Computational Aspects of Modeling Fluid Flow in Micro-junctions

OU Supercomputing Symposium

Oct. 7, 2008

Evan Lemley & Tim Handy
Department of Engineering and Physics
University of Central Oklahoma

Overview

Background / Current Research

Problem Description

2D Simulations

3D Simulations Mark I

3D Simulations Mark II

Conclusions and Future Work

Applications

Flow in microfluidic flow networks and flow in porous networks are of interest in many engineering applications.

Applications include porous media, micro-power generation, biomedical, computer chips, chemical separation processes, micro-valves, micro-pumps, and micro-flow sensors

Yanuka, M., Dullien, F.A.L., and D.E. Elrick, 1986, “Percolation Processes And Porous Media I. Geometrical And Topological Model Of Porous Media Using A Three-Dimensional Joint Pore Size Distribution,” J.Colloid Interface Sci., **112**, pp. 24-41.

Lee, W.Y., Wong, M., and Zohar, Y., 2002, “Microchannels in Series Connected Via a Contraction/expansion Section”, J. Fluid Mech., **459**, pp.187-206.

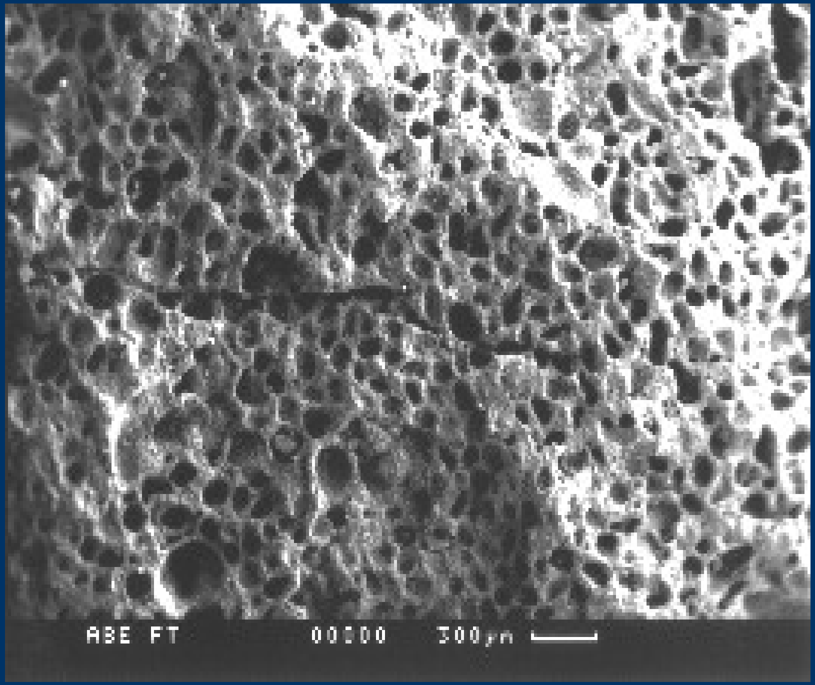
Judy, J., Maynes, D., and Webb, B.W., 2002, “Characterization of Frictional Pressure Drop for Liquid Flows Through Microchannels,” Intl. J. Heat Mass Trans., **45**, pp.3477-3489.

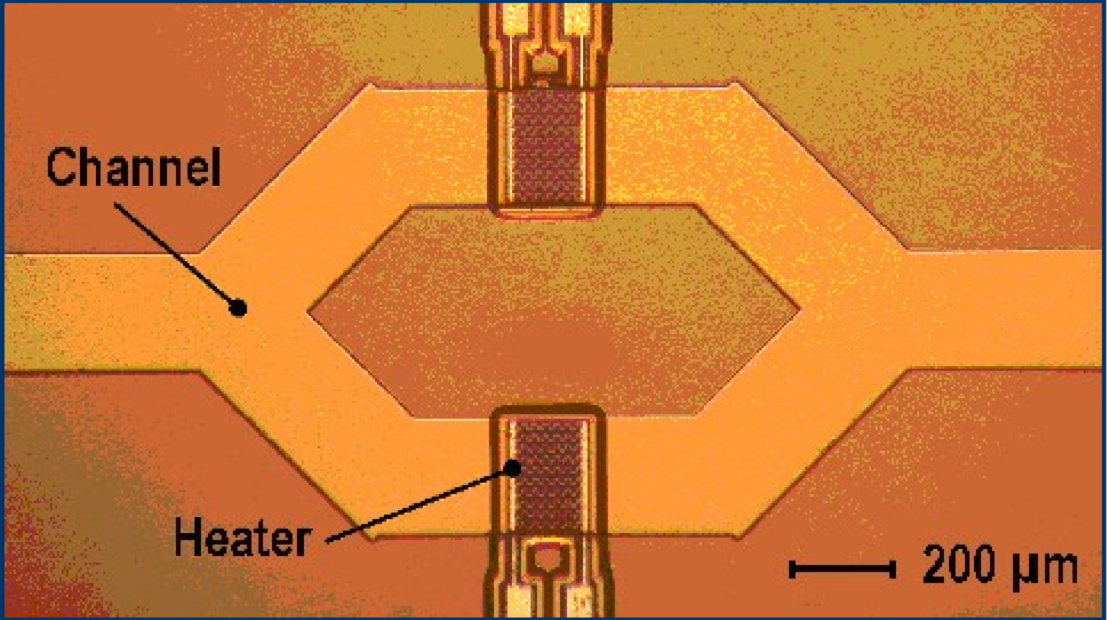
Flow in these applications is usually laminar

Graveson, P., Branebjerg, J., and Jensen, O.S., 1993, “Microfluidics a Review,” J. Micromech. Microeng., 3, pp.168-182.

Porous Media

Microfluidic Devices

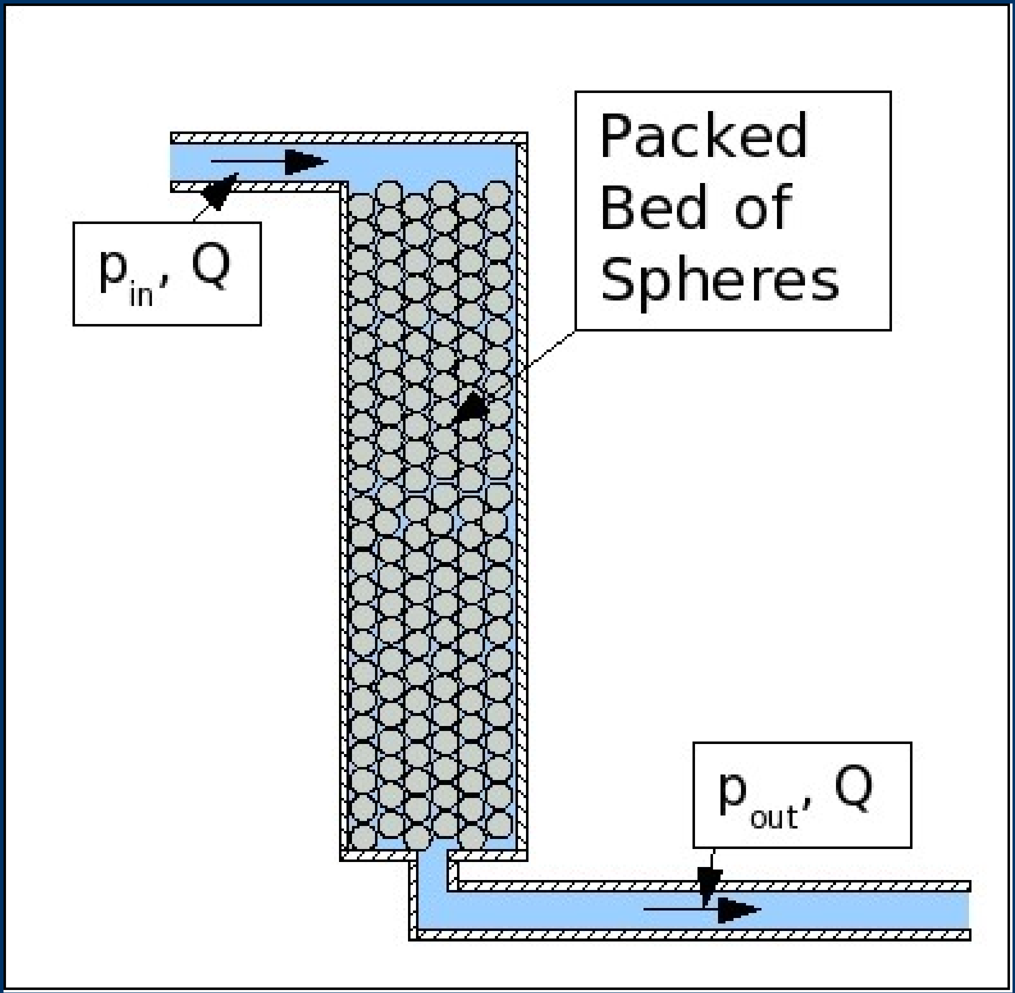




Highly porous magnesian limestone.
(www.dawntnicholson.org.uk)

Microfluidic Valve Structure.
(http://www.cchem.berkeley.edu/sjmgrp/people/boris/boris.htm)

