# Turbulent Flow Simulation on HPC-Systems

## Worksheet 1: Getting Started

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**Part 1: VTK Stencil**

Working on the very first worksheet of this course, I got familiar with the skeleton code that we will be using throughout the course. I have also thought about the parallelization via **MPI**.

After implementing the hands-on task in the class, **Double Pressure Stencil**, I understood what was expected of us in this worksheet. So at first, I started implementing the **apply** function. In this function, given a cell, we are expected to get the pressure (*at the center of the cell*) and velocity values (*average across the cell*) from **Flow Field**. After getting those values, I stored them in the object by making use of the **vector** data structure in order to access the values of the particular cells during the **write** operation. I also needed to know the **First Corner**, which is the start of the *White Region*. For that reason, I simply kept the first iterated *cell indexes*. The code snippet below shows the implementation of the **apply** function:

```
// Init data structures
FLOAT pressure; auto* velocity = (FLOAT*) malloc(3 * sizeof(FLOAT));

// Set the starting position, the first corner!
if (firstCornerInd_ == nullptr) setFirstCorner_(i, j, k);

// Get the pressure and velocity
if (parameters_.geometry.dim == 2) { // 2D
    flowField.getPressureAndVelocity(pressure, velocity, i, j);
    velocity[2] = 0.0; // Set z-velocity to 0!
} else if (parameters_.geometry.dim == 3) { // 3D
    flowField.getPressureAndVelocity(pressure, velocity, i, j, k);
} else {
    std::cerr << "This app only supports 2D and 3D geometry" << std::endl;
    exit(1);
}

// Store the data
pressures_.push_back(pressure); velocities_.push_back(velocity);
```

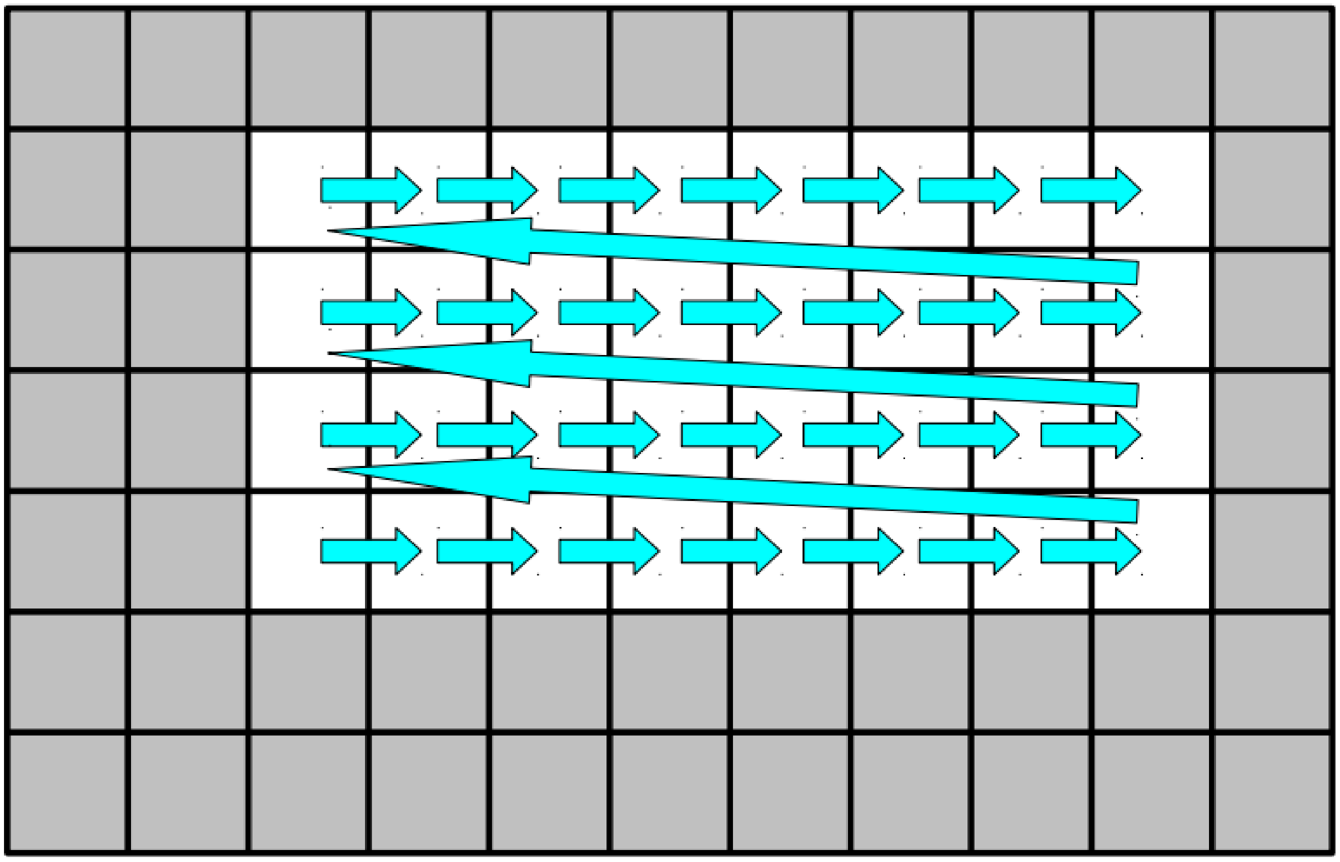
As a second step, I have implemented the **write** functionality, which writes **VTK** files with a time information (in *microseconds*) appended to the filename. For that I have created separate function for *writing the nodes/points*, *writing the pressures* and *writing the velocities* for readability purposes. For keeping this report as short as possible, I decided not to include the code blocks for this since it's longer than **apply**. However, feel free to check it here!

***Keep in mind** that we have more nodes than we have cell values because **VTK** differentiates between vertex (or node) and cell values, and we use quadrilateral or octahedral cells on a uniform grid. For example, if we had **20 * 10 = 200** cells in a **2D** space, we would have **(20 + 1) * (10 + 1) = 231** nodes.*

The functions **getPosX** and **getDx** are utilized to write the points.

**Part 2: Handling the Ghost Cells and always working in the White Region:**

As you might remember from the lecture, we have boundaries around our workable region (*for ease of coding and parallelization*). As can be seen in the picture below, in addition to the *default boundary* where the workable region is covered by a single cell space, we also have some additional ghost cells that we need to take care. For that reason, I have used the **lowOffset** and **highOffset** parameters of the **Iterator** class, which is *bounded iteration* where by default, the *1-layer of default boundary* is already handled. That's why instead of setting **lowOffset** to **2** and **highOffset** to **1**, I set them **1** and **0** respectively. After setting those values correctly, the **Iterator** now iterates only in the *White Region*.



**Part 3: Plotting the VTK when the "time" is right!**

- **dt_convergence** = adaptive time stepping, always changing.
- **dt_vtk** = time step size given in the parameters.
- **dt**, the actual time step.

