Electronic Supplementary Material (ESI) for Lab on a Chip

Using computational fluid dynamics to simulate Rayleigh Bénard convection

When a fluid is heated, its density changes. Often, spatial variations in temperature cause corresponding differences in density between neighboring hot and cold regions in the fluid. In a gravitational field, these density gradients produce spatial variations in the buoyancy force that provide a driving force for fluid motion. A familiar scenario involves heating a confined fluid from below such that the warmer fluid moves up and the colder fluid moves down. This process is known as **convection,** and is responsible for a wide range of physical phenomena such as heat transfer, flow in the atmosphere, oceans, planetary mantle, sun's surface, and even lava lamps (Figure 1). **Rayleigh Bénard convection** is a subclass of natural convection that occurs when a fluid is confined in an enclosure whose top and bottom surfaces are maintained at fixed temperatures. In our research, we have harnessed Rayleigh-Bénard convection to perform thermally actuated biochemical reactions that replicate DNA.

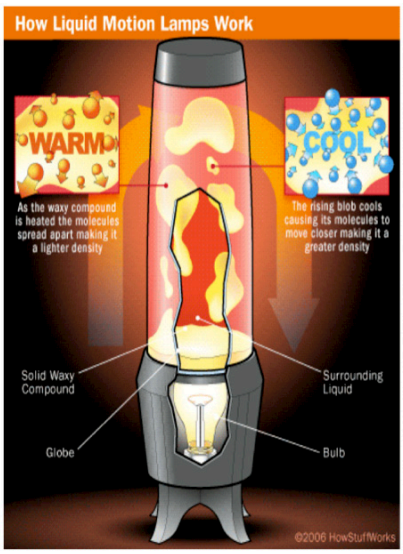


Figure 1: Convective flow in a lava lamp

The Polymerase Chain Reaction

The **polymerase chain reaction (PCR)** enables a known DNA sequence to be copied billions of times. The reaction involves a sequence of steps, each of which occurs at a different temperature. A complete sequence of steps is called a cycle, and each cycle consists of three steps; **denaturing** of the double stranded DNA (dsDNA) to produce two single stranded fragments (ssDNA), **annealing** of primers to the specific sequence in the single-stranded DNA yielding annealed DNA (aDNA), and enzymatic **extension** of the annealed DNA in the presence of nucleotides (E) to produce two double stranded copies (Figure 2). The simplified reaction model described in the references below illustrates this process, where k_d, k_a, and k_e are the rate constants associated with the denaturing, annealing, and extension steps, respectively.

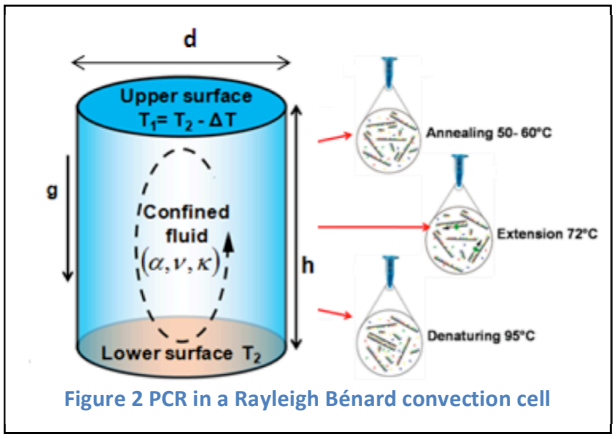


Figure 2 PCR in a Rayleigh Bénard convection cell

J. W. Allen, M. Kenward and K. D. Dorfman, *Microfluidics and Nanofluidics*, 2009, **6**, 121-130.
E. Yariv, G. Ben-Dov and K. D. Dorfman, *Europhysics Letters*, 2005, **71**, 1008-1014.

$$dsDNA \xrightarrow{k_d} 2ssDNA \qquad \text{Denaturing [94 - 98 °C]}$$

$$2ssDNA \xrightarrow{k_a} 2aDNA \qquad \text{Annealing [55 - 65 °C]}$$

$$aDNA + E \xrightarrow{k_e} ssDNA \qquad \text{Extension [70 - 75 °C]}$$

Rayleigh Bénard convection offers a promising approach to rapidly execute the PCR. These reactions are performed in an aqueous medium confined within micro-fluidic cylindrical cells of varying dimensions (Figure 2). The geometry of a cylinder can be determined completely by specifying its diameter (*d*) and height (*h*) or more practically its aspect ratio (*h/d*) and height (*h*). It should be kept in mind that the convective flow pattern developed within such cylindrical cells depends on the temperature difference between the bottom and the top surface, the geometry of the cell (cell aspect ratio and height) and the fluid properties (kinematic viscosity (ν = μ/ρ), thermal diffusivity (α), and thermal expansion coefficient (β)). For PCR, the top and bottom surfaces of the cell are maintained at fixed temperatures of 55 and 97 °C respectively, leaving the cell geometry as the main parameter that can manipulated to tune the internal convective flow profile.

Computational Fluid Dynamics

Computational fluid dynamics (CFD) will be used to analyze the flow field and the amplification of target DNA through reactions in these micro cylinders. For a defined geometry, the continuity equation (conservation of mass), Navier-Stokes equations (conservation of momentum) and the conservation of energy are solved for a particular set of initial and boundary conditions. Therefore for an incompressible fluid (water) these equations in Cartesian coordinates can be written as:

Continuity equation

$$\frac{\partial u}{\partial x}+\frac{\partial v}{\partial y}+\frac{\partial w}{\partial z}=0 \tag{1.1}$$

Navier-Stokes Equation

$$\begin{aligned}
&\frac{\partial u}{\partial t}+u\frac{\partial u}{\partial x}+v\frac{\partial u}{\partial y}+w\frac{\partial u}{\partial z}=-\frac{1}{\rho}\frac{\partial p}{\partial x}+f_x+\nu\left(\frac{\partial^2 u}{\partial x^2}+\frac{\partial^2 u}{\partial y^2}+\frac{\partial^2 u}{\partial z^2}\right)\\
&\frac{\partial v}{\partial t}+u\frac{\partial v}{\partial x}+v\frac{\partial v}{\partial y}+w\frac{\partial v}{\partial z}=-\frac{1}{\rho}\frac{\partial p}{\partial y}+f_y+\nu\left(\frac{\partial^2 v}{\partial x^2}+\frac{\partial^2 v}{\partial y^2}+\frac{\partial^2 v}{\partial z^2}\right)\\
&\frac{\partial w}{\partial t}+u\frac{\partial w}{\partial x}+v\frac{\partial w}{\partial y}+w\frac{\partial w}{\partial z}=-\frac{1}{\rho}\frac{\partial p}{\partial z}+f_z+\nu\left(\frac{\partial^2 w}{\partial x^2}+\frac{\partial^2 w}{\partial y^2}+\frac{\partial^2 w}{\partial z^2}\right)
\end{aligned} \tag{1.2}$$

Energy equation

$$\rho C_p\left(\frac{\partial T}{\partial t}+u\frac{\partial T}{\partial x}+v\frac{\partial T}{\partial y}+w\frac{\partial T}{\partial z}\right)=-k\left(\frac{\partial^2 T}{\partial x^2}+\frac{\partial^2 T}{\partial y^2}+\frac{\partial^2 T}{\partial z^2}\right) \tag{1.3}$$

In the above equations f_x , f_y = 0, but the driving force term in the z-direction is due to buoyancy. In Rayleigh-Bénard convection, this is typically expressed in terms of the Boussinesq approximation

$$f_z = g\beta\rho(T-T_o) \tag{1.4}$$

where *g, β, ρ* are the acceleration due to gravity, the thermal expansion coefficient of water and the density of water respectively.