Artificial Porous Media



Packed Beds, Gas and Liquid Filters

Sphere sizes μm to cm

Hold-up for chemical reaction, thermal processing, or filtering

Current Research

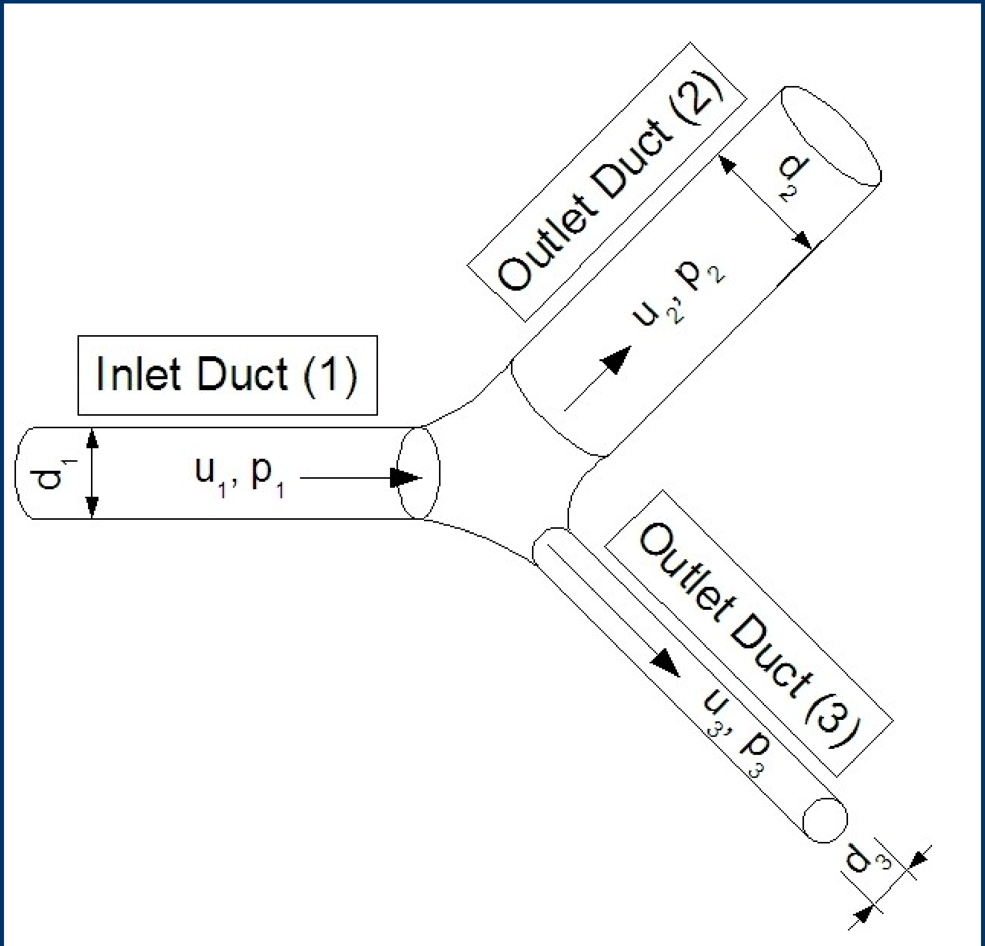
Collaborative Effort with Dimitrios Papavassiliou and Henry Neeman from OU (began Fall 2004)

Simulation of Flow of Fluids through Porous Media

Code FTPM – Flow Through Porous Media.

Solves for velocity and pressure at pore junctions in a randomly generated pore network.

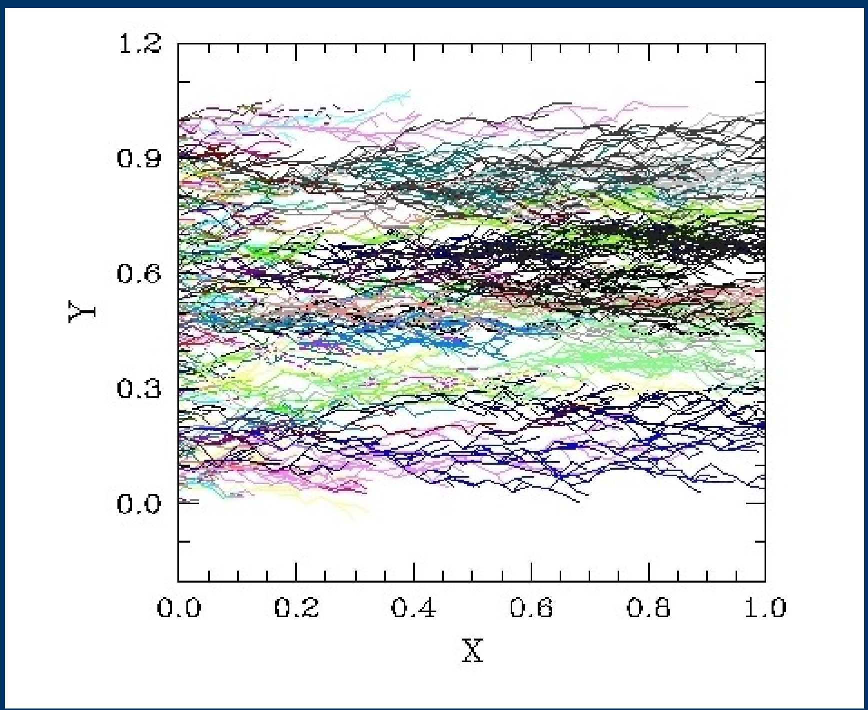
Flow Network Analysis



Design and Analysis of networks depends on knowledge of flow and energy losses in arbitrary branches.

No systematic studies to generalize these bifurcations

Porous Network Simulator (Collaboration with Univ. of Oklahoma)



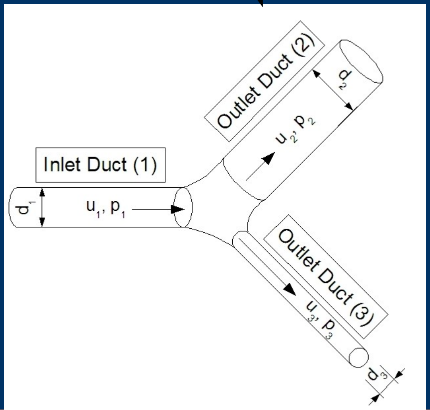
Projection on the xy plane of a 3D network that has 200 entry points at x=0, porosity equal to 10% and a range of ±60˚ relative to the x axis and ±30˚ relative to the y axis.

3D Monte Carlo networks from normal, beta, or empirical distribution (pore size pdf)

Coordination Number (1, 2, 3)

number of pores entering and leaving a junction

$\theta \pm 90^\circ$



Literature

T's and Y's – limited configurations and most are for turbulent flow

Basset, M.D., Winterbone, D.E., and Pearson, R.J., 2001, "Calculation of Steady Flow Pressure Loss Coefficients for Pipe Junctions," Proc. Instn. Mech. Engrs., Part C, Journal of Mechanical Engineering Science, **215** (8), pp. 861-881.

W.H. Hager, 1984, "An Approximate Treatment of Flow in Branches and Bends," Proc. Instn. Mech. Engrs., Part C, Journal of Mechanical Engineering Science, **198**(4) pp. 63-9.

Blaisdell, F.W., and Manson, P.W., 1967, "Energy loss at pipe junctions," J. Irrig. and Drainage Div., ASCE, **93**(IR3), pp. 59-78.

Schohl, G.A., 2003, "Modeling of Tees and Manifolds in Networks," *Proceedings of the 4th ASME/JSME Joint Fluids Engineering Conference*, **2**, Part D, pp. 2779-2786.

Bassett, M.D., Pearson, R.J., and Winterbone, D.E., 1998, "Estimation of Steady Flow Loss Cofficients for Pulse Converter Junctions in Exhaust Manifolds," *IMechE Sixth International Conference on Turbocharging and Air Management Systems*, IMechE HQ, London, UK, **C554**/**002**, pp.209-218.

Ruus, E., 1970, "Head Losses in Wyes and Manifolds," J. Hyd. Div., ASCE, **96**(HY3), 593-608.

Laminar loss coefficients and elbows, reductions, contractions – much *larger loss coefficients than turbulent case – strong dependence on Reynold's number*.

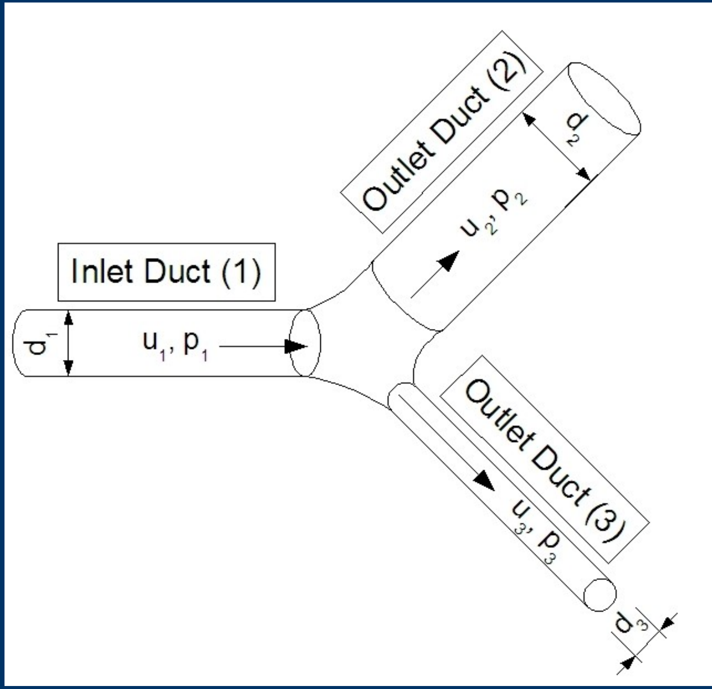
Edwards, M.F., Jadallah, M.S.M., and Smith, R., 1985, "Head Losses in Pipe Fittings at Low Reynolds Numbers," Chem. Engr. Res. Des., **63**(1), pp. 43-50.

Importance of roughness at microscale

Problem Description

Stagnation Loss Coefficient

$$K_2 = \frac{\left[\left(\frac{p_1}{\rho} + \frac{u_1^{\,2}}{2}\right) - \left(\frac{p_2}{\rho} + \frac{u_2^{\,2}}{2}\right)\right]}{\frac{u_1^{\,2}}{2}}$$



Parameters:

d_2/d_1, d_3/d_1

θ_2 and θ_3

f_2 (this sets f_3) – (why? other literature and possibility of simulations where this is unknown initially)

Automation of Geometry Generation and CFD Runs

Custom Code was written to:

(a) create GAMBIT journal files that instantiate the desired geometry *based on existing 2D geometries.*

(c) create a script that loads journal files into GAMBIT and meshes

(d) create all necessary preprocessing files for FLUENT.