We always wish things that cannot always happen, like having **dt_convergence** and **dt_vtk** same all the time! Since we are required to plot **every 0.01 seconds (or whatever is set in the parameter)**, I had to handle the cases where **dt_convergence** and **dt_vtk** are not the same:

#### 1) dt_convergence = dt_vtk

Everything works as expected!

#### 2) dt_convergence > dt_vtk

**dt_vtk** acts as an upper bound for **dt**. We simply set **dt** = **dt_vtk** here.

```
// If dt is larger than timeVtk, set dt = timeVtk!
if (floor(parameters.timestep.dt, 2) > floor(parameters.vtk.interval, 2)) {
    parameters.timestep.dt = parameters.vtk.interval;
}
```

#### 3) dt_convergence < dt_vtk

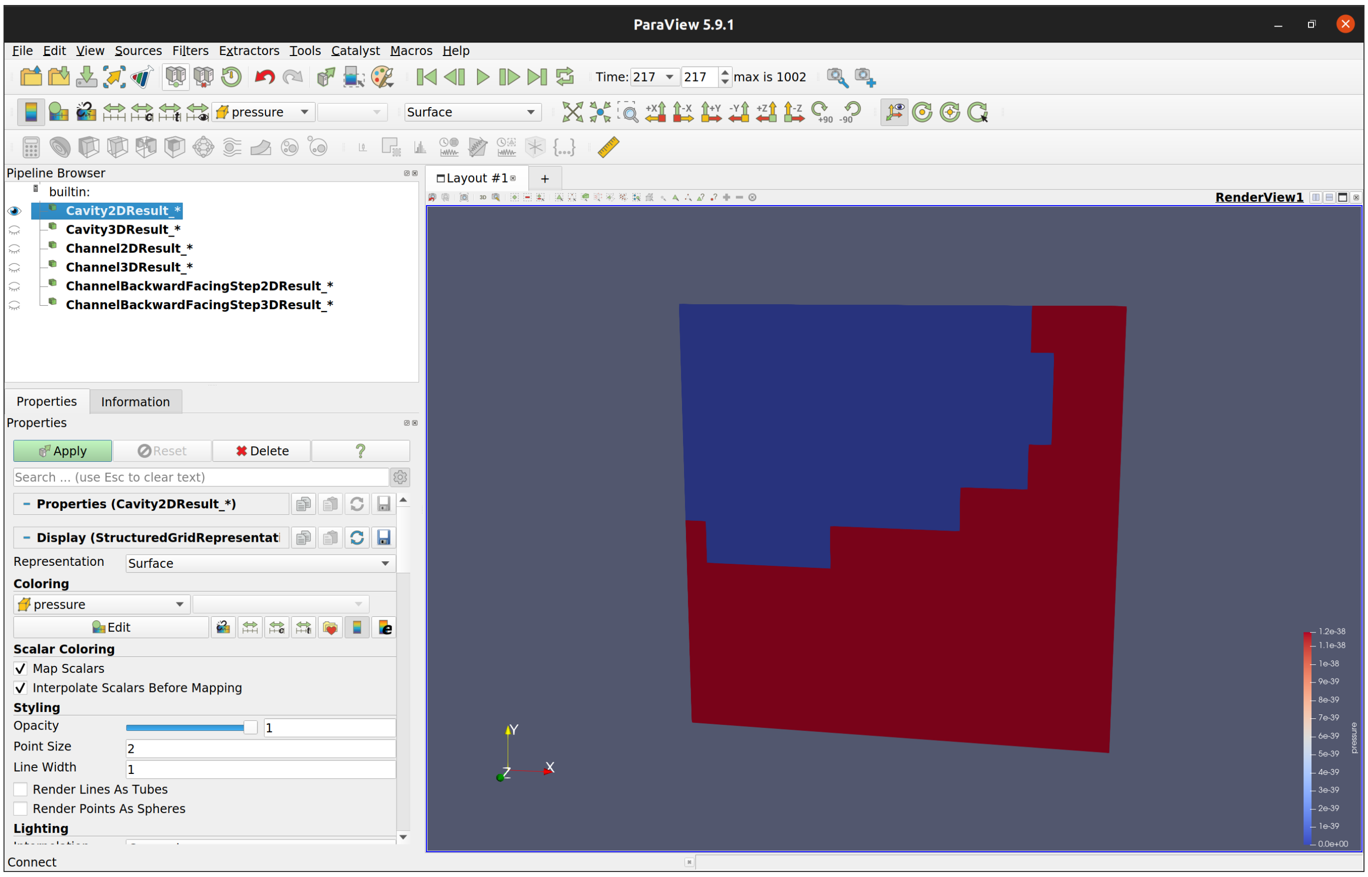
The most problematic case. In this case, we are doing as many time steps as we can until we reach the next point in time to plot.

```
// In case dt is smaller than timeVtk, wait for the right time to plot!
FLOAT time_before = time;
do {
    time += parameters.timestep.dt;
} while (floor(time, 2) < floor(time_before + parameters.vtk.interval, 2));
```

### Part 4: The results on ParaView

As can be seen below, I used ParaView to check my results. I have both printed 2D and 3D and analyzed both pressure and velocity.