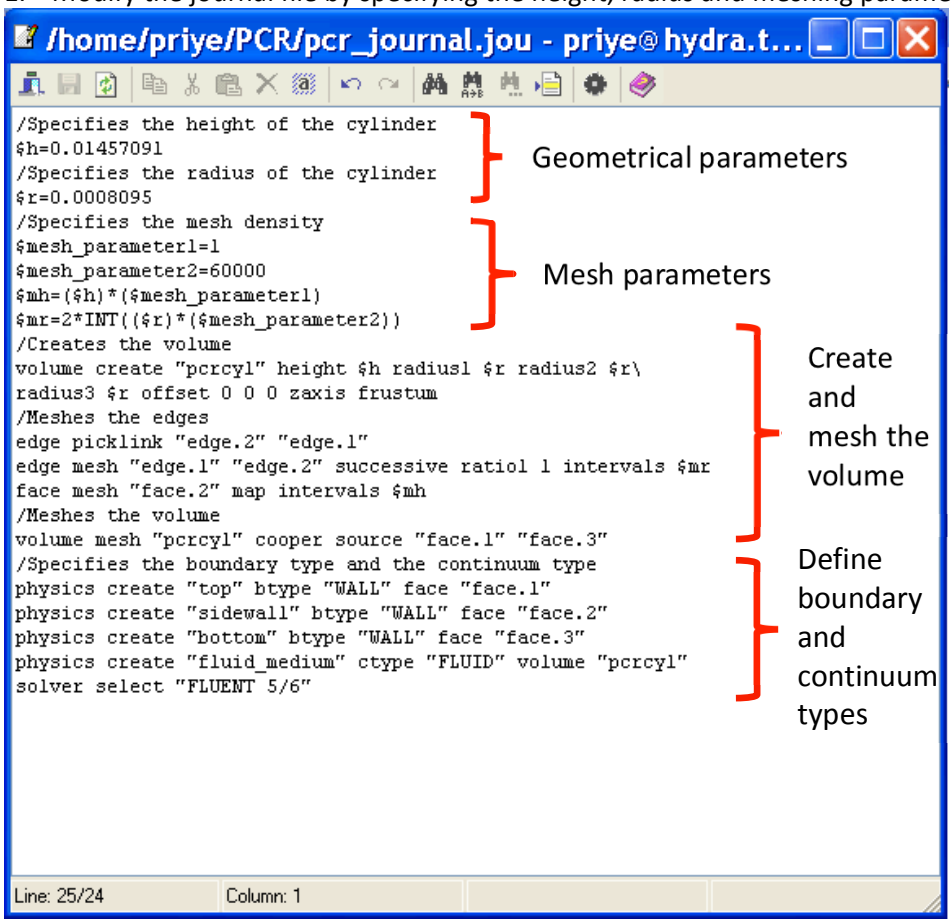
The equations above are partial differential equations and the variables are non linearly coupled. An analytical solution to the above set of equation is not possible in general. Therefore we can only obtain a solution by numerically solving the above equations over discrete nodal points generated within a geometry. This is where computational fluid dynamics (CFD) plays a very important role. In general, CFD analysis involves three components: pre-processing, solving and post-processing.

Pre-processing

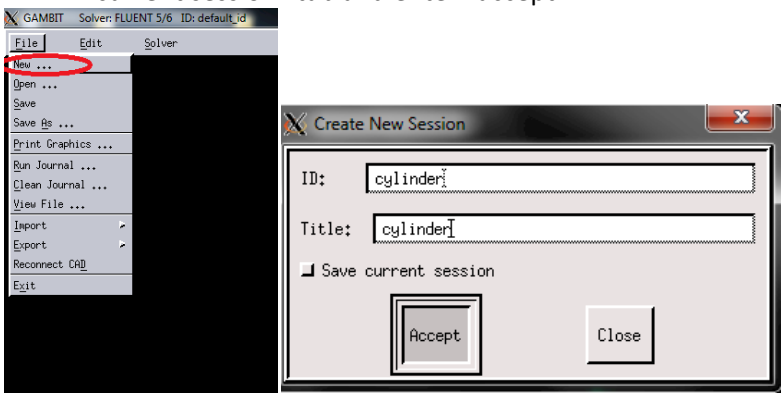
First we need to create the geometry and discretize it into numerical cells. This process is known as **grid generation or meshing**. Gambit (ANSYS) will be used to create a cylinder of a given diameter and height, and then mesh it. The mesh density is specified on the edges. Quadrilateral elements are used to mesh the complete volume. The volume inside is specified to be a fluid continuum and the faces are identified as boundaries. These instructions are written in a journal file (.jou file). All the parameters can be changed in this journal file and then it can be read by the Gambit compiler to create and mesh the required geometry. A step by step instruction is given on how to modify and run the journal file.

Meshing instructions

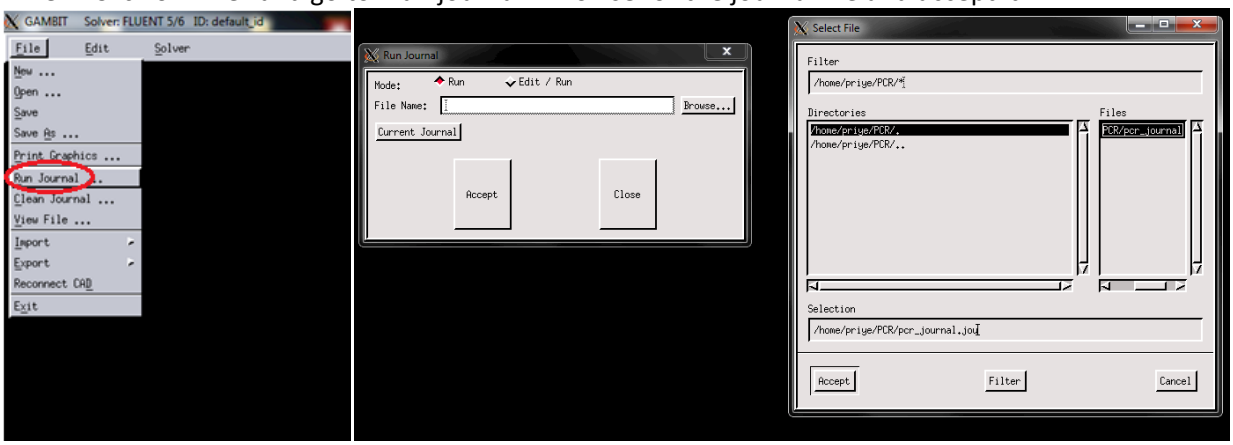
1. Modify the journal file by specifying the height, radius and meshing parameters. Then save it.