(e) create post-processing files for FLUENT results and to tabulate results for a complete set of runs

Solution Methodology

2D Geometry Generalization

$L_1 = 5\ d_{max}$

L_2 and $L_3 = 10d_{max}$

If $d_2 > d_{avg}$,

then $r_2 = 3d_2$;

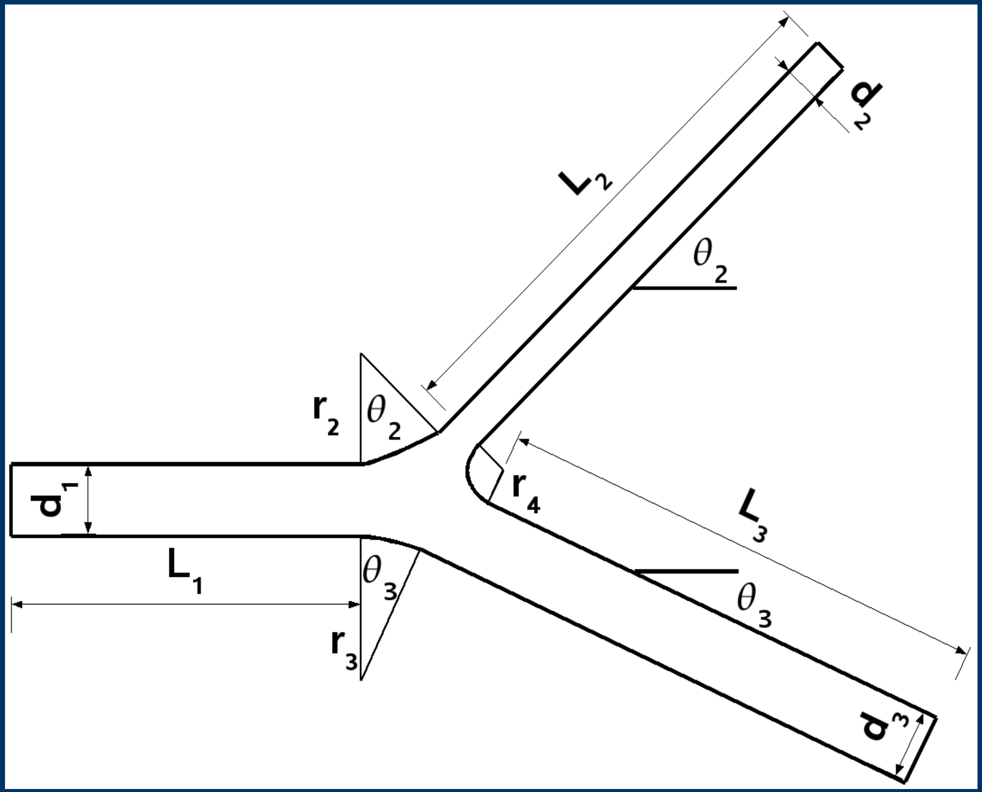
else $r_2 = 2d_2$

If $d_3 > d_{avg}$,

then $r_3 = 3d_3$;

else $r_3 = 2d_3$

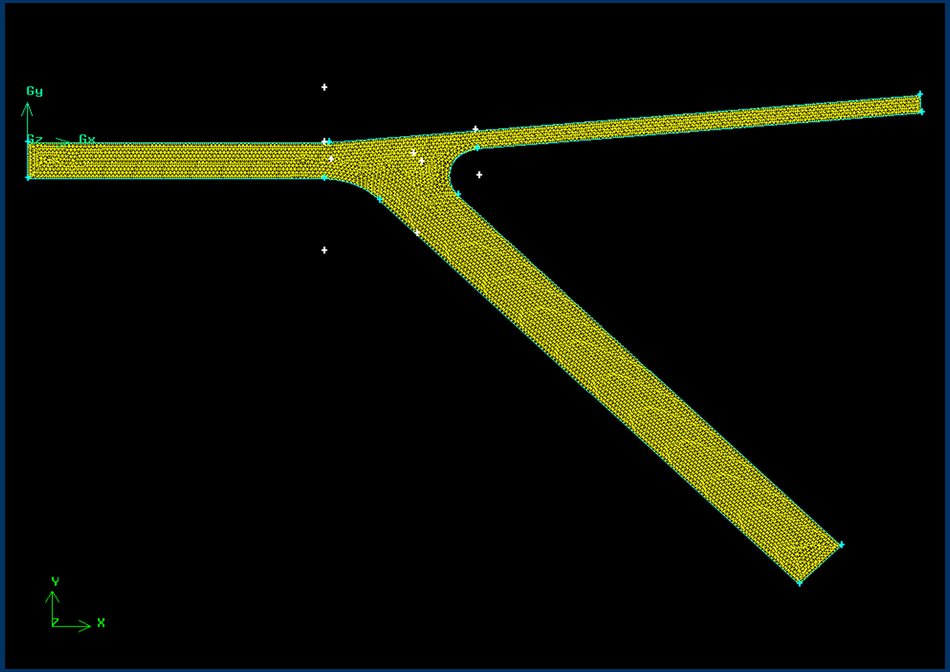
$r_4 = d_{max}/2$

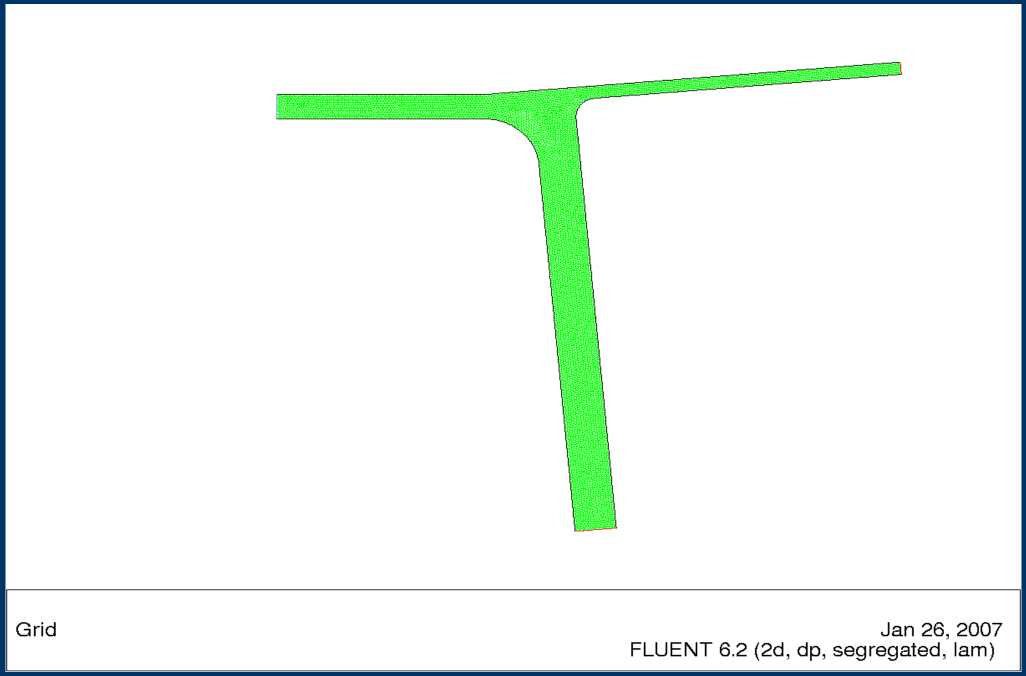


Generalized Geometry

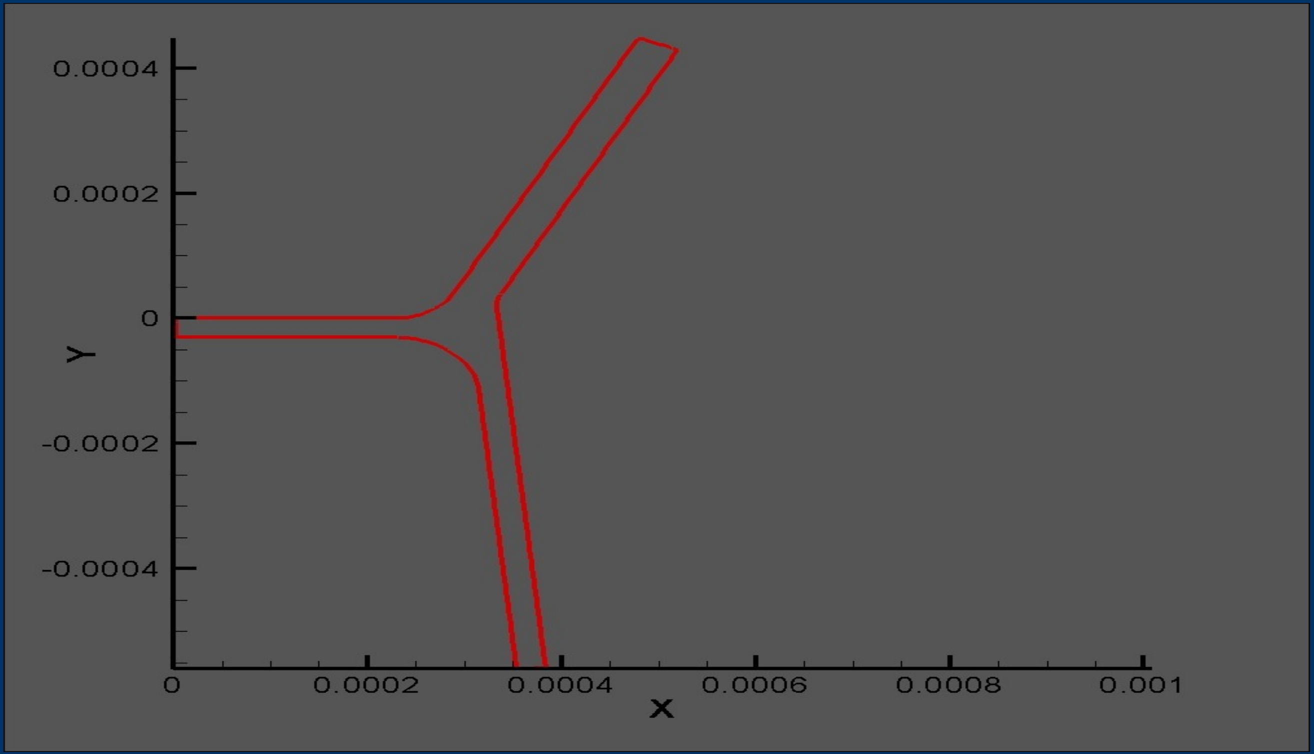
larger and smaller outlet ducts ; 2Dim. - 3Dim are underway