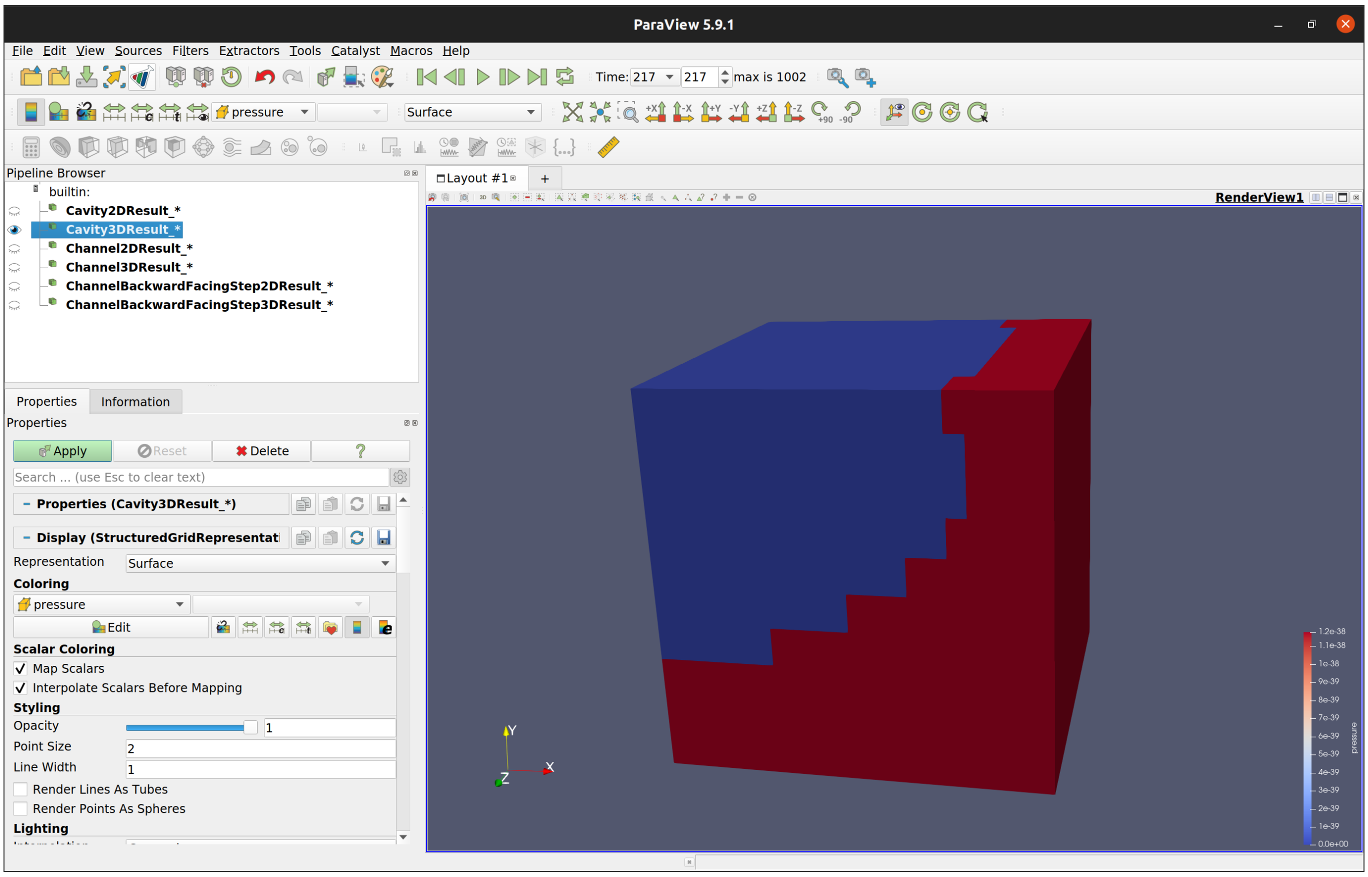
**Cavity2D - Pressure:**



Pipeline Browser
builtin:
Cavity2DResult_*
Cavity3DResult_*
Channel2DResult_*
Channel3DResult_*
ChannelBackwardFacingStep2DResult_*
ChannelBackwardFacingStep3DResult_*

Properties (Cavity2DResult_*)
Display (StructuredGridRepresentat
Representation Surface
Coloring
pressure
Scalar Coloring
✓ Map Scalars
✓ Interpolate Scalars Before Mapping
Styling
Opacity 1
Point Size 2
Line Width 1
Render Lines As Tubes
Render Points As Spheres
Lighting

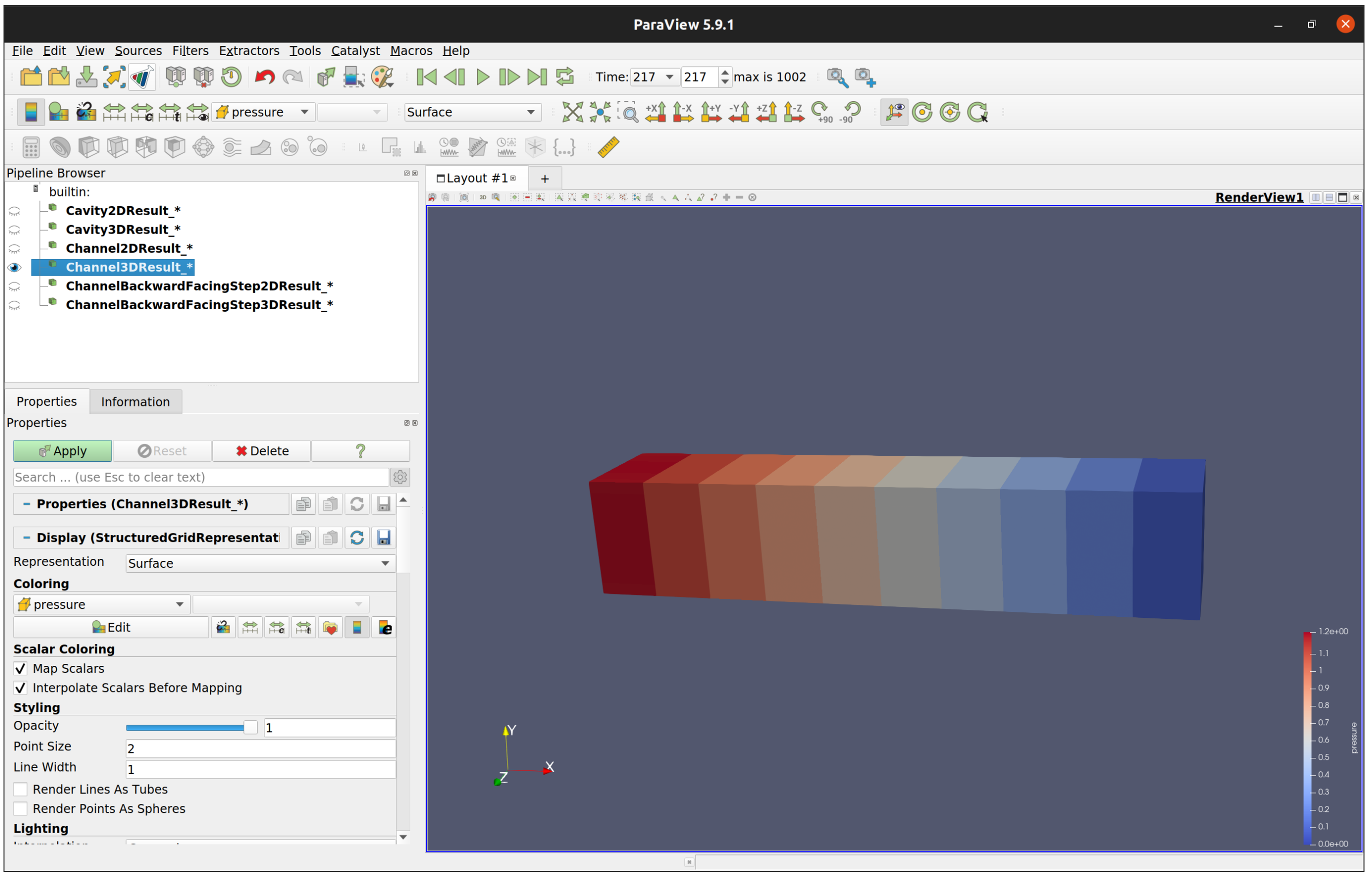
## Cavity3D - Pressure:



Pipeline Browser
builtin:
Cavity2DResult_*
Cavity3DResult_*
Channel2DResult_*
Channel3DResult_*
ChannelBackwardFacingStep2DResult_*
ChannelBackwardFacingStep3DResult_*