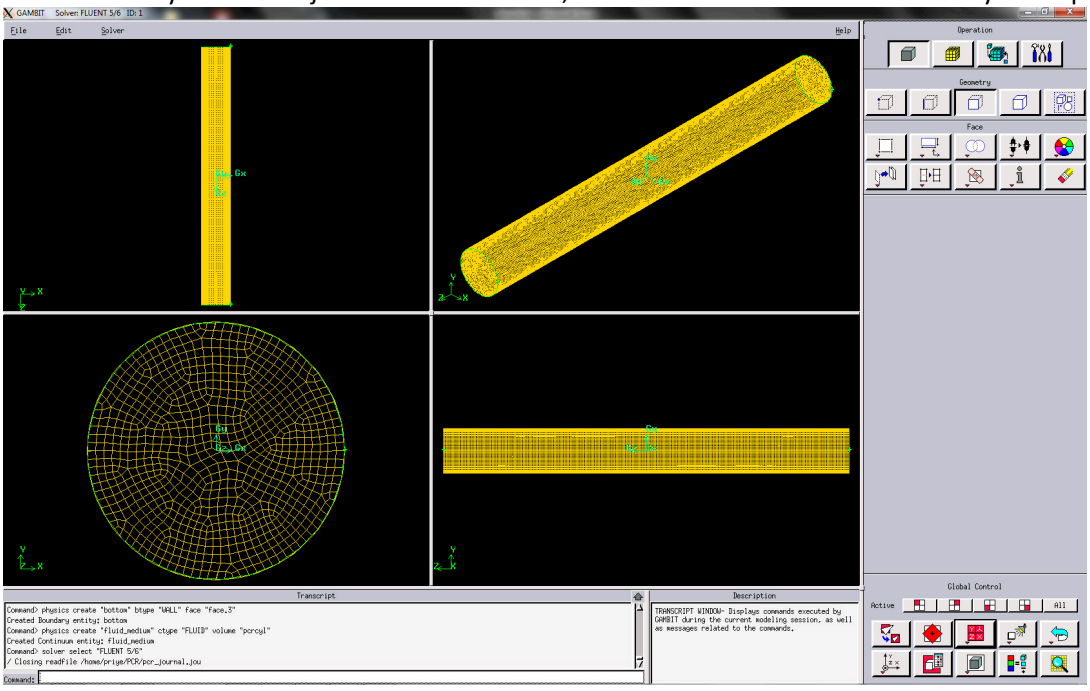
2. Go to "file" tab and select "new". Type in a desirable name for the geometry, deselect the “save current session” tab and enter “accept”.



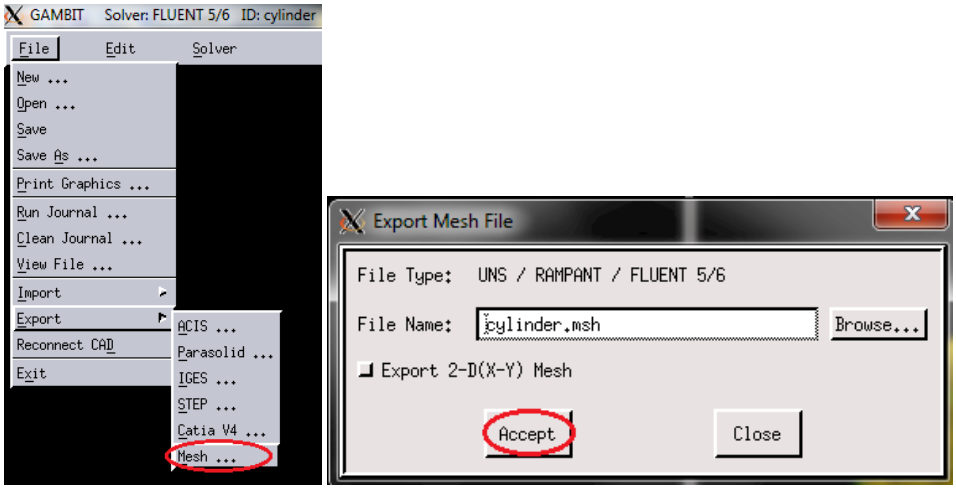
3. Click on "file" and go to "run journal". Browse for the journal file and accept it.



4. After you run the journal file in Gambit, the mesh will be created and ready for export.



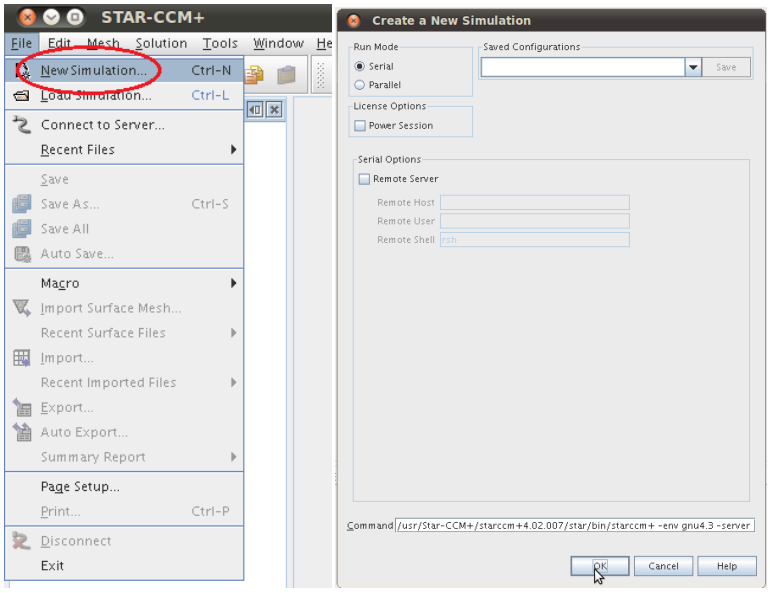
5. Name your mesh and export it as “file_name.**msh**”.