avoid sharp edges ; 5 – 90 degrees for angles



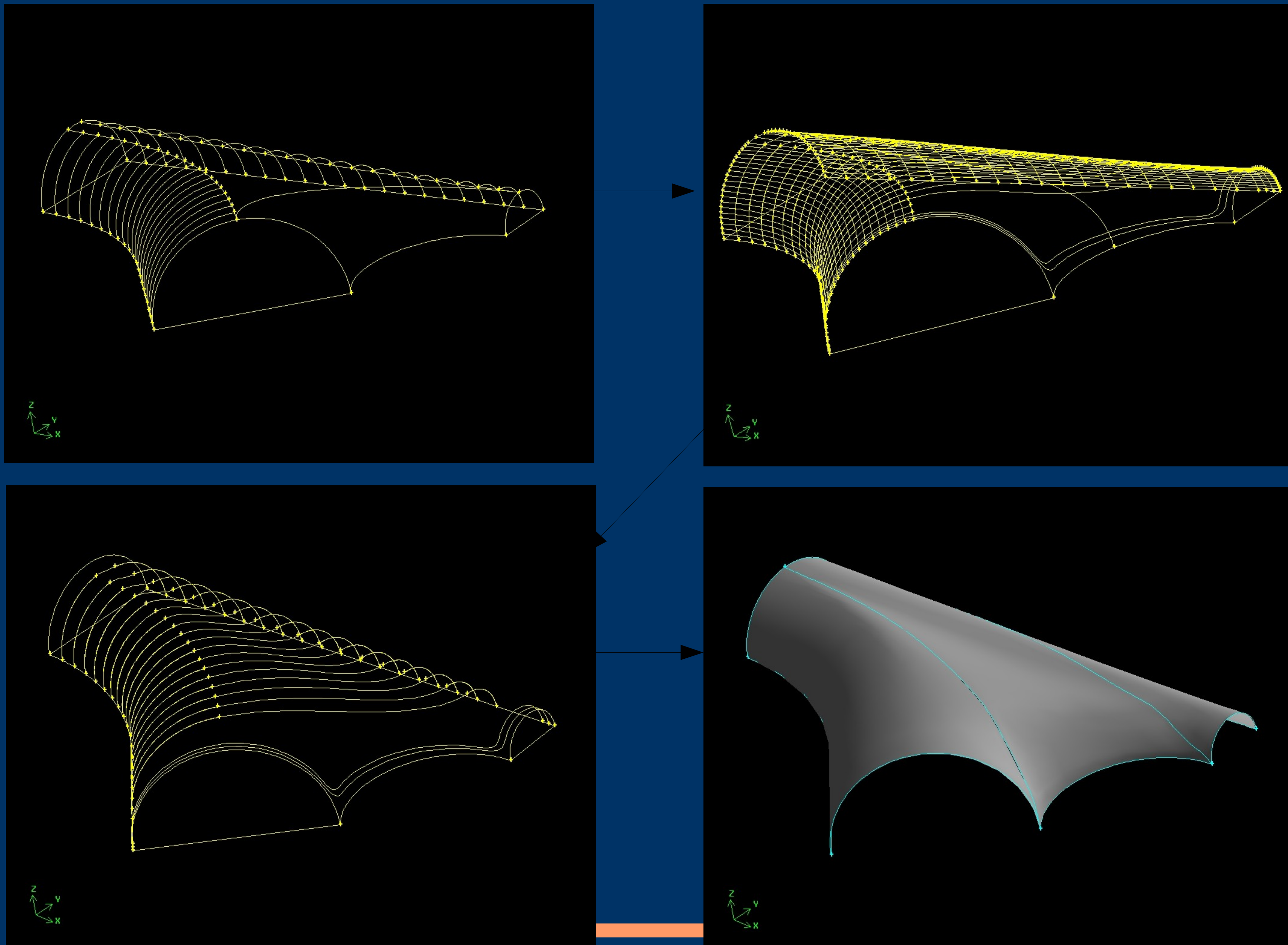


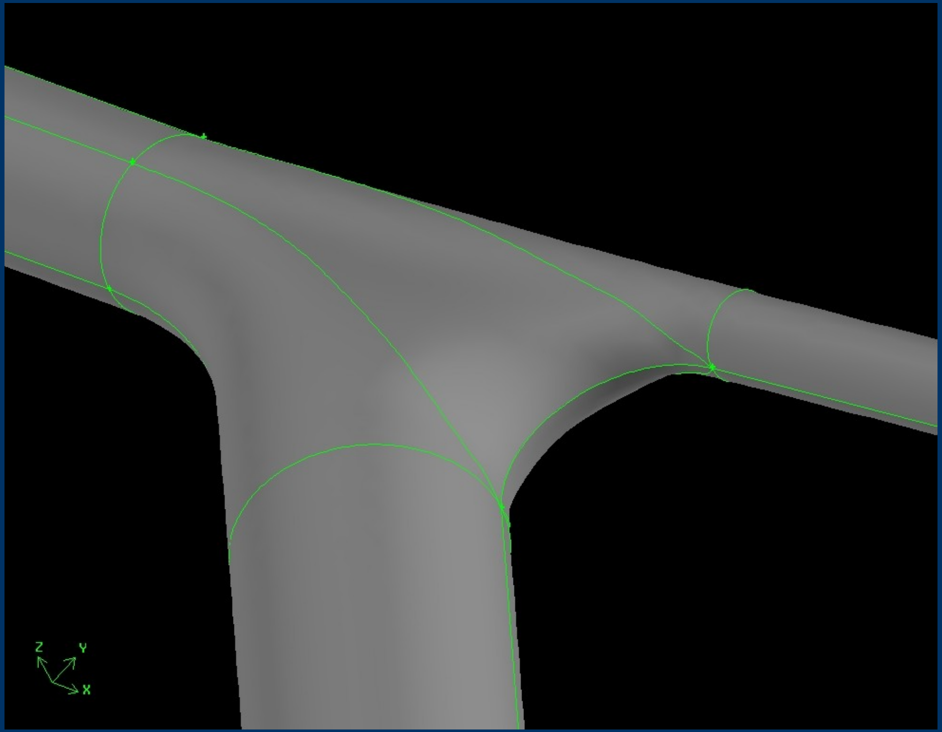
Grid
Jan 26, 2007
FLUENT 6.2 (2d, dp, segregated, lam)

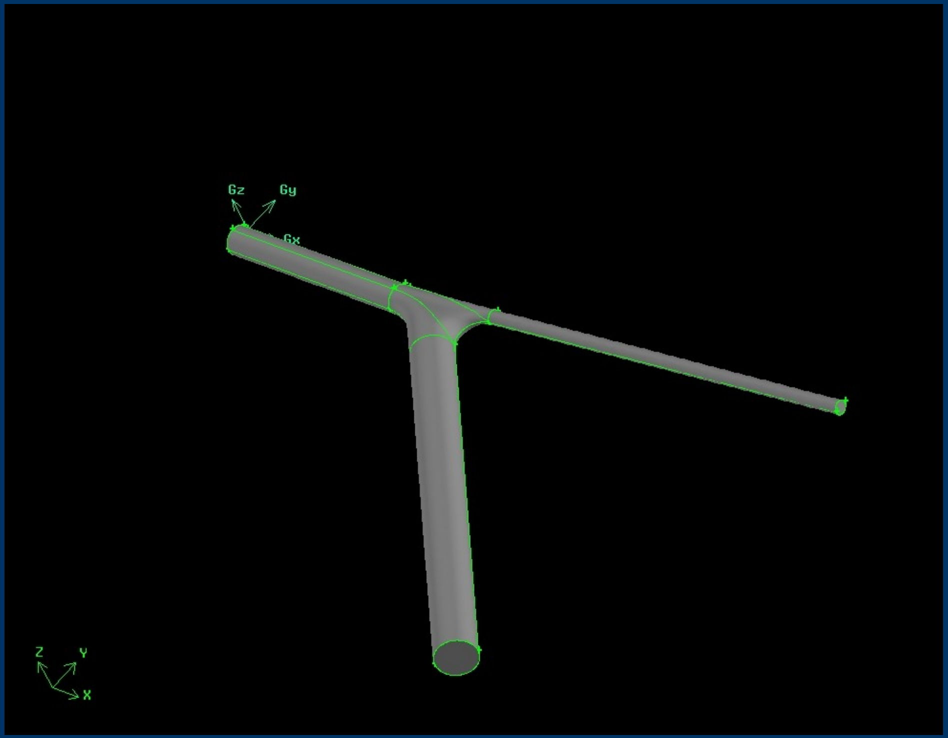


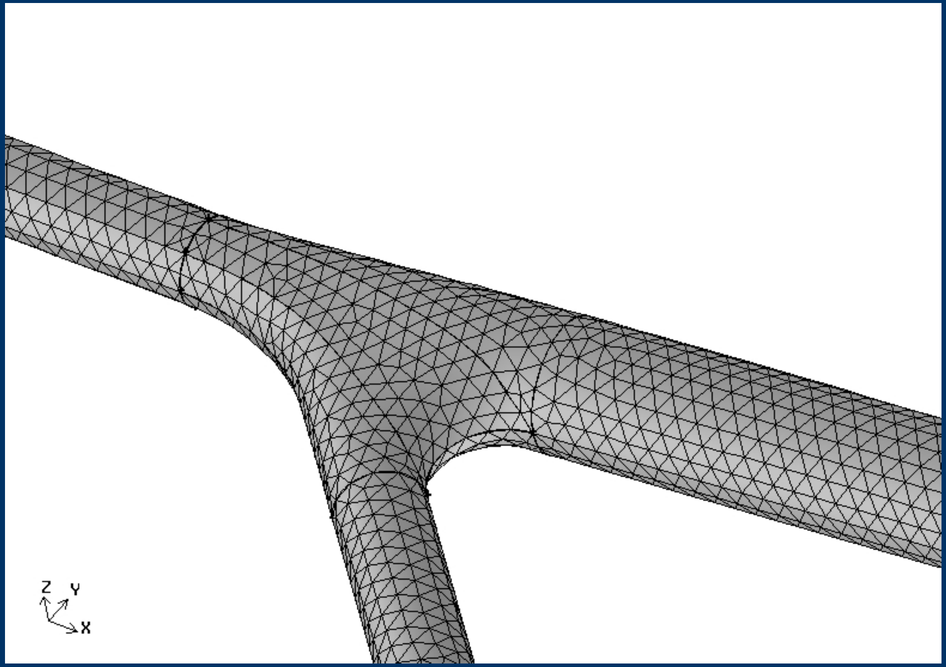
0.0004
0.0002
0
-0.0002
-0.0004
Y
0
0.0002
0.0004
0.0006
0.0008
0.001
X

