Computational Fluid Dynamics (CFD) how-to for Membranes project
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This document is about using Citrix Receiver on a Mac to simulate flow through a pore in a membrane at the University of Louisville. The tutorial shows the setup along with some Mac/Citrix specific quirks.

Set up preferences in Citrix for "read and write" to you local computer. Otherwise it might ask you each time, or sometimes fail to even give you that option. Then you won't be able to save your things. The login is your usual university one.

Then get ANSYS Workbench, Fluent and other software on Citrix using the "add" button. It's not installing anything locally so this doesn't take long at all.

You might need a 2nd monitor. The first time I used it, Citrix was creating ANSYS windows off screen, and I could not work until plugging in that 2nd monitor. If you still never get that window or get an error message, just keep trying and restart Citrix if you need to. Do not totally give up at this point.

Click away that getting started message if you've seen it a lot before.

This tutorial is based on an online nozzle tutorial:
https://confluence.cornell.edu/display/SIMULATION/FLUENT+-+Compressible+Flow+in+a+Nozzle
But with some changes:
-Laminar flow with water instead of air
-There are some new tips for getting it to work at the microscale
-At the end of this tutorial are some tips for adding a moving wall
-Added specifics for getting it to work via Citrix, and also for Mac users
-The exact meshing steps in the nozzle tutorial didn't work with my setup so that part has been modified too.

All the following videos are at this YouTube playlist:
https://www.youtube.com/playlist?list=PLU_9JEJNLVb_oY0A7QFFQus4xd9ox1KOH

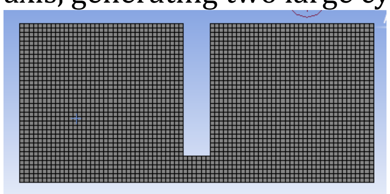
See the video, **1_SetUpNewWorkbenchProject.mov**. Steps in that video are: start ANSYS Workbench, drag a Fluent project over from the left menu to the white area, and name and save your project

I save it on the remote computer instead of my laptop, because some of these programs don't work well with path names > 256 characters.

Next, draw up some geometry for the pore wall, end caps, and axis. You can do this in a text editor. The default units are meters but we can scale down later. Each line is given a Group ID, a point number, and then the x, y, z coords. This example has 8 line

segments each defined by two points. The end point has to match up w/ the start point of the next group. If you put 3 or more points in a group, ANSYS tries to draw a curved line.
In this tutorial, we are trying to draw the outline of this blocky shape. (Then we will fill it with the little squares later) We don't really need curved lines for this shape.

The pore is represented by the low spot in the middle of the gray shape. This makes little sense until you take the shape and rotate it 360 around the bottom horizontal axis, generating two large cylinders connected by a little cylinder: the pore.



(Group Point x y z –don't stick these labels in the text file)

1	1	-0.200	0.180	0
1	2	-0.015	0.180	0
2	1	-0.015	0.180	0
2	2	-0.015	0.030	0
3	1	-0.015	0.030	0
3	2	0.015	0.030	0
4	1	0.015	0.030	0
4	2	0.015	0.180	0
5	1	0.015	0.180	0
5	2	0.200	0.180	0
6	1	0.200	0.180	0
6	2	0.200	0	0
7	1	0.200	0	0
7	2	-0.200	0	0
8	1	-0.200	0	0
8	2	-0.200	0.180	0

OK save that .txt file somewhere you can find, whether on your local machine or elsewhere. Local machine is probably easiest.

However, you **can** navigate directories using Windows on the remote computer if you're in Workbench, go to View->Files, then files should show up at the bottom of the screen. Right click (or 2- finger click—mac) on a file name and you get an option to "Open Containing Folder," then you can browse & copy and paste files within Windows.

Now it's time to work through the Geometry section.