Properties (Cavity3DResult_*)
Display (StructuredGridRepresentat
Representation Surface
Coloring
pressure
Scalar Coloring
✓ Map Scalars
✓ Interpolate Scalars Before Mapping
Styling
Opacity 1
Point Size 2
Line Width 1
Render Lines As Tubes
Render Points As Spheres
Lighting

## Channel3D - Pressure:

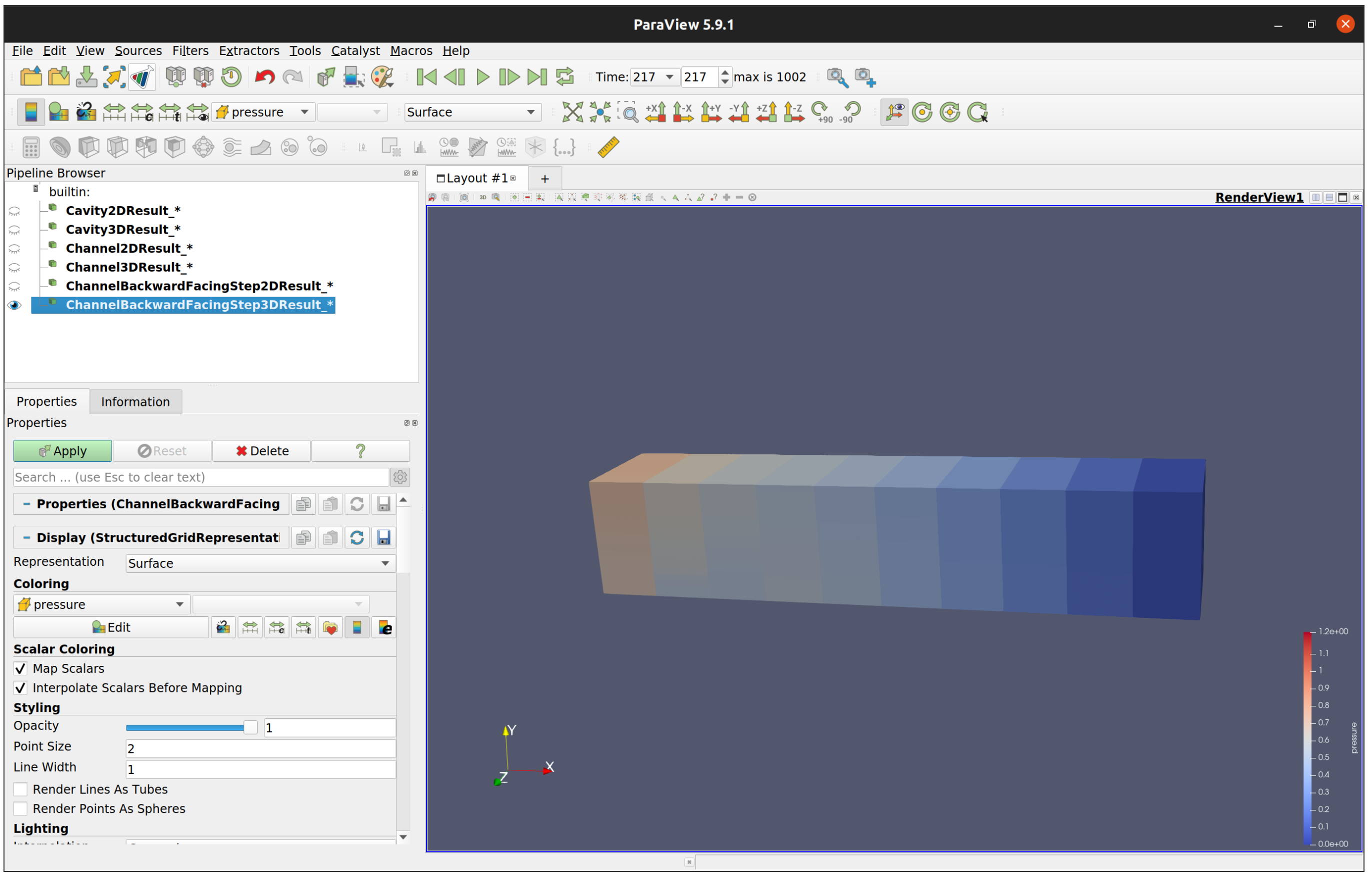

ParaView 5.9.1

Time: 217 217 max is 1002

Pipeline Browser
builtin:
Cavity2DResult_*
Cavity3DResult_*
Channel2DResult_*
Channel3DResult_*
ChannelBackwardFacingStep2DResult_*
ChannelBackwardFacingStep3DResult_*

Properties (Channel3DResult_*)
Display (StructuredGridRepresentat
Representation Surface
Coloring pressure
Scalar Coloring
✓ Map Scalars
✓ Interpolate Scalars Before Mapping
Styling
Opacity 1
Point Size 2
Line Width 1
Render Lines As Tubes
Render Points As Spheres
Lighting