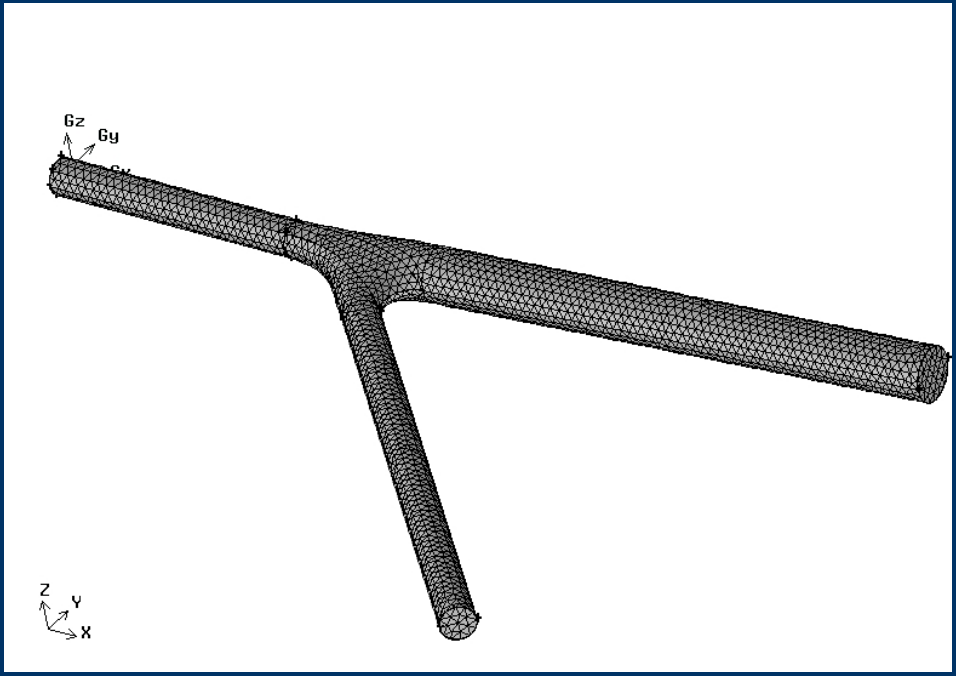
3D Geometry – Mark I




Z Y
X


Gz Gy
Gx
Z Y
X


Z Y
X


Gz
Gy
Z Y
X

Simulation Parameters

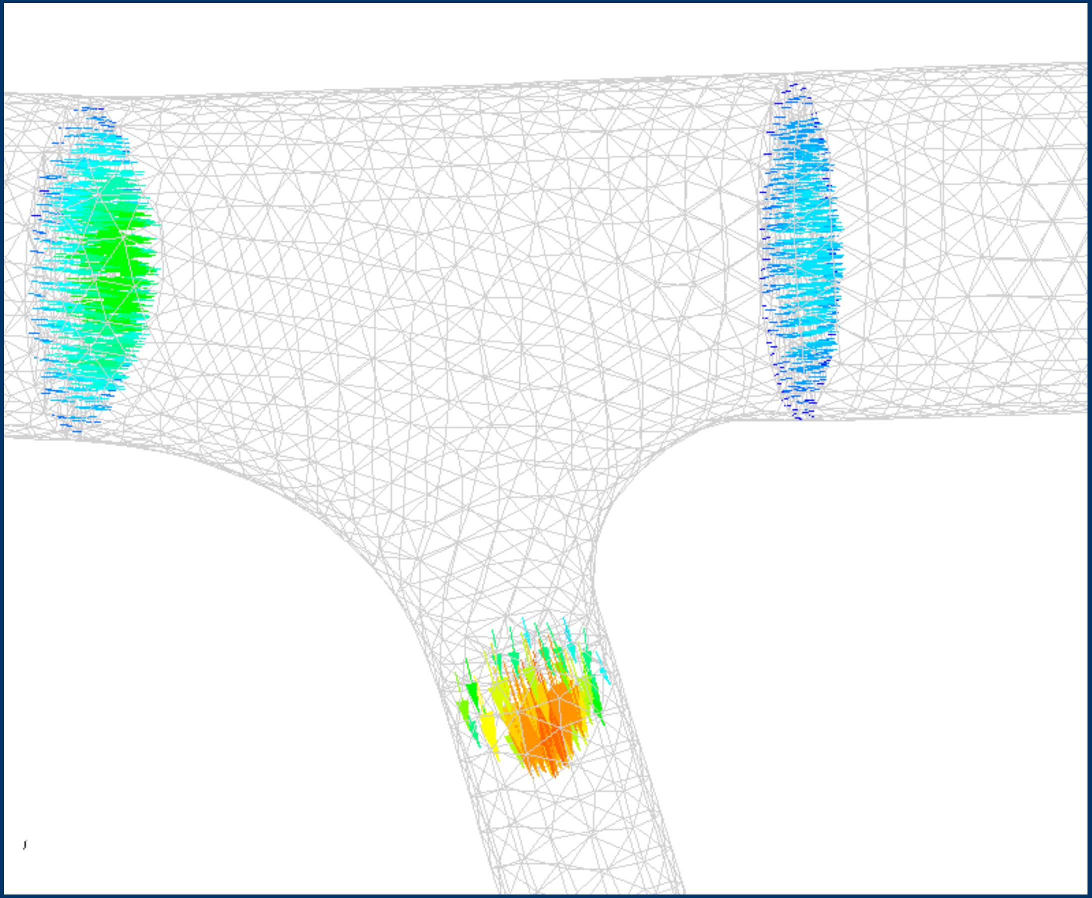
Re_D was maintained at constant value at the inlet duct

d_1 was 30 microns. The fluid was chosen to be liquid water at 20˚C. The inlet flow velocity, $u_{1,}$ was set to 0.5 m/s giving a Reynolds number of 15

$Le_D = 0.06Re_D$ D --- gives 0.9 D for $Re_D = 15$

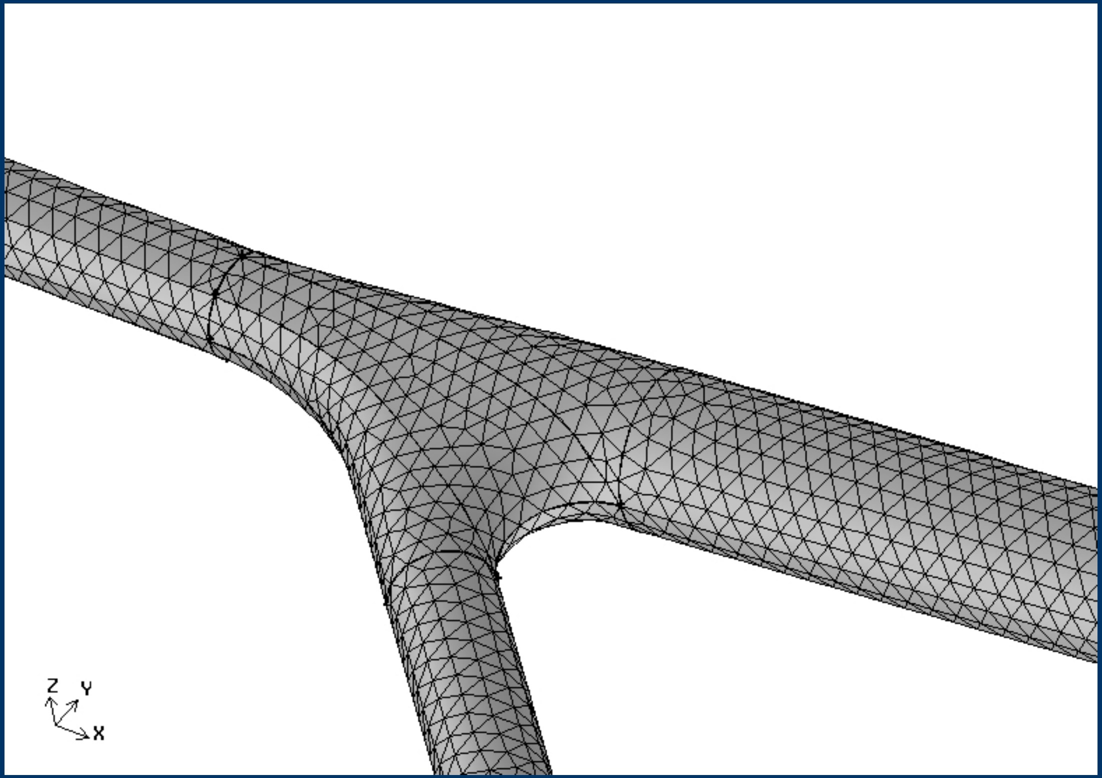
FLUENT output files contain surface averaged static pressure and magnitude of flow velocity at duct cross-sections at the duct inlets and exits.

Duct Inlet/Outlets



Duct inlet and exit sections considered to be where geometry of duct is the same as the downstream portion for outlets and upstream portion for inlet.

Mesh Automation



- Mesh was set to 1/4 of smallest duct
- Tetrahedral Mesh
- Large number of tests to assess ability to generalize the mesh (1/4 factor determined in this manner)
- Some testing to verify no change in results with change in mesh size.
- Inlet was specified as velocity inlet
- Outlets were outflow boundaries – allowed specification of flow fraction

Numerical Methods

Finite Volume solution of integral Navier Stokes

Steady-State 3D

Implicit

SIMPLE for pressure velocity coupling

1st order upwind scheme of momentum discretization

Max number of iterations

Convergence criterion = 0.1%

Parameter Values

d_2/d_1 and d_3/d_1 = 0.5, 1.0, 1.5

f_2 = 0.1, 0.3, 0.5, 0.7, 0.9

θ_2 and θ_3 = 5˚, 25˚, 45˚, 65˚, 85˚

600 runs attempted – 475 completed (*geometry issues on remainder*)

Suite of C++ procedures to create geometries, input files, read and collate results

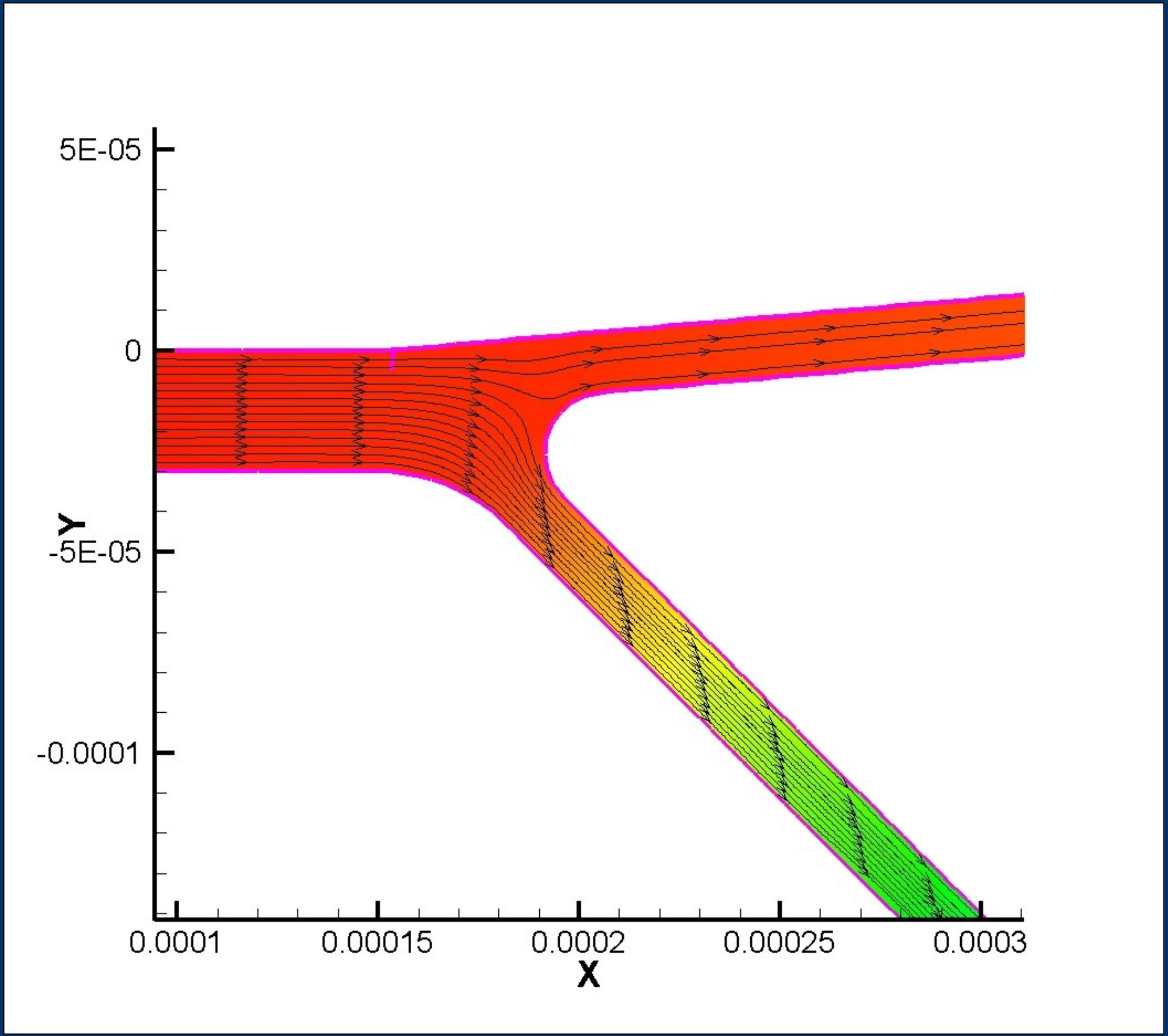
Create GAMBIT script to create geometries