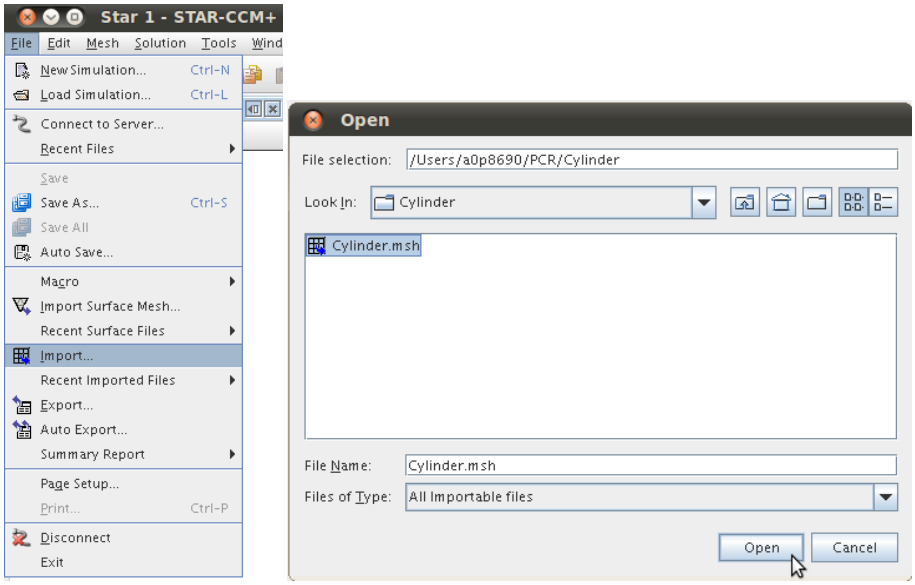
Solver

Once the geometry is created, meshed and exported, it will then be imported into the CFD Solver (STARCCM+). The objective of the solver is to obtain a solution to the equations (1.1 to 1.3), for a given set of boundary and initial conditions.

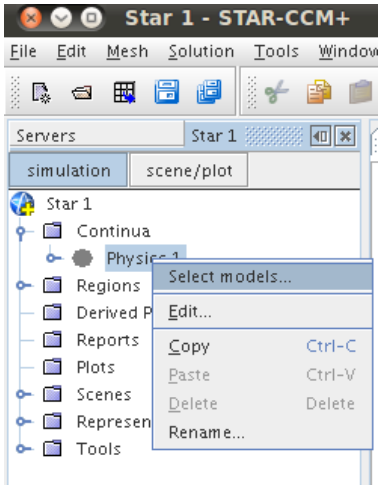
1. Go the "file" tab and click on “New Simulation” followed by “ok”



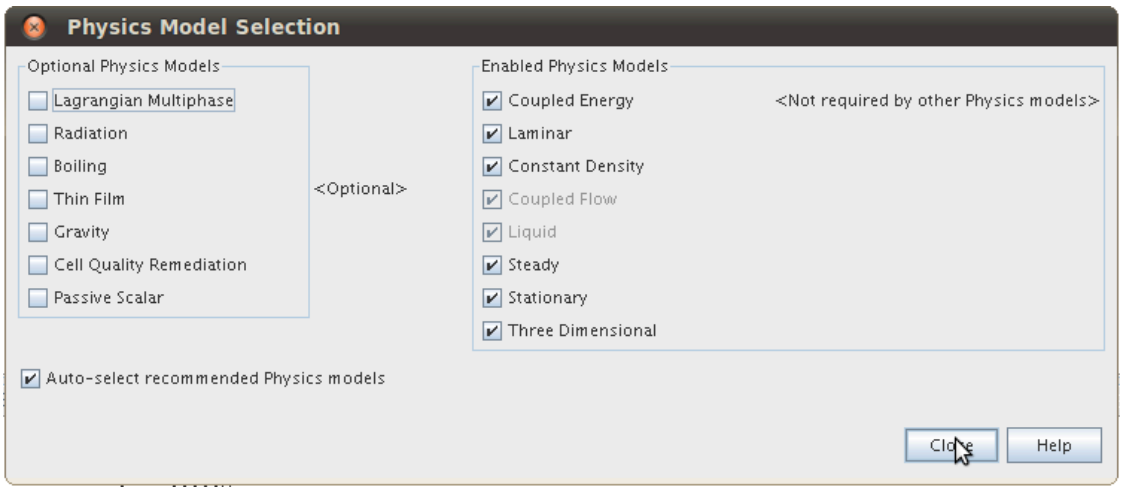
2. To import the geometry, go to the "file" tab and click "import geometry". Browse for the geometry and select “open”.



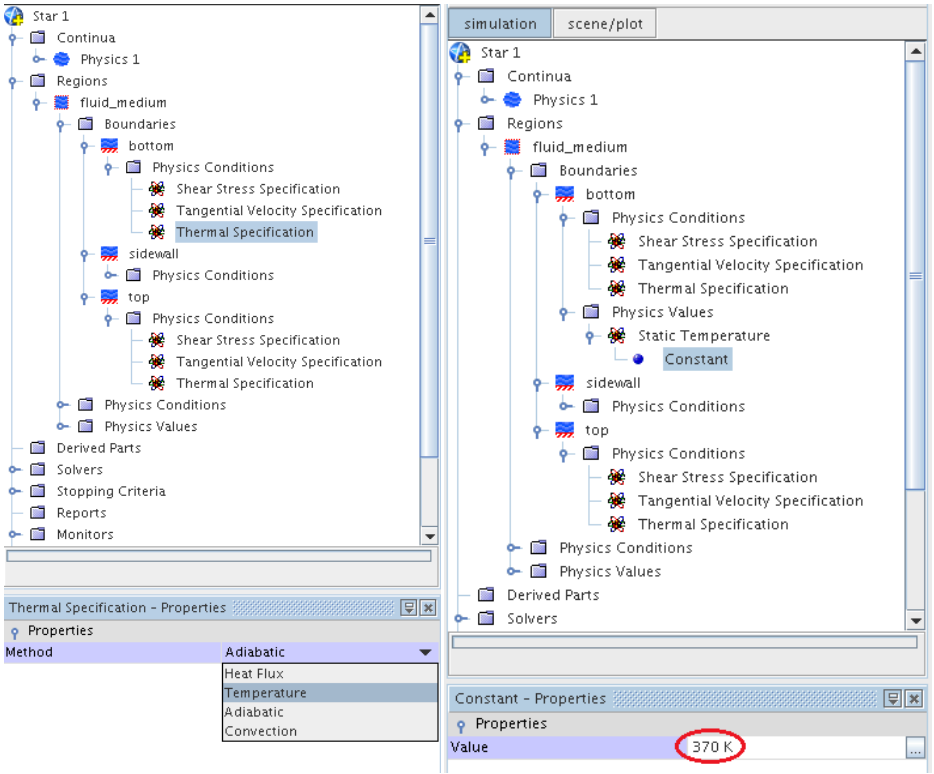
3. Go to continua, right click “physics 1” and choose “select models”.