## ChannelBackwardFacingStep3D - Pressure:

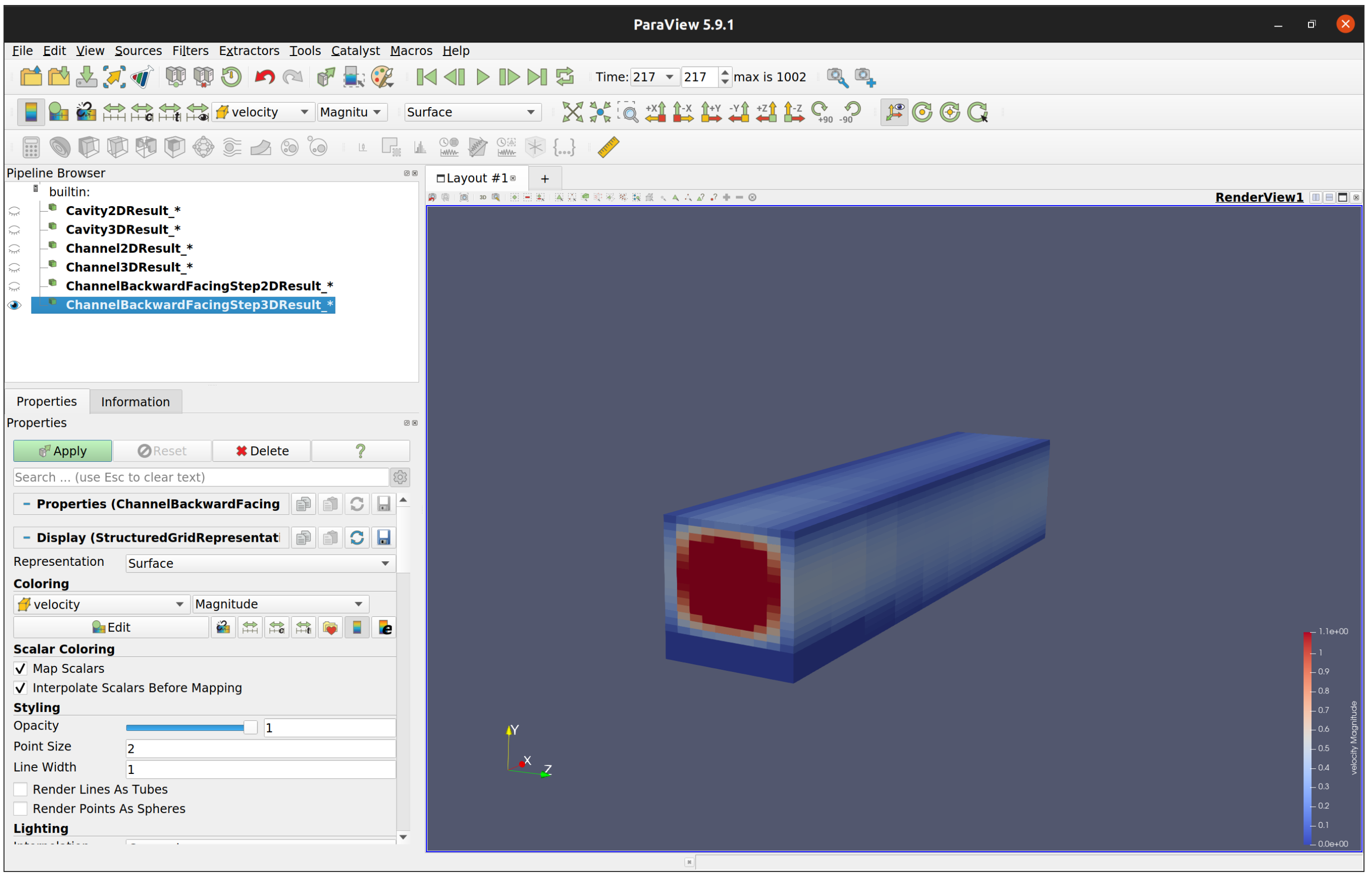

ParaView 5.9.1

Time: 217 217 max is 1002

Pipeline Browser
builtin:
Cavity2DResult_*
Cavity3DResult_*
Channel2DResult_*
Channel3DResult_*
ChannelBackwardFacingStep2DResult_*
ChannelBackwardFacingStep3DResult_*

Properties (ChannelBackwardFacing
Display (StructuredGridRepresentat
Representation Surface
Coloring pressure
Scalar Coloring
✓ Map Scalars
✓ Interpolate Scalars Before Mapping
Styling
Opacity 1
Point Size 2
Line Width 1
Render Lines As Tubes
Render Points As Spheres
Lighting

## ChannelBackwardFacingStep3D - Velocity:



builtin:
- Cavity2DResult_*
- Cavity3DResult_*
- Channel2DResult_*
- Channel3DResult_*
- ChannelBackwardFacingStep2DResult_*
- ChannelBackwardFacingStep3DResult_*

Properties (ChannelBackwardFacing

Display (StructuredGridRepresentat

Representation: Surface

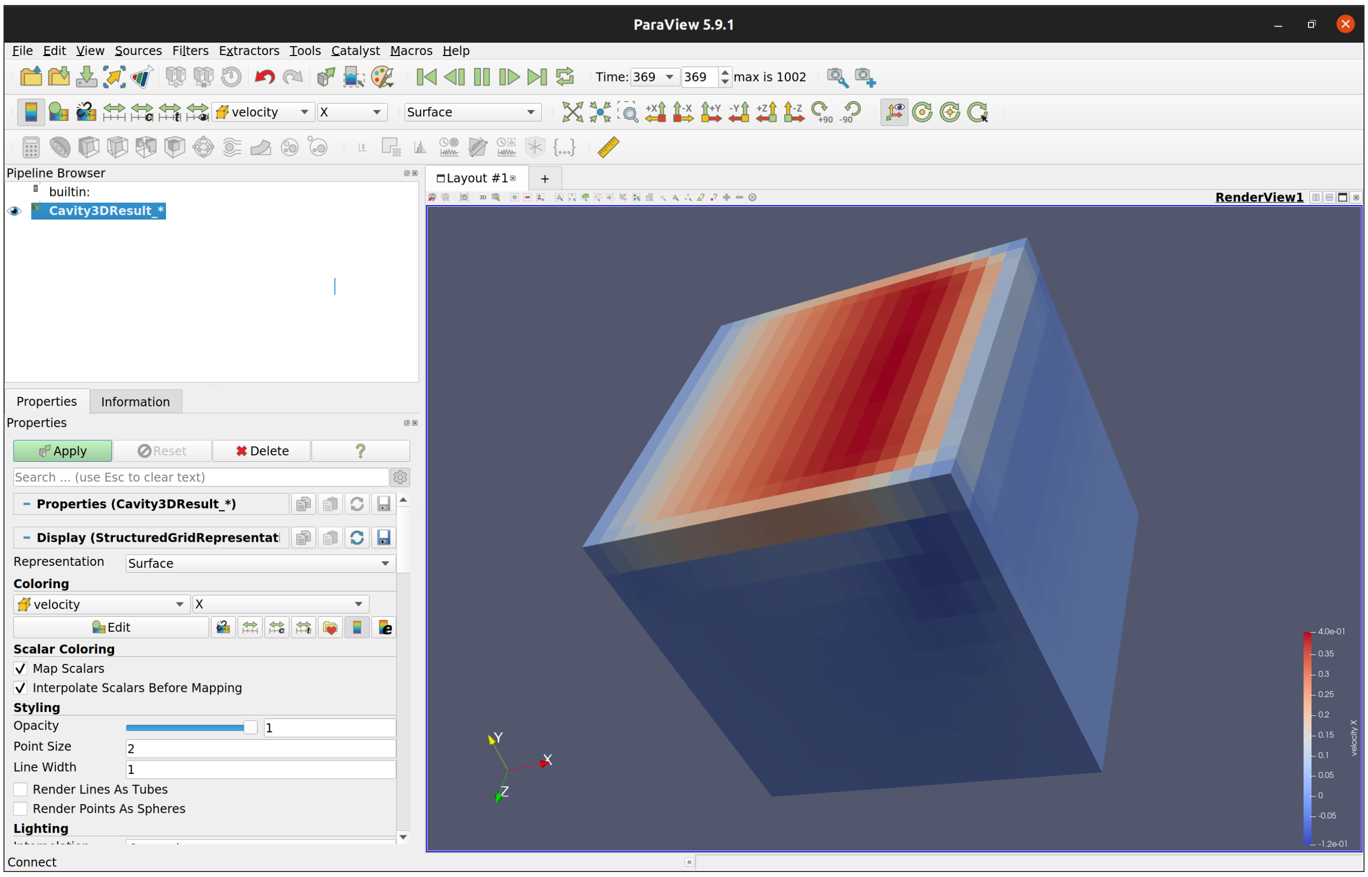
Coloring: velocity, Magnitude

Scalar Coloring
- ✓ Map Scalars
- ✓ Interpolate Scalars Before Mapping

Styling
- Opacity: 1
- Point Size: 2
- Line Width: 1
- Render Lines As Tubes
- Render Points As Spheres