Create input files for GAMBIT and FLUENT

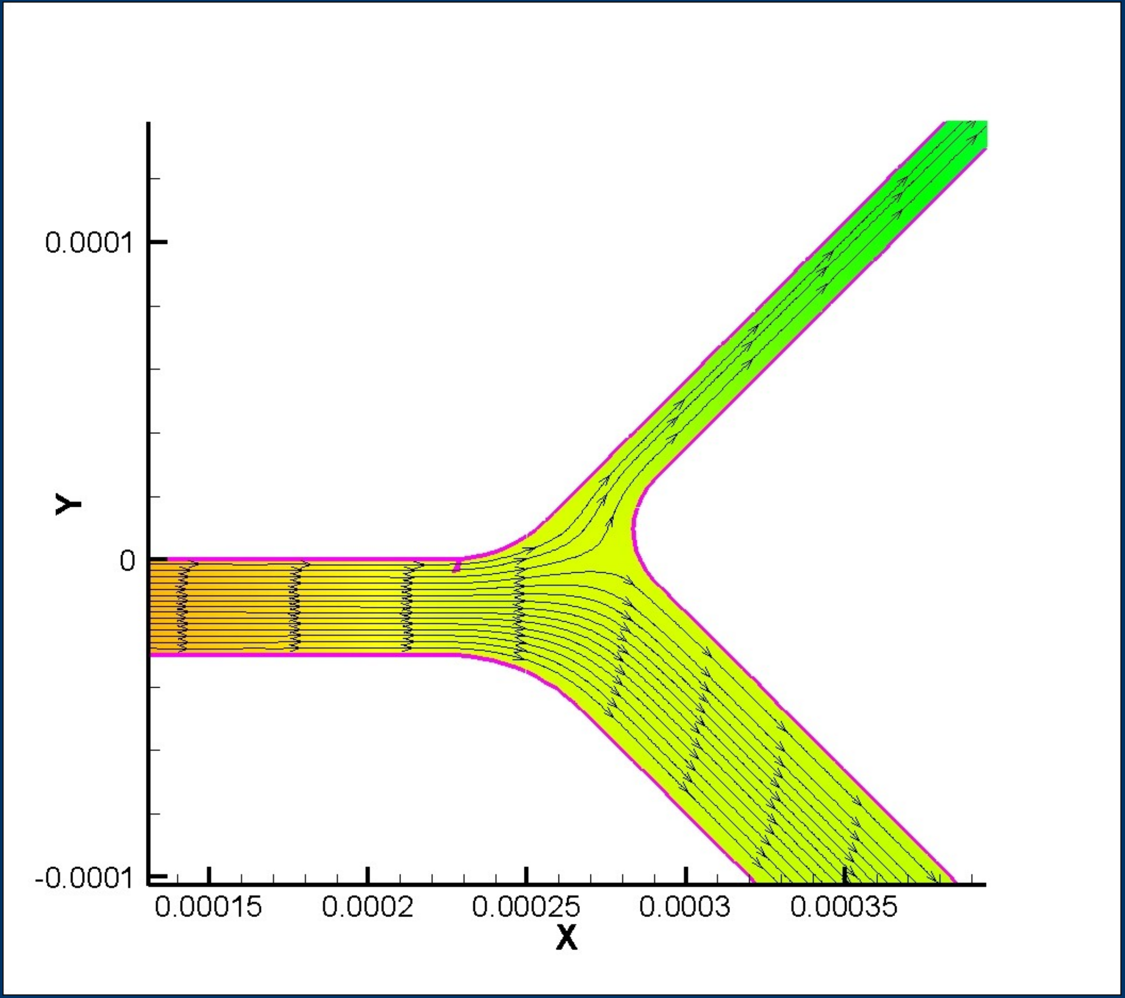
Read results files for static pressures and velocities averaged over surfaces in and out of junctions.

Fluent Result

f2 = 0.1, d2/d1 = 0.5, θ2 = 5˚, d3/d1 = 0.5, and θ3 = 45˚

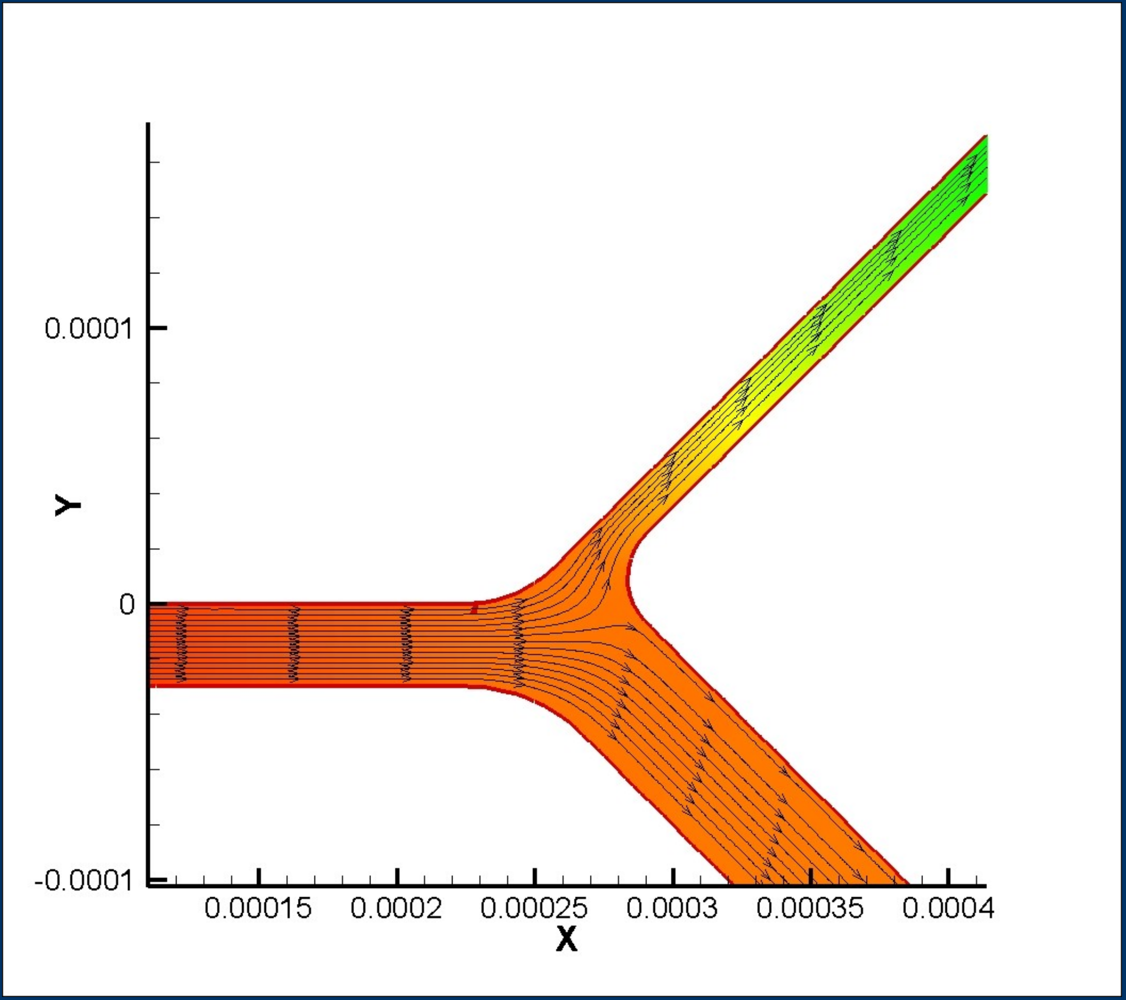


f2 = 0.1, θ2=45°, θ3=45°, d2/d1=0.5, d3/d1=1.5.