4. From the list of models, activate the models which are required. For our case the models to be selected are:
    - 3 Dimensional
    - Motion = Stationary
    - Time = Steady
    - Material = Liquid
    - Flow = Coupled flow
    - Equation of state = Constant density
    - Viscous regime = Laminar
    - Optional physical models = Coupled Energy



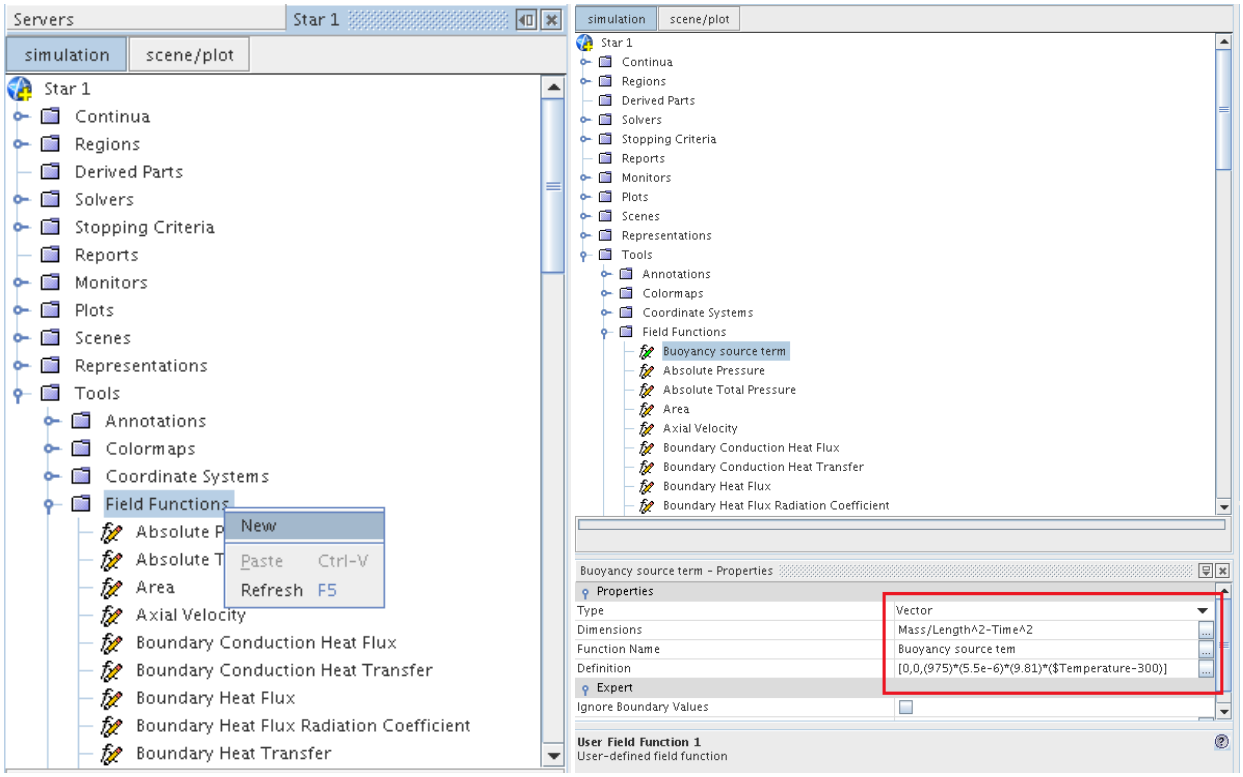
5. Now it is necessary to assign boundary conditions along all sidewalls. As an illustration let's consider the bottom surface. The bottom temperature is to be maintained at 97 °C (370 K). Expand the "Regions" tab, expand the "Boundaries" tab and then expand the "bottom" tab. Under "Physics Conditions" select "Thermal Specification". Choose "Temperature" from the options available. Expand the newly created tab "Physical Values". Set the bottom temperature to 370 K. Similarly set the top temperature to 325 K. By default, no slip boundary conditions are applied to all the walls. Also by default, the initial temperature and velocity in the domain is set to 300 K and 0 m/s respectively.



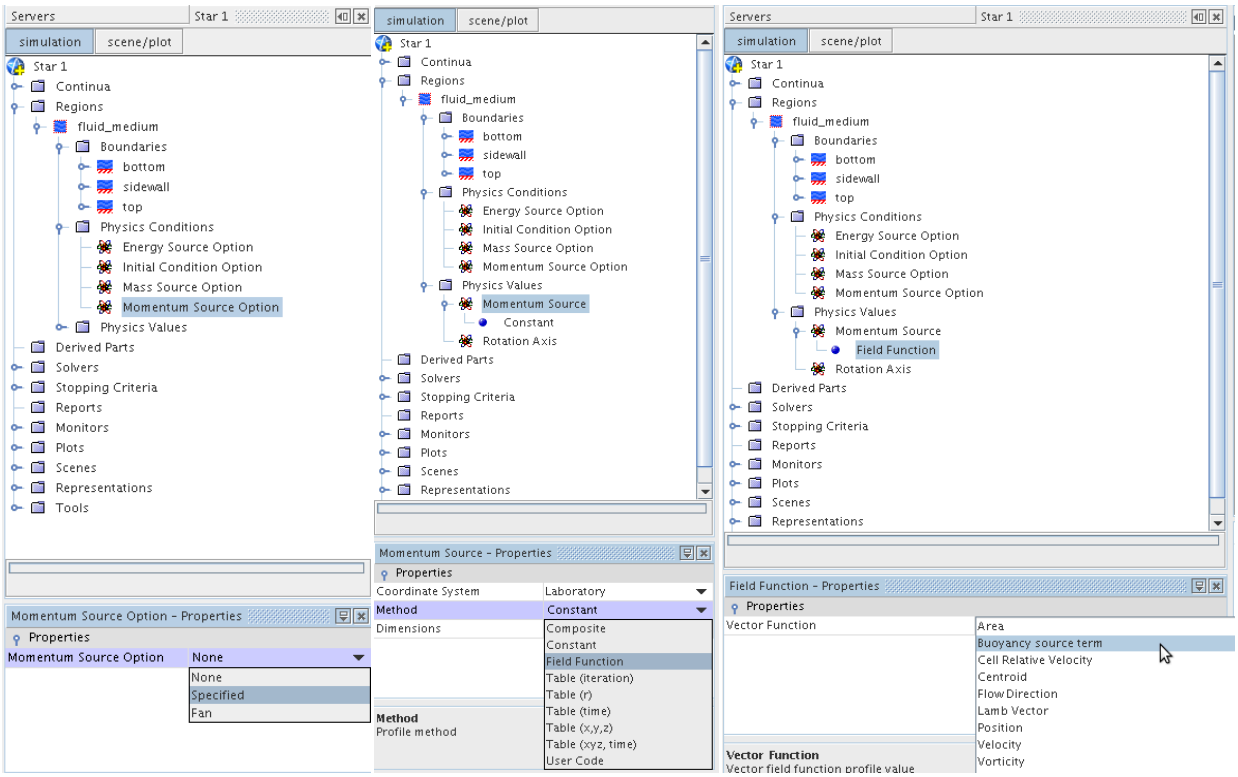
6. Now we need to incorporate the buoyancy driving force. Notice that we did not choose "gravity" in the selection of models. In this problem, the density change with temperature is accounted for by introducing a **momentum source term**. We will use the Boussinesq approximation, where all properties of the fluid except density do not change with temperature. Since this force is a function of the fluid temperature, we will create a new user defined function for it. Create a new "field function" under the "Tools" tab. Rename it "Buoyancy source term". In the properties of this field function make the "Type" a vector, give it the correct dimensions (force/volume). Change the function name to "Buoyancy source term" and finally, in the "Definition" tab enter the following.