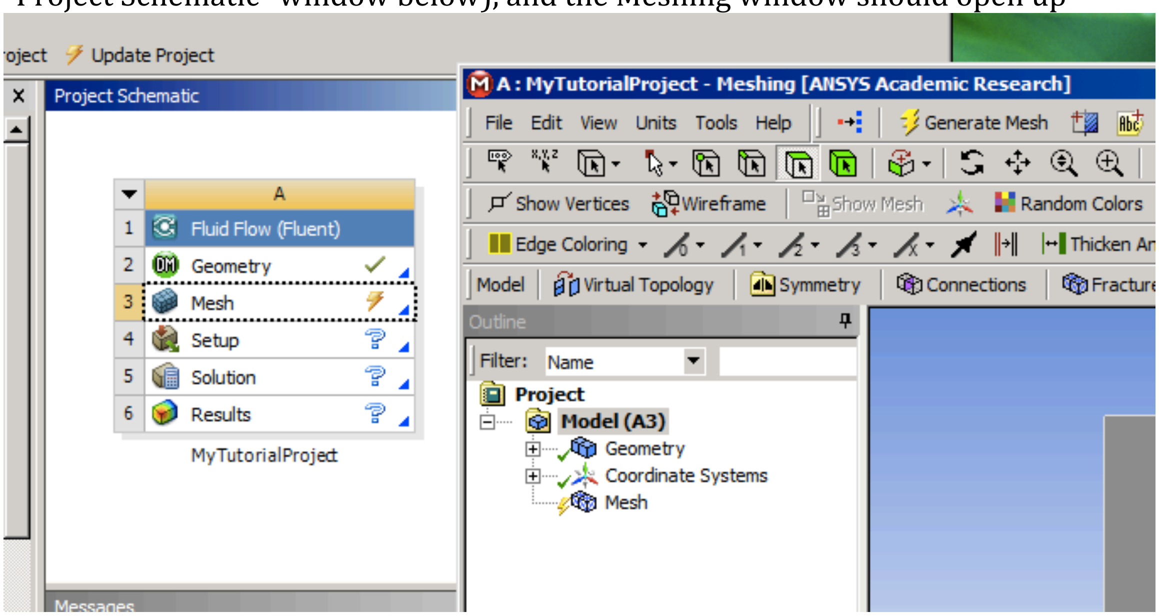
See the videos **2_GeometryPart1.mov** and**3_GeometryPart2.mov** about how to turn the above text file into a sketch.

After we draw up the geometry, there are some arrows that need to be removed.

4_CreatingSurfaceInDesignModeler.mov shows the steps

Now you should have two windows open, DesignModeler and Workbench, and you can click back on the Workbench. Geometry should now have a check mark. Time to move to Mesh. You can close DesignModeler.

Back in Workbench, double click on Mesh (step 3 in MyTutorialProject in the "Project Schematic" window below), and the Meshing window should open up



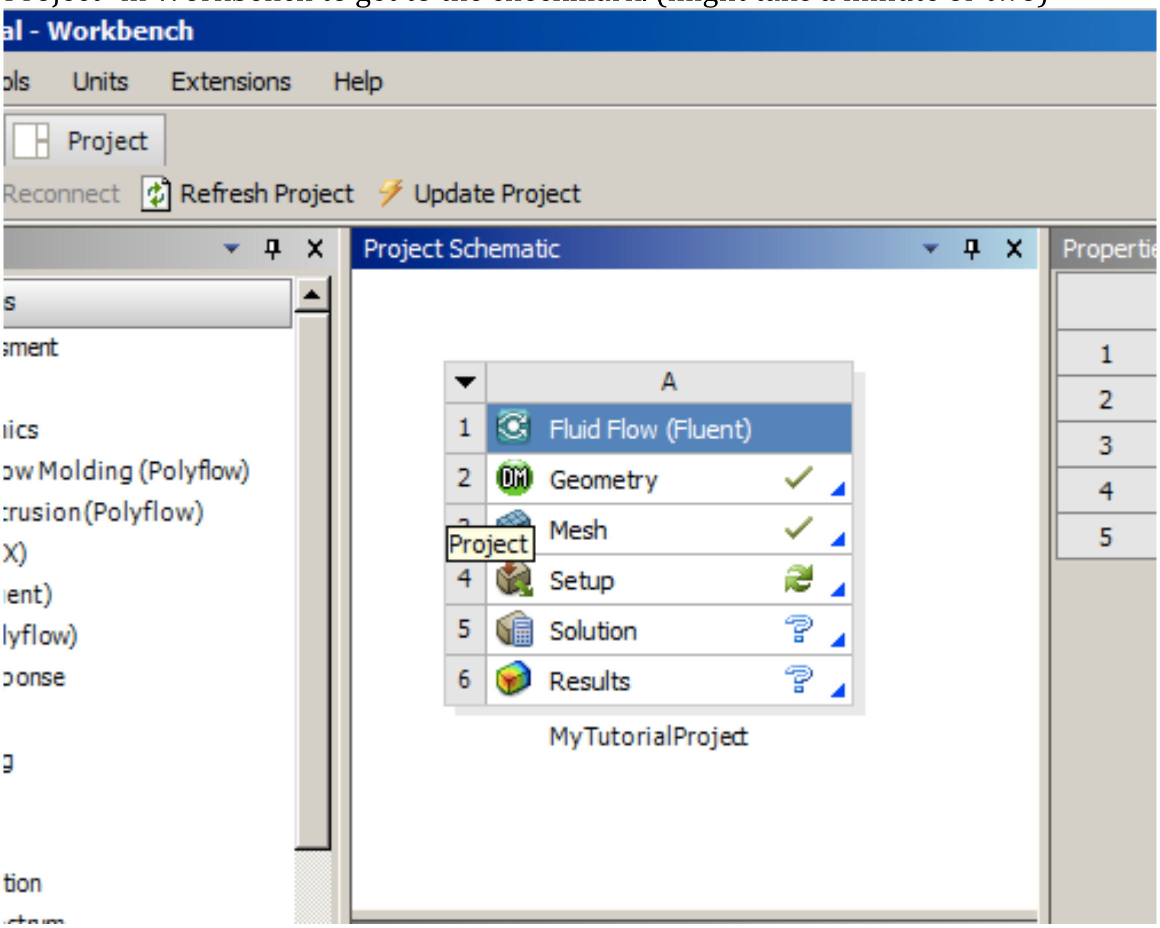
(Meshing window pops up with your surface loaded)