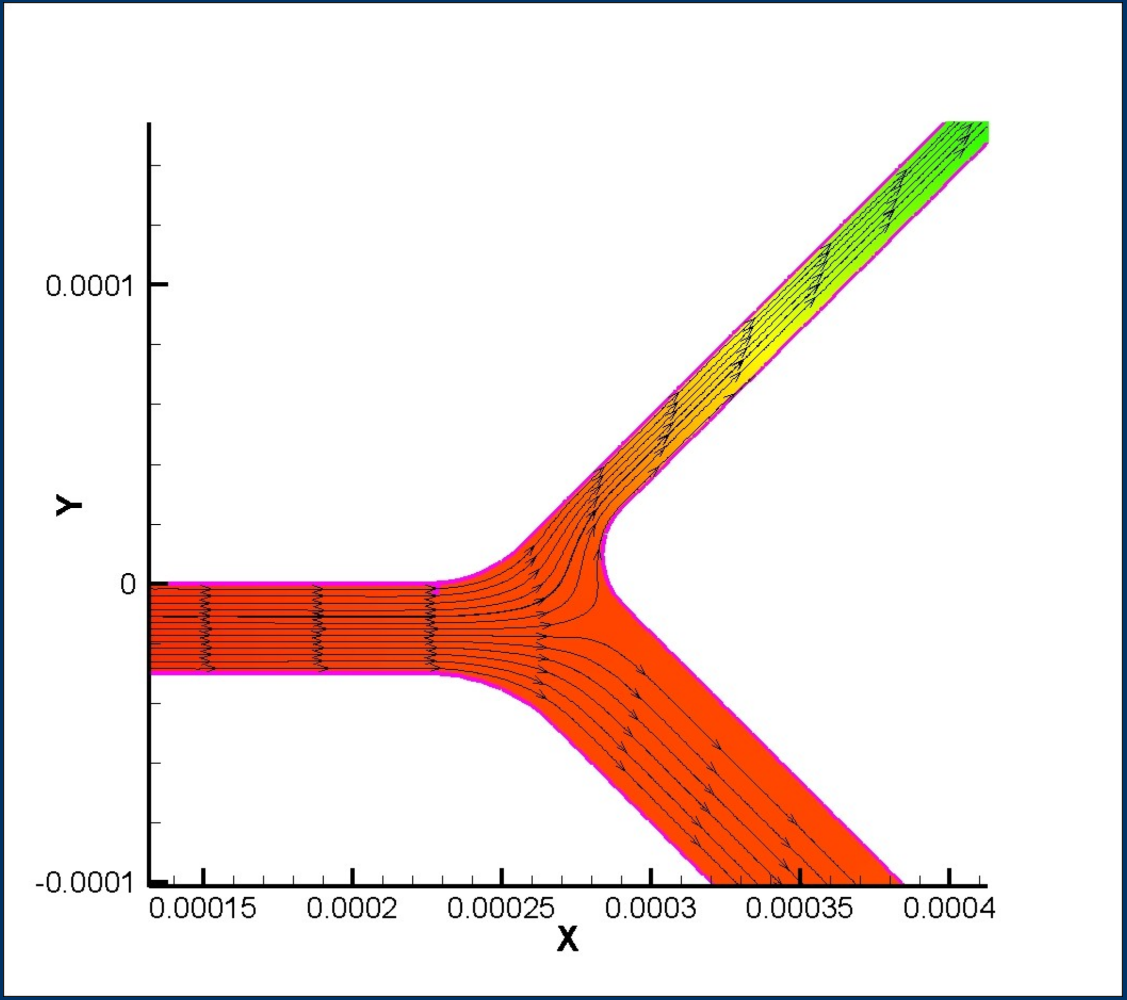
$K_2 = 5.47$

f2 = 0.3, θ2=65°, θ3=45°, d2/d1=0.5, d3/d1=1.5.



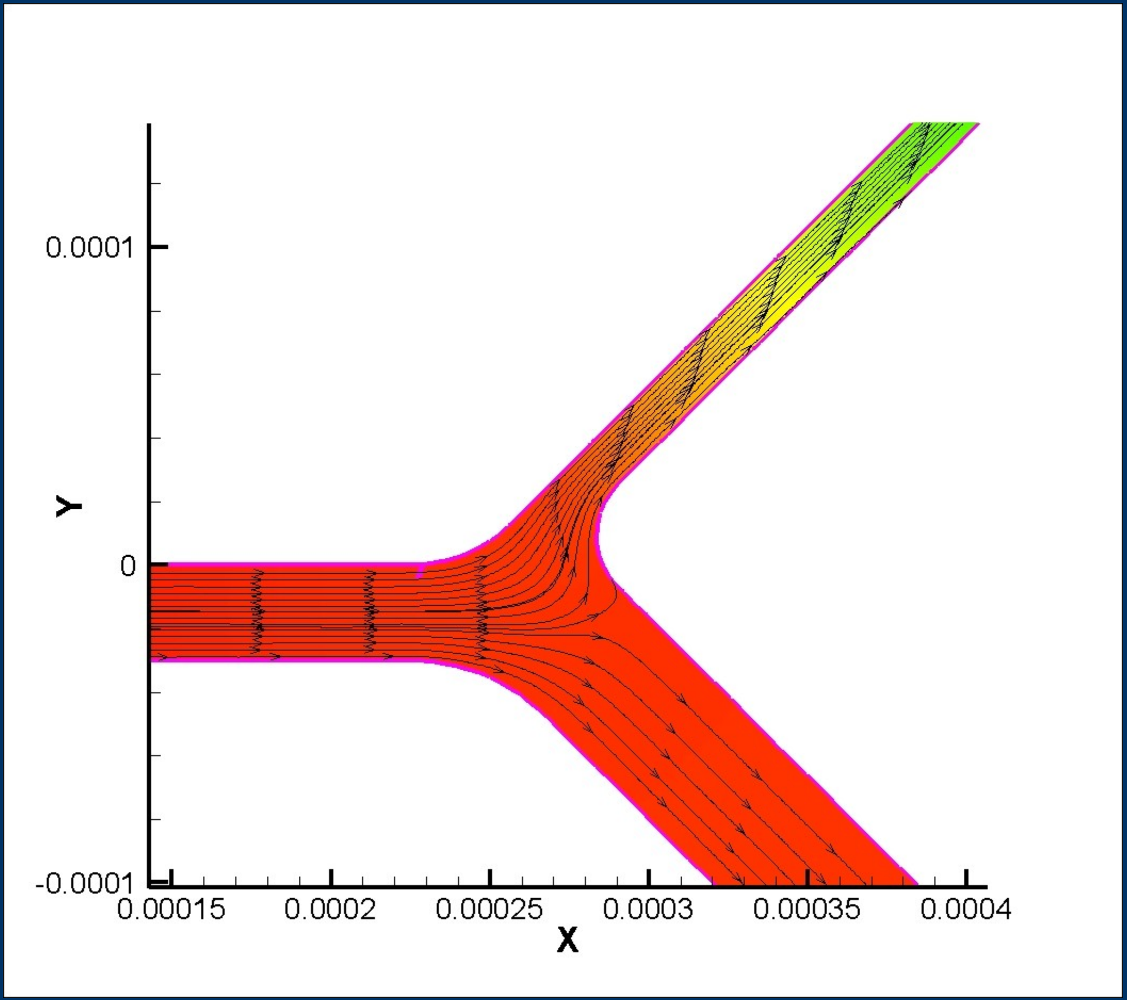
$K_2 = 11.6$

f2 = 0.5, θ2=65°, θ3=45°, d2/d1=0.5, d3/d1=1.5.



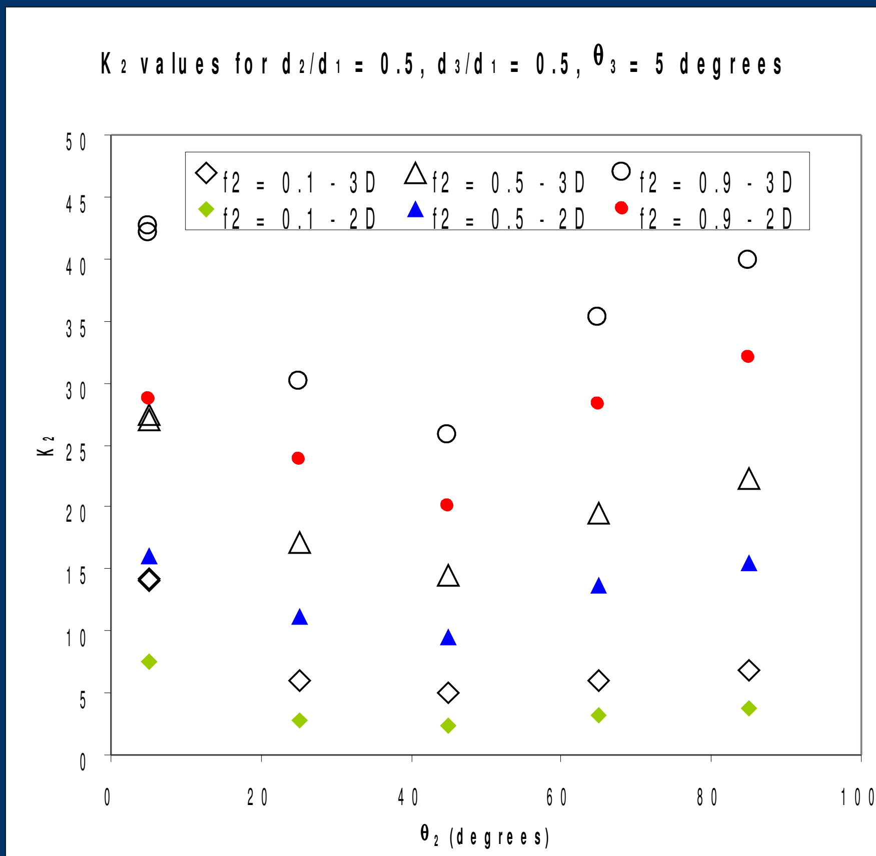
$K_2 = 18.4$

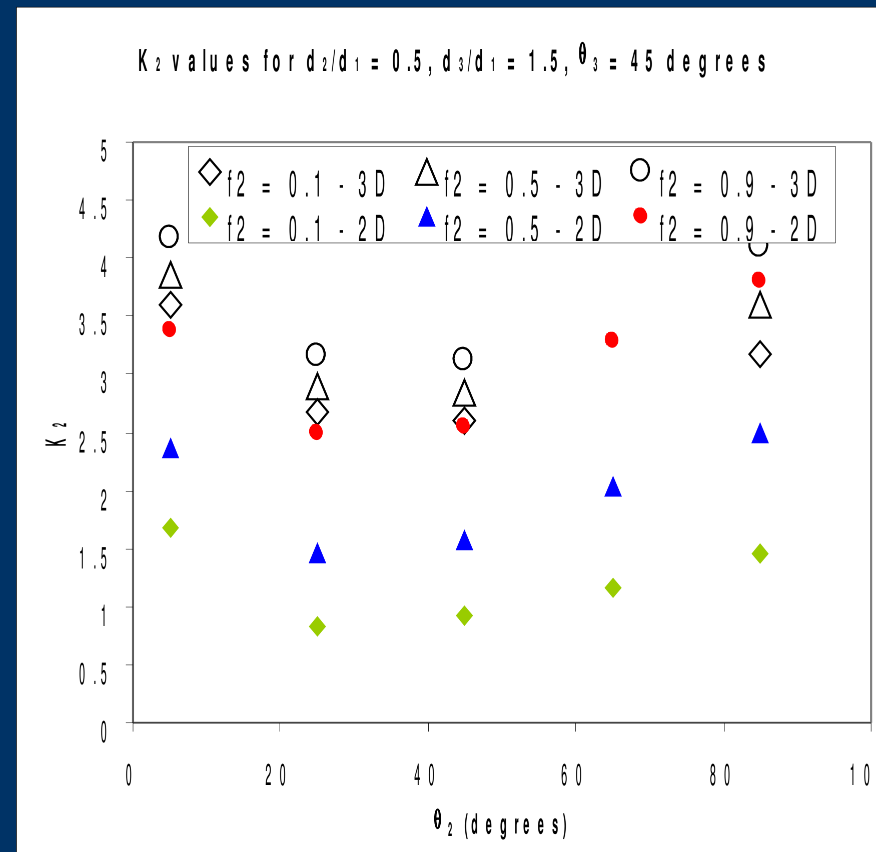
f2 = 0.7, θ2=65°, θ3=45°, d2/d1=0.5, d3/d1=1.5.