   [0,0,(975)*(5.5e-4)*(9.81)*($Temperature-300)]

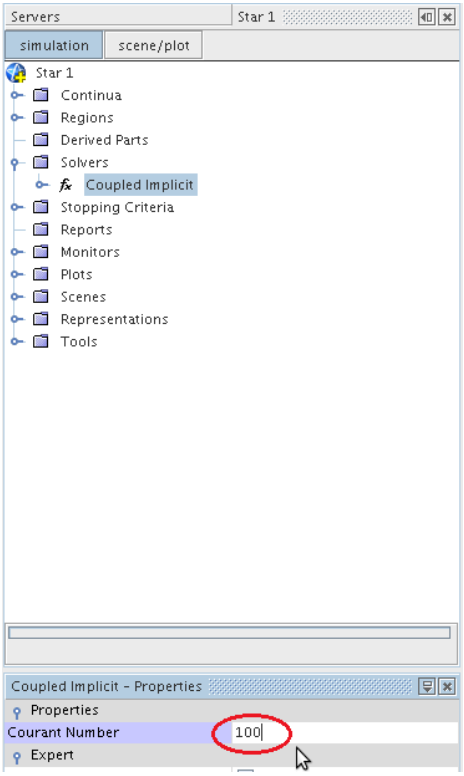
   This specifies that the buoyancy force, as described in Equation 1.4, acts only along the z axis.



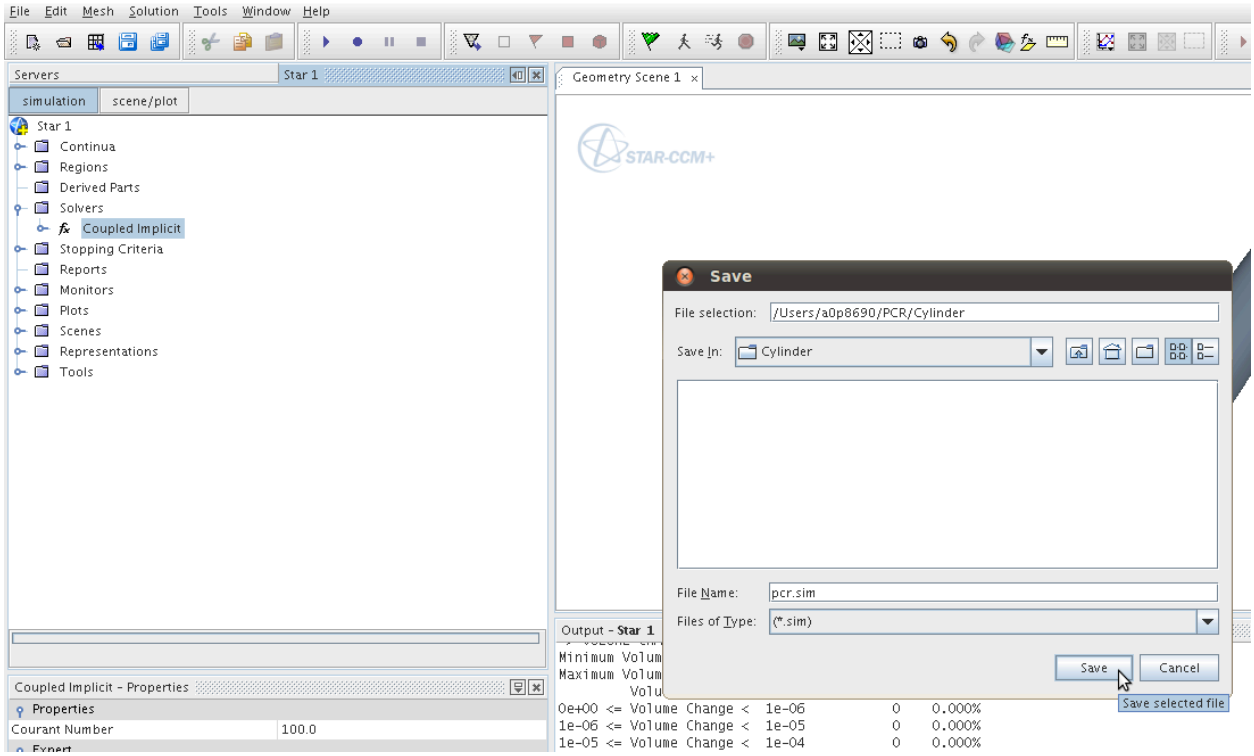
7. Now under "fluid_medium" in "Regions" tab, change the "Momentum Source Option" from "none" to "specified". Now under the "Physical Values" tab change the method of the "Momentum Source" to "Field Function" from the default "Constant". Select "Buoyancy source term" from the list of available field functions.