Lighting

## Cavity3D - Velocity (x):



builtin:
- Cavity3DResult_*

Properties (Cavity3DResult_*)

Display (StructuredGridRepresentat

Representation: Surface

Coloring: velocity, X

Scalar Coloring
- ✓ Map Scalars
- ✓ Interpolate Scalars Before Mapping

Styling
- Opacity: 1
- Point Size: 2
- Line Width: 1
- Render Lines As Tubes
- Render Points As Spheres

Lighting

## Part 5: Flow Physics and Profiling (Questions Answered)

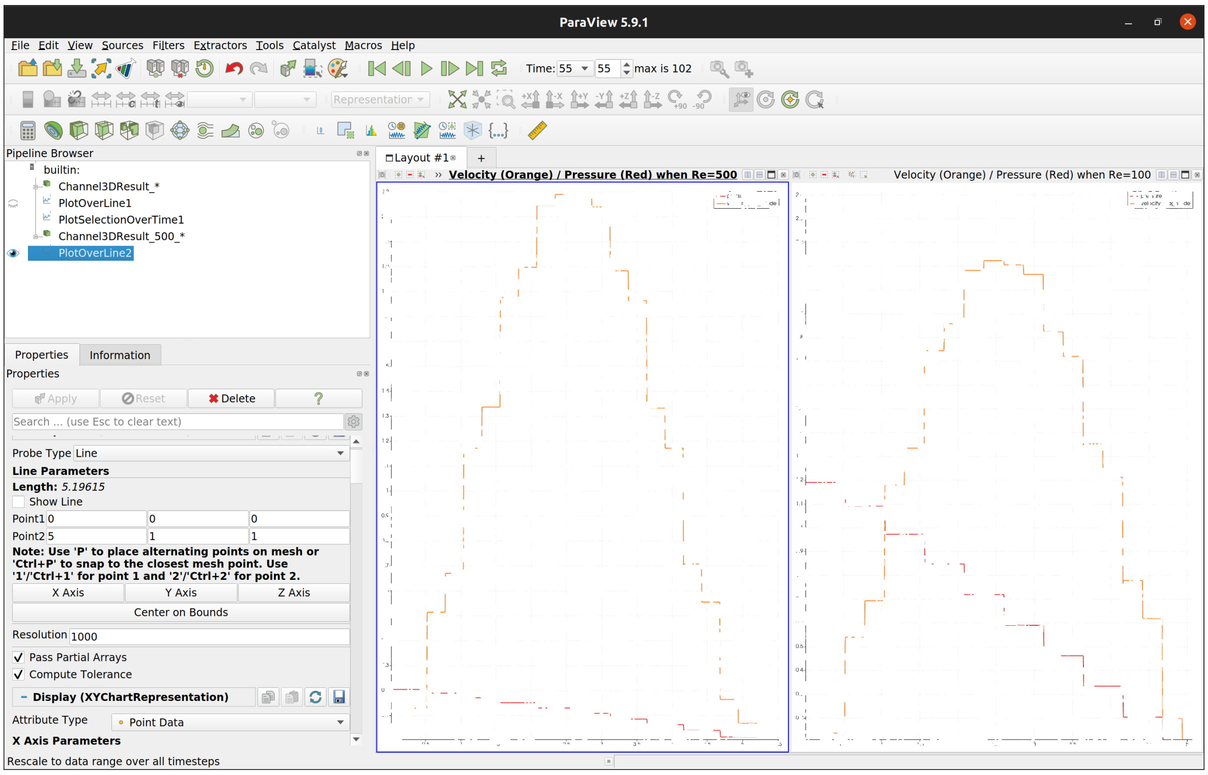
### 1) Study of the scenarios cavity, channel and channel with backward-facing step in more detail:

- ***The influence of the Reynolds number on the velocity and pressure field. In particular,***
    - ***How many vortices can you observe in the cavity scenario, depending on the choice of the Reynolds number? Where are these vortices located?***

      As we increase the *Reynolds number*, the vorticity distribution seems more homogeneous. That is, the vortices are distributed more evenly throughout the surface. In contrast, lower *Reynolds number* resulted in more inhomogeneous distribution where the vortices lie mostly around the borders.

    - ***How does the velocity/pressure field of the channel flow depend on the Reynolds number?***

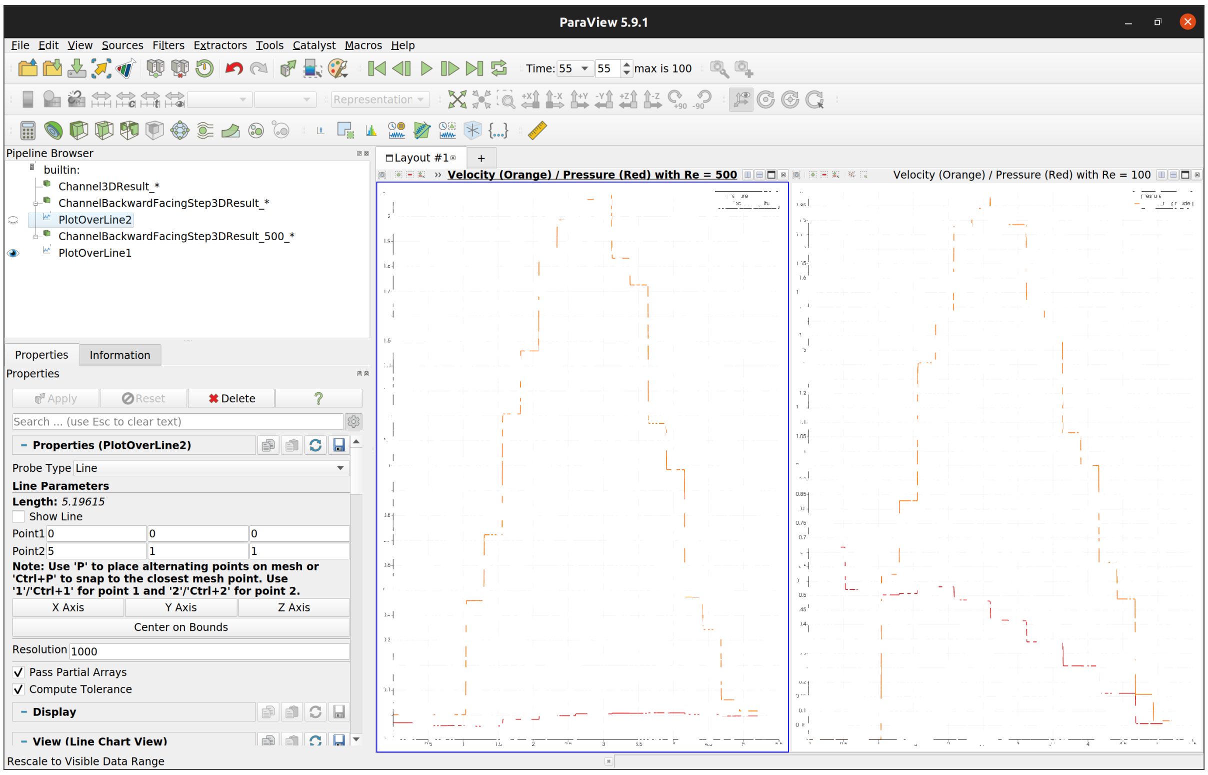
      As can be seen in the graph below where **Velocity (Orange)** is plotted over **Pressure (Red)** with the *Reynolds number* set to **500 (Left)** and **100 (Right)**, it is not hard to deduce that setting the *Reynolds number* high resulted in a higher **velocity/pressure field** as **velocity** values got bigger while **pressure** values got smaller. In a nutshell, **velocity/pressure field** and the *Reynolds number* has a positive correlation.