The meshing part of the nozzle example I had been using did not work consistently with the weird Citrix/Mac/Ansys15 setup, and I often got stuck generating a mesh. Luckily, once you get past this point you don't often have to revisit.

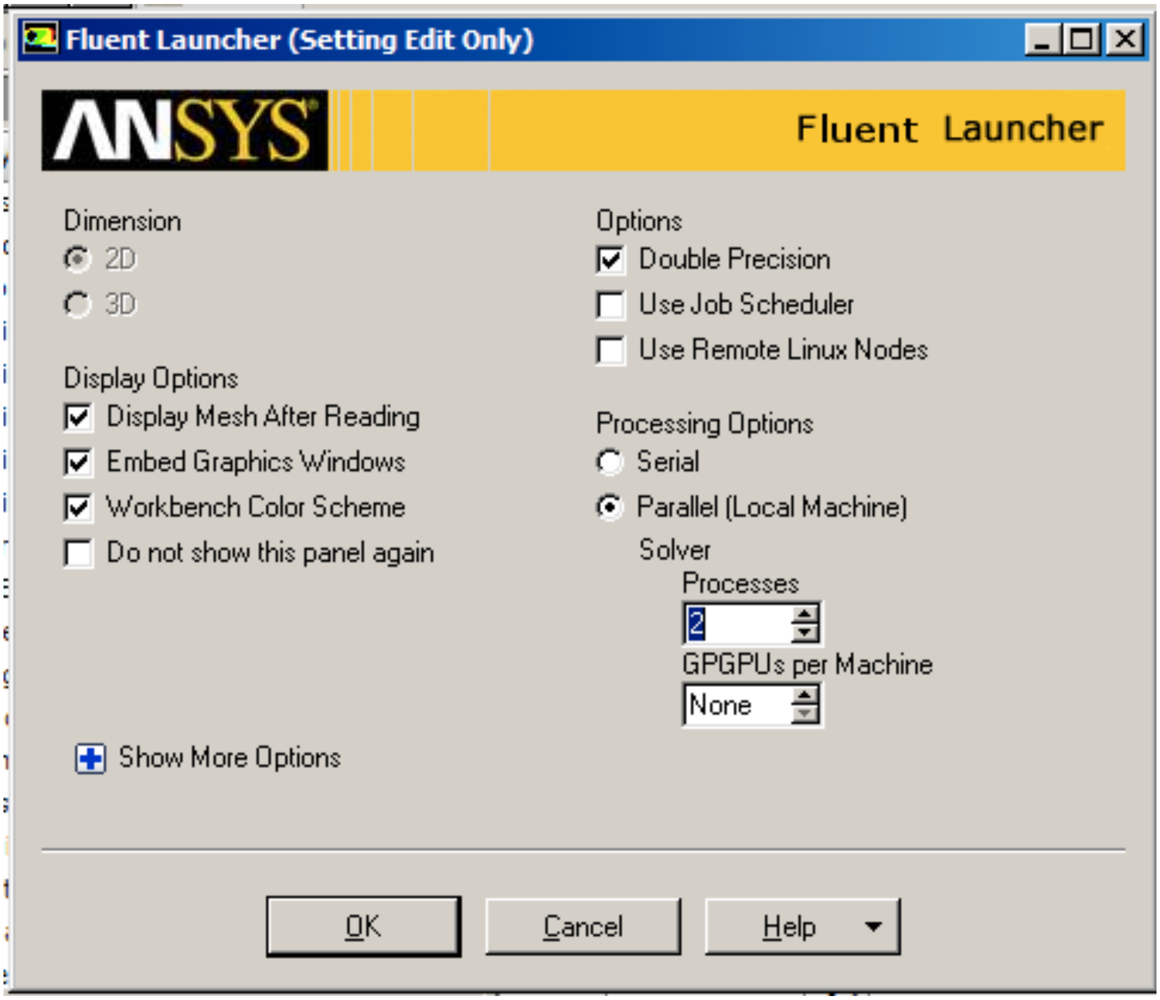
6 or 7 takes later, I now have a sequence that works well with this setup. If you're following the Nozzle example and getting stuck, see the video:

5_TheMeshingMovie.mov
6_MeshingPart2NamedSelections.mov then shows how to label wall sections so we can refer to them later in Setup.

Back to the Workbench window, the Mesh step should now have a checkmark. If you went back and forth a few times between Workbench and Mesh to create those named selections, there might be a lightning bolt next to Mesh. If so hit "Update Project" in Workbench to get to the checkmark. (might take a minute or two)



Time for Setup. THE BEST PART. Double click the Setup step in the Project Schematic window.
You'll see a Fluent Launcher window; edit the settings like this



Click OK, then you will see the setup window.

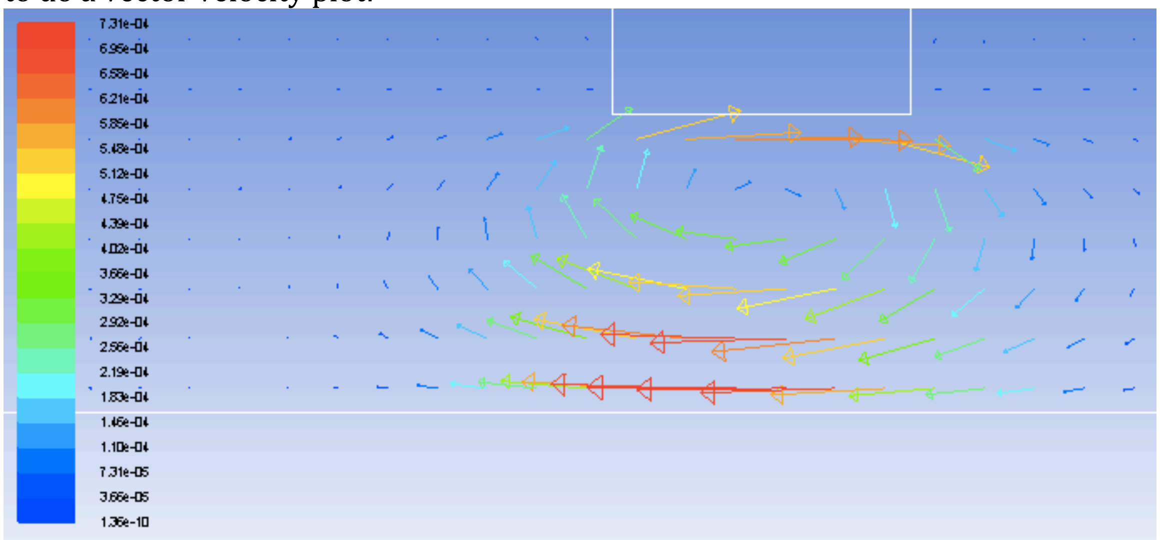
At this point I had to leave campus and this can lead to a session that's still open but unreliable. If moving between networks, you should save and close everything, then restart Citrix back at the new wi-fi location. Log Off works better than Disconnect if it gives you that choice.

