below the main pull-down menus increase the functionality of ParaView. The function of each button can be easily understood by its icon (Figure D-4), also any button description can be found in the Help menu (keeping the mouse over an icon without clicking on it will also give a short explanation on its functionality).

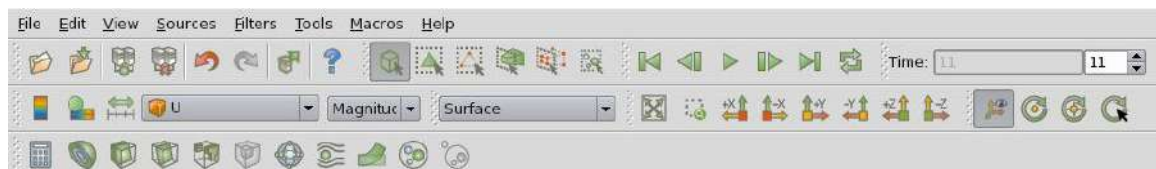


Figure D-4 Toolbars in ParaView

Manipulating the view

View settings

The View menu from Edit menu contains three items: General, Lights and Annotation.

The General panel includes the following items (which are often set at startup):

- The background color, from arrow down Choose Color button.
- Parallel projection is the usual choice for 2D, CFD simulations.

The lighting controls are in Lights panel in the Light Kit panel. For producing images with strong bright colors (e.g. isosurface) Headlight of strength 1 is appropriate.

For including annotations in the image Annotation panel should be used. The Orientation Axes feature controls an axes icon in the image window (e.g. to set the color of the axes labels x, y and z).

General settings

Some default behavior of ParaView can be controlled in the General panel. The Auto Accept button enables accepting the changes without pressing the Apply button (not a very good option for big cases because re-rendering the image after each change takes a long time)

The Render View panel contains three sub-items: General, Camera and Server. The level of detail (LOD) is included in the General panel which controls the rendering of the image while it is being manipulated (e.g. rotated or resized); lower levels allow cases with large numbers of cells to be re-rendered quickly during manipulation.

The Camera panel includes control settings for 3D and 2D movements. The user can edit the rotation, translation and the zoom map to make it suitable for these needs. This can be used by a combination of mouse, Shift and Control keys.

Contour plots

Selecting Contour from the Filter menu at the top menu bar creates a contour plot.

If the case is a 3D case module, the contours will be a set of 2D surfaces that represent a constant value. There is Isosurface list in the Properties panel that the users can edit by New Range window in the most convenient way. The chosen scalar field is selected from a pull down menu.

Introducing a cutting plane

Creating contour plots across a plane is more convenient than isosurfaces. Cutting planes are the tools which can be used for this purpose, to create surfaces. This can be done by Slice filters, using cutting Plane, Box or Sphere options. A cutting plate can be manipulated like other by mouse. In a similar way, the contour lines can also be derived out of planes.

By default ParaView triangulate the cells and shows them as triangles. For disabling this uncheck “triangulate the slice” option in the properties window of slice.

Vector plots

The Glyph filter is used for creating vector plots. Scale Mode menu in the properties panel is used for:

- Setting the length of a vector, weather to be proportional to vector magnitude or not, all with the same length (Vector).
- Controlling the base length of the glyphs (set Scale Factor).

Plotting at cell centers

Vectors at cell centers are more common, for this purpose the Cell Centers filter should be applied before Glyph filter.

Streamlines

Creating tracer lines, using the Stream Tracer filter create streamlines. Tracer points can be along a line or point which are shown in white, and can be choose from Tracer Seed panel. Usually, some trial and error is needed for achieving the desired streamlines, the length of steps tracer takes can be changed in the main Stream Tracer panel, a smaller length increase calculation time but increase smoothness. For having high quality images Tubes filter can be used after tracer lines have been created. There are different types of tubes, not only cylindrical.

Image output

For creating a screenshot of the graphs the easiest way is Save Screenshot from File menu. After selecting it in the opened window the picture resolution can be set, and by locking the aspect ratio, changing image resolution in one direction cause change in its resolution in the other direction respectively. For high quality images a resolution of more than 1000 pixels is a good choice.

Animation output

Some animations can be also created using ParaView in the File menu by choosing animation and setting the resolution, and also frames per time step. You can save your animation by assigning a name and choosing file format, and then the captured pictures are saved with this format:

“<fileRoot>_<imageNo>.<fileExt>”

In the newer versions of ParaView (4.3.1), it is possible to export directly as animation with .ogv or avi format. Do the same as before, except in the saving window select .ogv or .avi for file format.