Probe Type Line
Line Parameters
Length: 5.19615
Show Line
Point1 0 0 0
Point2 5 1 1
Note: Use 'P' to place alternating points on mesh or 'Ctrl+P' to snap to the closest mesh point. Use '1'/'Ctrl+1' for point 1 and '2'/'Ctrl+2' for point 2.
Resolution 1000
✓ Pass Partial Arrays
✓ Compute Tolerance
Display (XYChartRepresentation)
Attribute Type Point Data
X Axis Parameters
Rescale to data range over all timesteps

    - ***How is the velocity/pressure field behind the backward-facing step affected by the choice of the Reynolds number?***

      As can be seen in the graph below, the results look similar with that of channel flow. Again, we can say that **velocity/pressure field** and the *Reynolds number* has a positive correlation.



Time: 55 55 max is 100

builtin:
Channel3DResult_*
ChannelBackwardFacingStep3DResult_*
PlotOverLine2
ChannelBackwardFacingStep3DResult_500_*
PlotOverLine1

Velocity (Orange) / Pressure (Red) with Re = 500

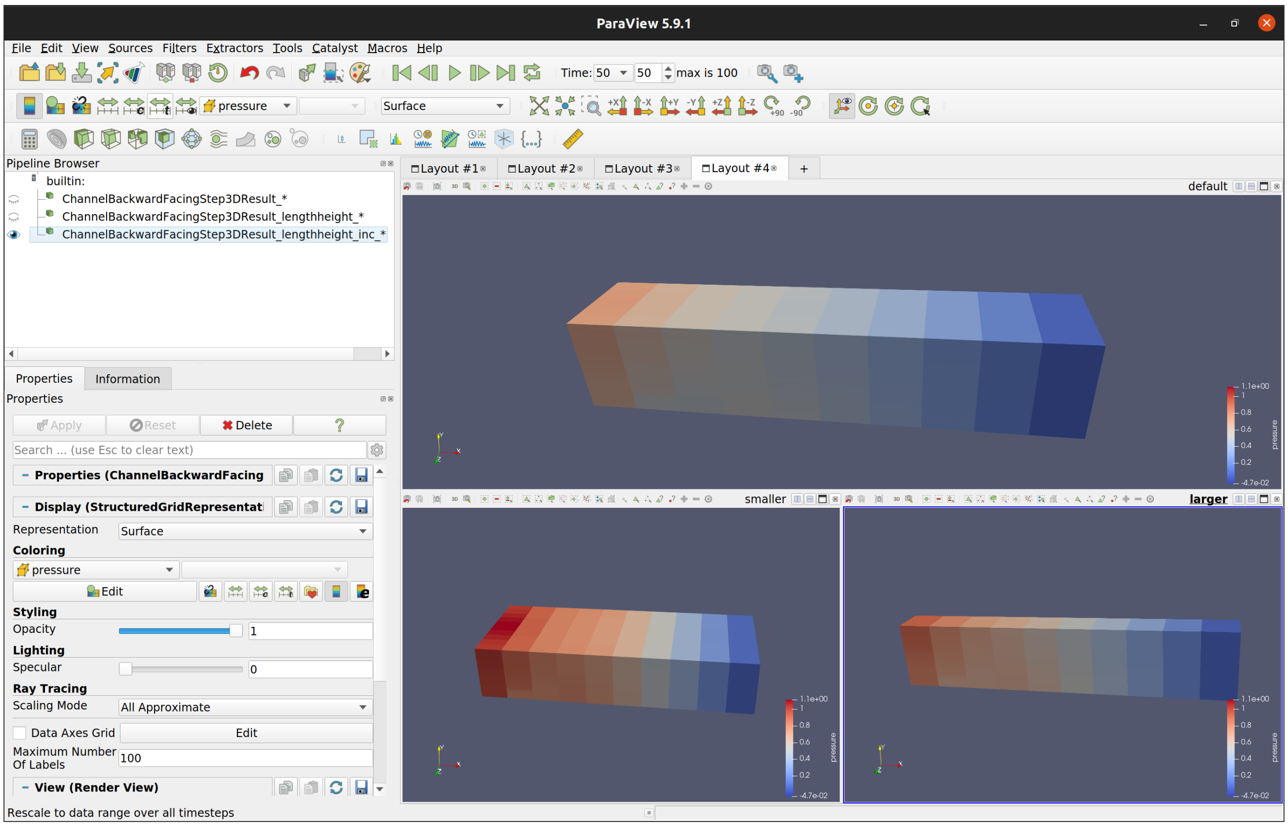
Velocity (Orange) / Pressure (Red) with Re = 100

Properties (PlotOverLine2)
Probe Type Line
Line Parameters
Length: *5.19615*
Show Line
Point1 0 0 0
Point2 5 1 1
Note: Use 'P' to place alternating points on mesh or 'Ctrl+P' to snap to the closest mesh point. Use '1'/'Ctrl+1' for point 1 and '2'/'Ctrl+2' for point 2.
Resolution 1000
✓ Pass Partial Arrays
✓ Compute Tolerance
Display
View (Line Chart View)

- ***The influence of the length and height of the backward-facing step on the flow field.***

  As can be seen in the graphs below, I have tested different length and height settings of the backward-facing step. It definitely has an influence on the flow field. When we look at the flow field at the top (the default one), we can see that the pressure is getting closer to **0.8**. However, when we look at the ones at the bottom, in both cases, the pressure gets to a point higher than default one.

  On the bottom left, we have smaller length and height values. As can be seen easily, the pressure is getting closer to even **1.0** whereas on the bottom right, where we have larger length and height values, the pressure was lower (close to **0.9**).