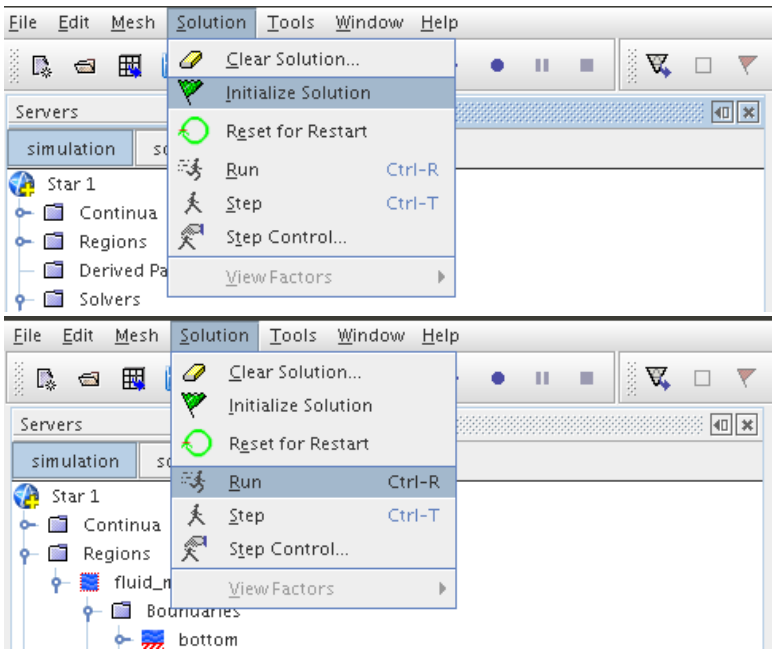
8. Next to set the “Courant Number” in the “Coupled Implicit” tab of the “solver” properties to 100 for faster convergence.



9. Save your simulation.



10. "Initialize" your solution from the solution tab and then "run" the solver.

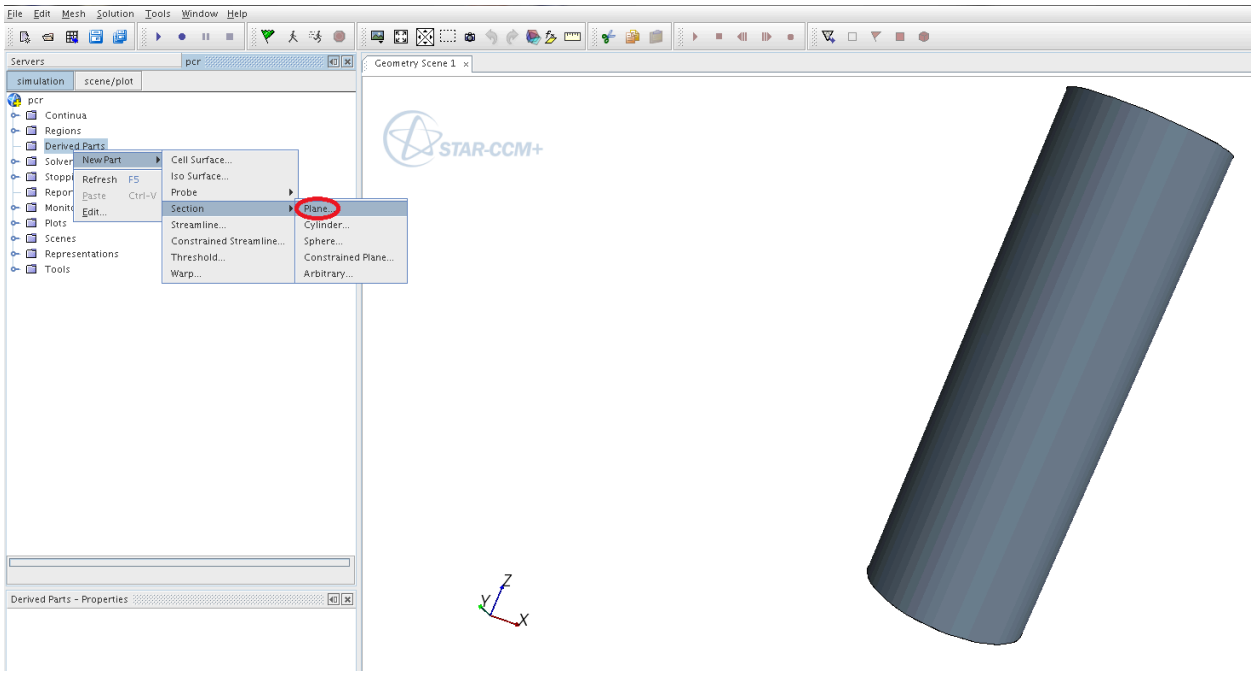


11. The residuals should continually decrease as the number of iterations increases. When they have reduced below a certain minimum value (10^{-3} or lower). You may stop the iterations and view the results.

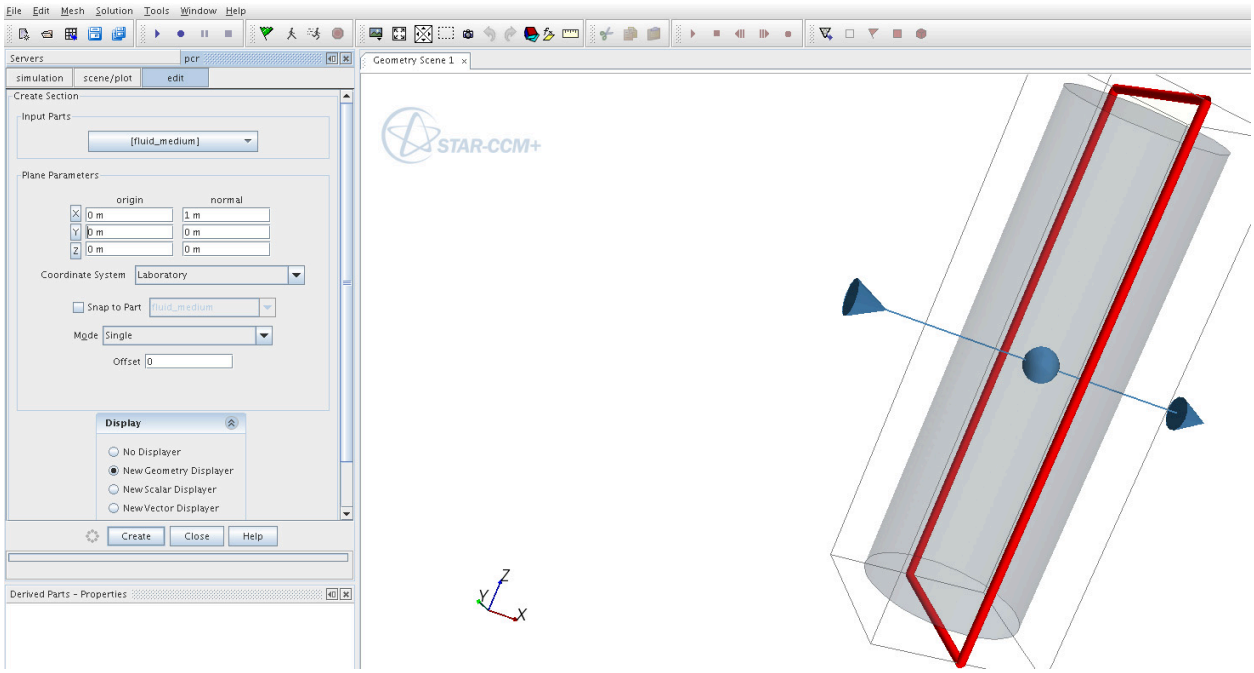
Post processing

Finally we will analyze our results. To do this, we first create a plane at the desired location in the geometry and view contours of the physical parameter of interest.