Watch **7_SetupAndCalculate.mov** for the next step. This video shows you how to
-Scale the domain down to 400 microns x 180 microns
-Choose settings: pressure-based, absolute, steady and axisymmetric
-Choose the Viscous-Laminar model
-Set the material to be water instead of the default air, with density 998.2 kg/m3 and viscosity 0.001003 kg/m-s.
-Set the solver to ignore convergence criteria; important for this microscale simulation so it doesn't think it's converged after step 1 or 2
-Set it to iterate 500 times (200 would have probably been okay)
-Calculate

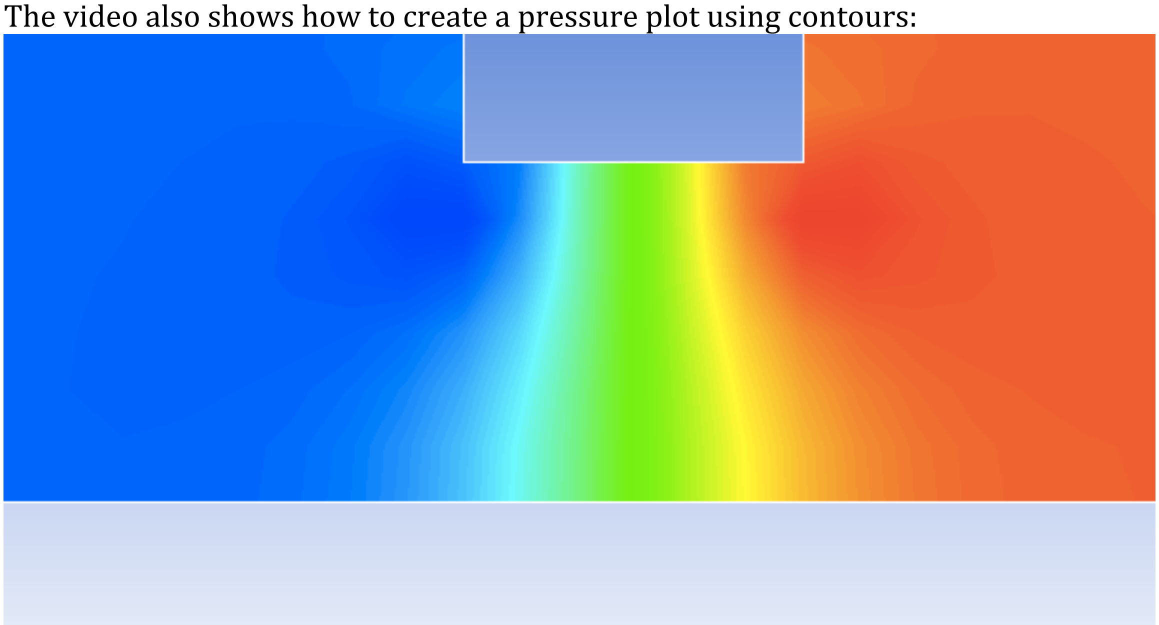
-Display velocity vectors.
This part is long so I split it into 2 videos. Next up:

8_ ShowVelocityAndPressureInSolution.mov

This video shows how to use the Graphics and Animations part of the Setup window to do a vector velocity plot:



The video also shows how to create a pressure plot using contours:



In the Graphics and Animations window, there are a lot of features like Options, Scene, Views, Lights, Colormap and Annotate. I didn't do anything in the video with these options, but they make it possible to
-Mirror the simulation around the axis so you can see a cross-section of a full pore

-Make it look nicer, you can remove the white line at the axis and you can also space out the legend on the colormap so the numbers aren't smushed together
-I couldn't get Annotate to work with my setup, and decided to write on the images later using the mac.

When you want to save images from the output, you can do screenshots like I did here, but more professional results can be had by going to File-> Save Picture
You can save vectors in .ps format, it's going to make your colorbar and legend look really great.
You can also save images in web-friendly .jpg format, great for pressure contours, but your colorbar and text will be bitmapped junk and should be re-done for publication.