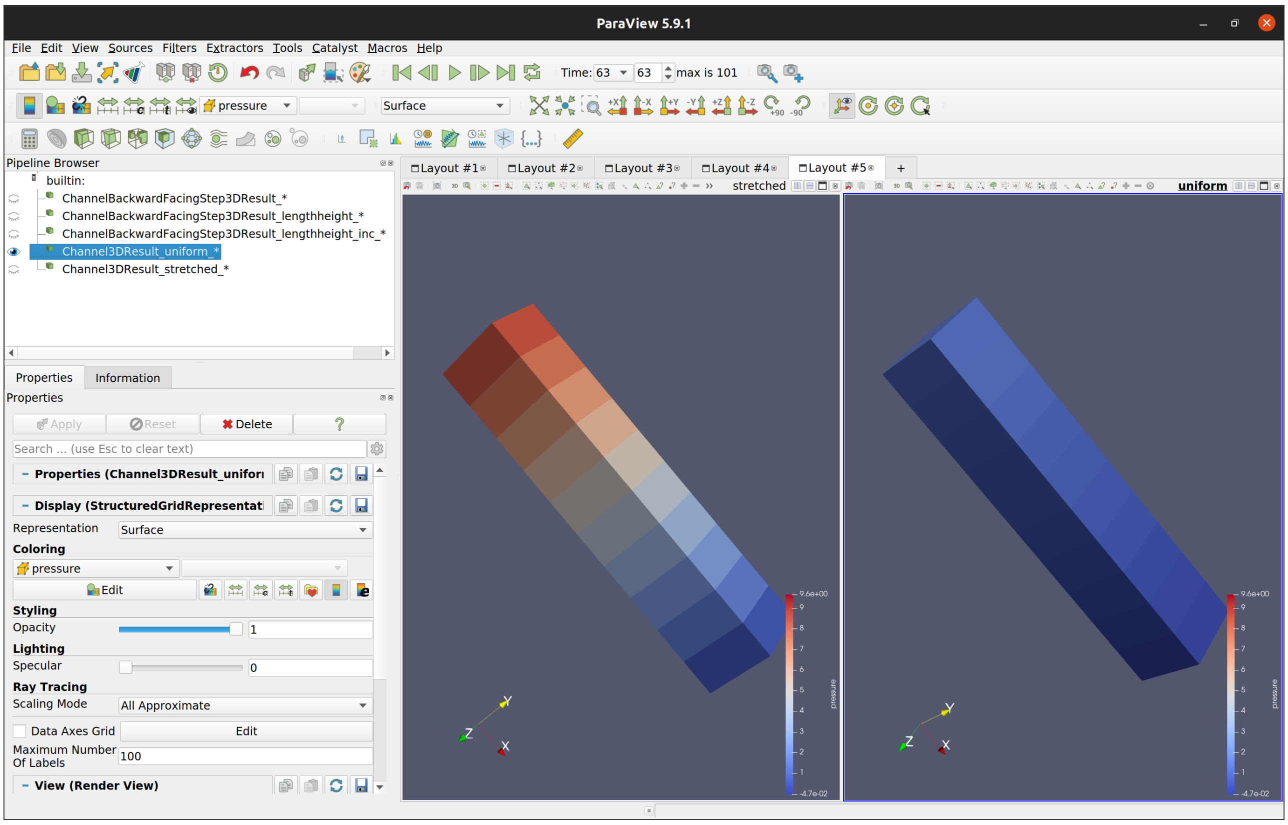
Time: 50 | 50 | max is 100

builtin:
ChannelBackwardFacingStep3DResult_*
ChannelBackwardFacingStep3DResult_lengthheight_*
ChannelBackwardFacingStep3DResult_lengthheight_inc_*

Properties (ChannelBackwardFacing
Display (StructuredGridRepresentat
Representation: Surface
Coloring: pressure
Styling
Opacity: 1
Lighting
Specular: 0
Ray Tracing
Scaling Mode: All Approximate
Data Axes Grid: Edit
Maximum Number Of Labels: 100
View (Render View)
Rescale to data range over all timesteps

- ***The influence of the used mesh on the overall accuracy and time step size. You may restrict your considerations to the channel flow scenario for this sub-task.***

  The mesh structure used has a significant effect on the overall accuracy and time step size. One can see how the **stretched mesh (left)** converged faster (*More accurate!*) than **uniform mesh (right)**. According to the time step, **stretched mesh (left)** has a **dt** of *0.000228466* whereas **uniform mesh (right)** has a **dt** of *0.0496032*, which is higher.



Time: 63 | 63 | max is 101

builtin:
ChannelBackwardFacingStep3DResult_*
ChannelBackwardFacingStep3DResult_lengthheight_*
ChannelBackwardFacingStep3DResult_lengthheight_inc_*
Channel3DResult_uniform_*
Channel3DResult_stretched_*

Properties (Channel3DResult_unifor
Display (StructuredGridRepresentat
Representation: Surface
Coloring: pressure
Styling
Opacity: 1
Lighting
Specular: 0
Ray Tracing
Scaling Mode: All Approximate
Data Axes Grid: Edit
Maximum Number Of Labels: 100
View (Render View)

**2) Investigation of the sequential performance using gprof:**

### Expected:

The **write** routine takes most of the time not because we have some loops (*They are not computationally-expensive*), but because we are writing to the file **at each iteration**! This is something that slows down our computation. As an improvement, instead of writing to the file at each iteration, we could *append* each line to a string, and then write the whole string **at the end of the iteration**.

### Actual:

As can be seen in the output of the **gprof** command (*Performance analysis for Cavity 2D*) below, the case is not as expected. Actually, the **write** routine takes absolutely no time compared to the other routines. I ran the performance analysis for each of the example cases, and the results are not that different and the routines that takes most of the time are the same.

For the Cavity2D case, the **apply** routine took *37,50%* of the time followed by **getVelocity** that took *25,00%* of the time. When I checked my implementation of the **apply** routine and the implementation of **getVelocity**, I saw no possible improvements since I believe they are implemented in the best way possible. However, as you can see under the *calls* section, there are too many calls to those routines. **apply** is called **231231** time and **getVelocity**, which gets called under **apply**, is called **3051048** times. So, we immediately can see there is room for improvement. We can for example make use of the **MPI** to parallelize the simulation so that multiple processes work on those *bottleneck* routines.

```
Performance Analysis for Cavity2D
For more, check Doc/WS1/data/prof

Each sample counts as 0.01 seconds.
  %   cumulative   self              self     total
 time   seconds   seconds    calls  us/call  us/call  name
 37.50      0.03     0.03   231231     0.13     0.19
NSEOF::Stencils::FGHStencil::apply(NSEOF::FlowField&, int, int)
 25.00      0.05     0.02  3051048     0.01     0.01
NSEOF::FlowField::getVelocity()
 12.50      0.06     0.01   231231     0.04     0.04
NSEOF::Stencils::RHSStencil::apply(NSEOF::FlowField&, int, int)
 12.50      0.07     0.01     1001     9.99     9.99
NSEOF::Solvers::PetscSolver::solve()
 12.50      0.08     0.01
NSEOF::Solvers::computeMatrix2D(_p_KSP*, _p_Mat*, _p_Mat*, void*)
```

I thank you for the opportunity of gaining hands-on experience with such algorithms, and I truly appreciate your effort.

***Batuhan Erden***