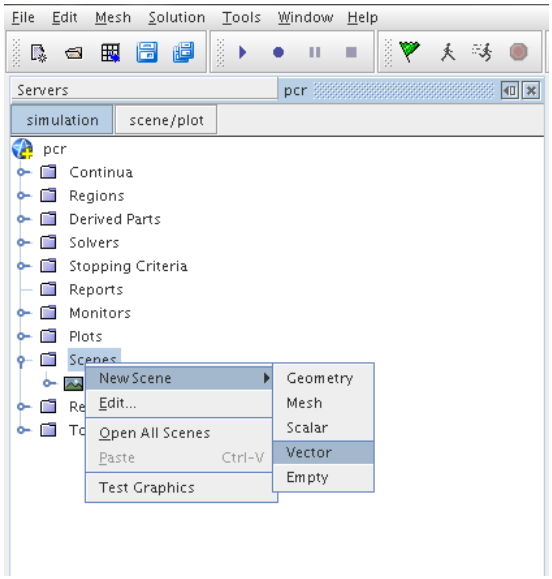
1. We will choose the y-z plane for analysis. To create a plane, right click "derived parts", navigate to "new part", "section" and then "plane".



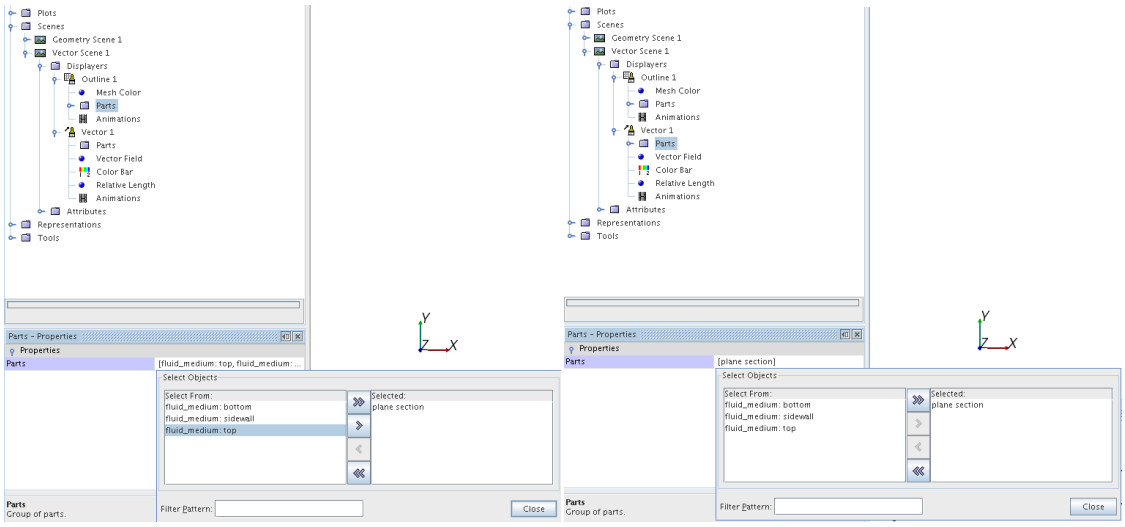
2. For the "input parts" choose the “fluid_medium” parameter and make sure the "normal" to the x component is 1. click on "create".



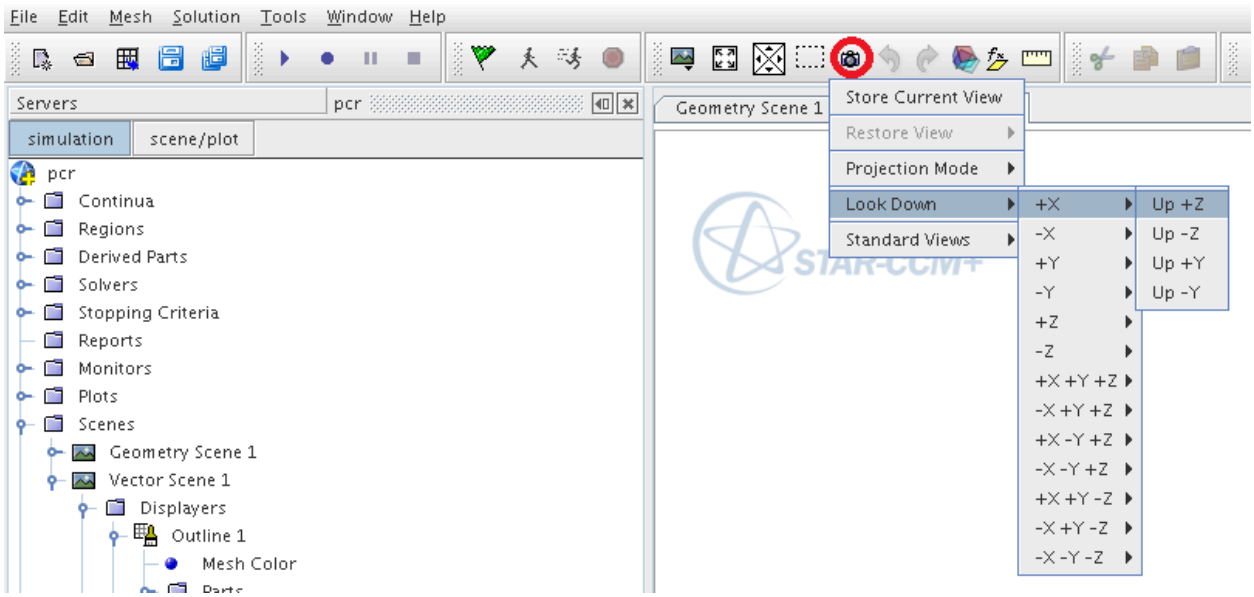
3. Now we can view data on the plane we created. To do this, right click on "scenes", followed by "new scene" and choose a "vector".



4. In the newly created vector scene, expand "Displayers" followed by "Outline 1" and click on "parts". From the properites menu of parts, select only the "plane section" that was just created from the list. Next under "vector 1" in the parts menu, select only "plane section" again. The vector field is the velocity field by default.



5. Now we will change the view orientation. To do this, click on the tiny camera from the widgets at the top as shown. Navigate to "look down" followed by "+X" and finally "UP +Z". This will ensure that we are looking at the y-z plane.



6. A similar scalar field can be created to view the temperature profile within the plane.