Back in the Workbench window, there's a Results task. It can produce some astonishing 3D renderings.

What next besides pretty pictures? The goal is to calculate pressures and volumetric flow rates vs various parameters (E-field, diameter, pore length, pore density, and so on) for comparison with pumping rate and pressure-sensor experiments

Get it to compute **volumetric flow rate Q** like this:
The task is to integrate up the velocity vectors' dot product with any surface that spans the channel and determine how much fluid is crossing the surface per unit time. (Also known as the flux).
Since we have an incompressible fluid, mass flow rate (kg/s) and volumetric flow rate Q(m3/s) are proportional. You can get mass flow rate in Setup->Results->Reports->Fluxes. For the above simulation, the mass flow rate at the outlet comes out about 0, that's great but not too interesting. It is more interesting when we create 0 pressure drop, then it should give Qmax.

Add a moving wall velocity **profile** that creates a non-uniform velocity that comes from the electric field simulation. When I tried this, the scaling in the setup did not work predictably with the profile, so I created a NEW geometry file with the geometry in meters (meaning, it was filled with very small numbers) and also created a profile containing some x-y points and x-velocities in meters/s.

For example, here is a velocity profile based on using a Laplace solver (MATLAB) to get the surface charge density, then converting charge density to a surface velocity using the Helmholtz-Smoluchowski equation. For the 30 micron long, 50 micron diameter pore with 1V transmembrane potential (1V/30 micron tangential field) the velocities were pretty small (4 microns/s) . It had 18 points for x, and y, separated by tabs, **here's the format of a profile ANSYS will read:**

```
((pore-prof point 18)
(x  -1.6758e-05                 -1.5008e-05   -1.3038e-05   -1.0988e-05   -8.9283e-06
        -6.9083e-06   -4.9283e-06   -2.9383e-06   -9.0833e-07   1.1317e-06
        3.1117e-06    5.0817e-06    7.1117e-06    9.2017e-06    1.1212e-05
        1.2982e-05    1.4552e-05    1.6022e-05)
(y  2.523e-05 2.4976e-05    2.4934e-05    2.4964e-05    2.5009e-05    2.5029e-05
        2.5017e-05    2.4994e-05    2.4977e-05    2.4981e-05    2.5013e-05
        2.5042e-05    2.5013e-05    2.4933e-05    2.4945e-05    2.5188e-05
        2.5629e-05    2.6153e-05)
(u  4.4824e-09          -5.9123e-08   -1.1938e-07   -1.7635e-07   -2.3411e-07   -
2.9754e-07    -3.7204e-07   -4.617e-07    -5.7332e-07   -7.1212e-07   -8.8239e-07
        -1.0932e-06   -1.3694e-06   -1.812e-06    -2.4668e-06   -3.0756e-06   -
3.868e-06       -4.4907e-06))
```

When setting the **tangential wall velocity** in Setup, you use the profile instead of a fixed velocity. To do that, you need to go to “Define” in the menu, select Profile, click Read, and locate your profile file, then click Apply. I had it use the inverse distance option. It will appear to do nothing, but if you can see the x, y, and u, it’s probably working. Then go to Setup, and in the boundary conditions section, select Components instead of constant velocity. You should be able to select the “u” profile for x-velocity. Along the PoreWall, Ansys will interpolate the profile to set a non-uniform wall velocity. This is simpler than the “user defined functions” you may come across on the forums, but profiles can’t change with time or with other conditions, just spatially. This profile could be further improved by using profiles for both the x- and y-components. In this example the x-components dominate, but there are small y components on the pore edges.

Validate by creating a simulation that can be compared to a well-known experimental or analytical result. For instance, a long tube with moving walls will represent an electrokinetic pump made from a glass capillary (and studied for decades.) Do we get the same vector field and pressure drop as expected?

Simulate pores in series (should be easy to draw multiple pores in a row) and **in parallel**. The parallel one –for example, two pores side by side-- may be a full 3D simulation, rather than this 2D axisymmetric simulation. 3D can take a lot of computer time. We should carefully use periodic boundary conditions to cut down on the number of mesh cells that have to be calculated. For instance, it might be more work to simulate two pores side-by-side, than an infinite field of pores on a square grid.

Integrate electric and fluid simulations, this will really pay off if doing a ton of simulations for a Ph.D. thesis.