$K_2 = 25.7$

2D vs. 3D Differences





$$\left[\frac{k_2^{3D}}{k_2^{2D}}\right]_{average} = 1.55 \quad (std.\ \ dev.) = 0.45$$

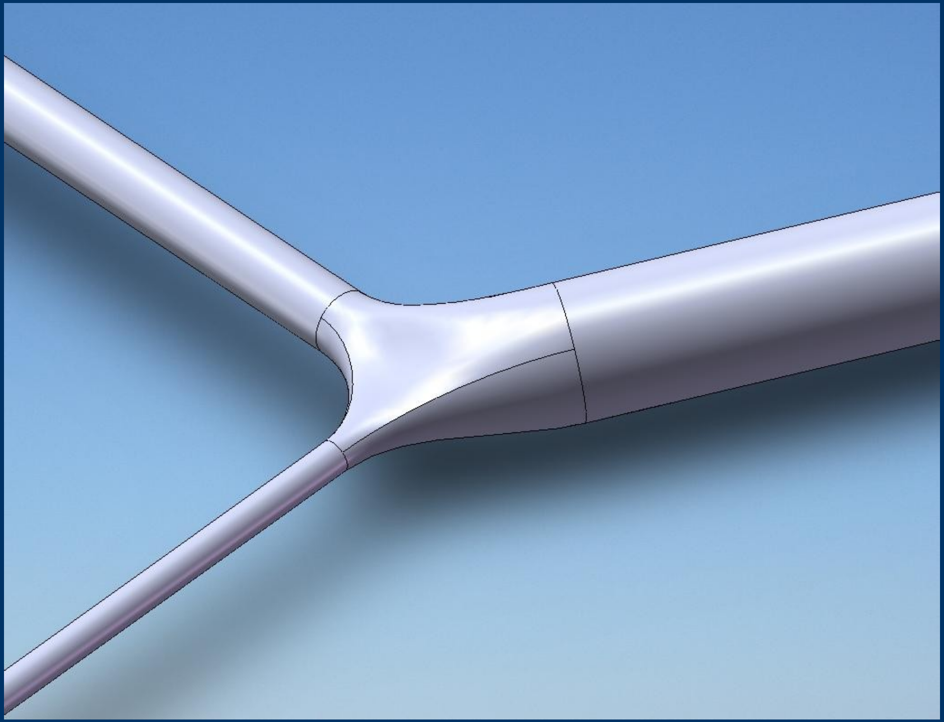
$$k_2 = \frac{\Delta p/\rho}{u_1^2/2} - \frac{u_2^2}{u_1^2} + 1$$

pressure effects

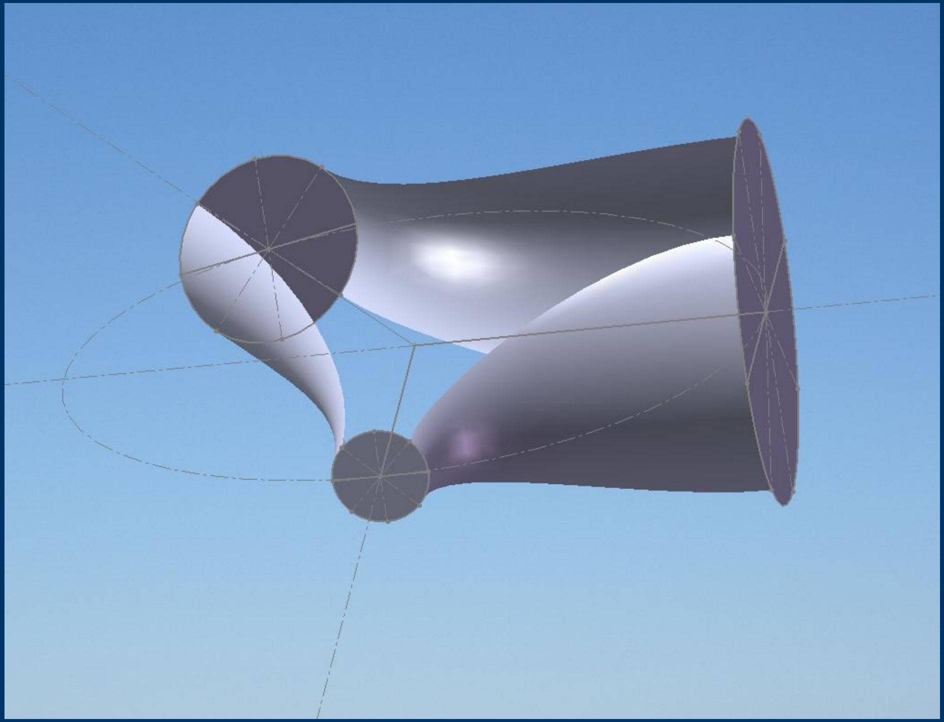
kinetic energy effects

3D Geometry Mark II - Junction Algorithm

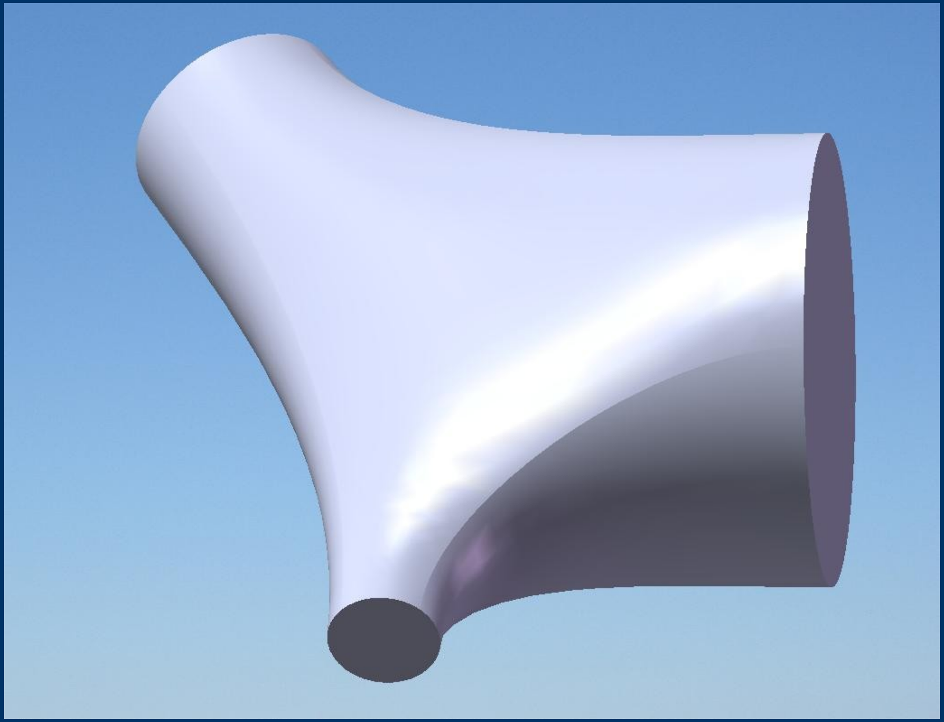
- No angle dependence
- C++, VBA, SolidWorks, GAMBIT
- Automated
- No failed geometries



3D Mark II Junction



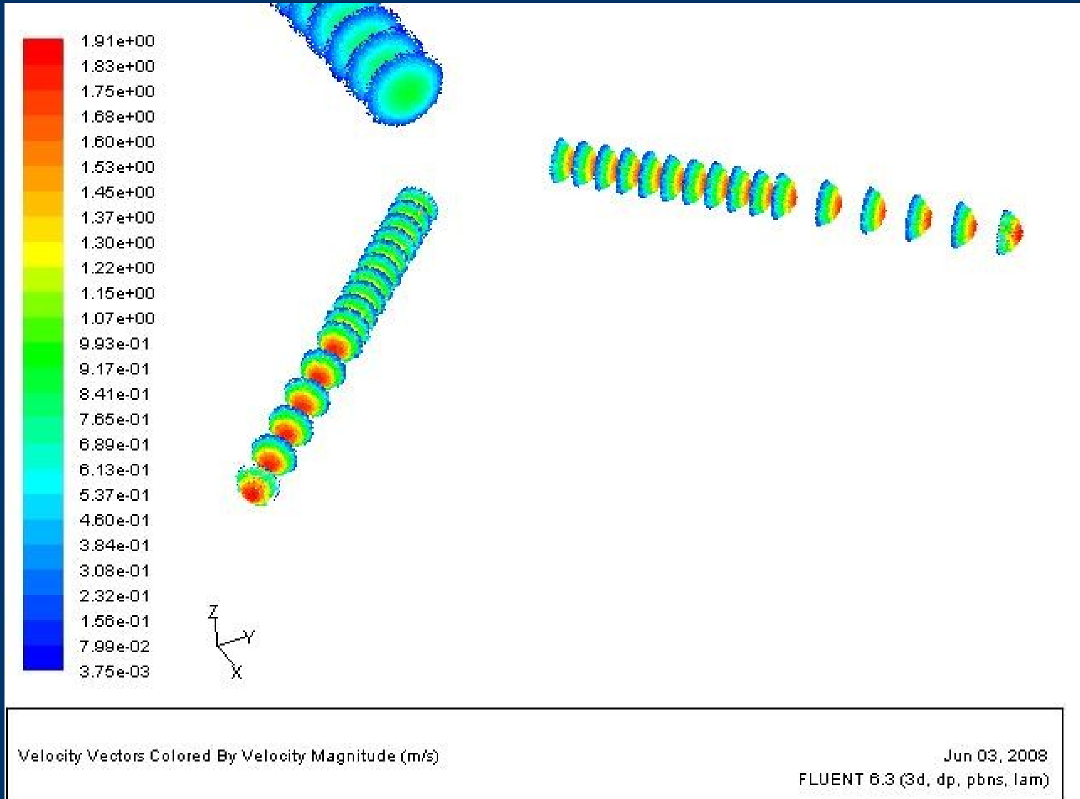
Junction Without Surface Fills



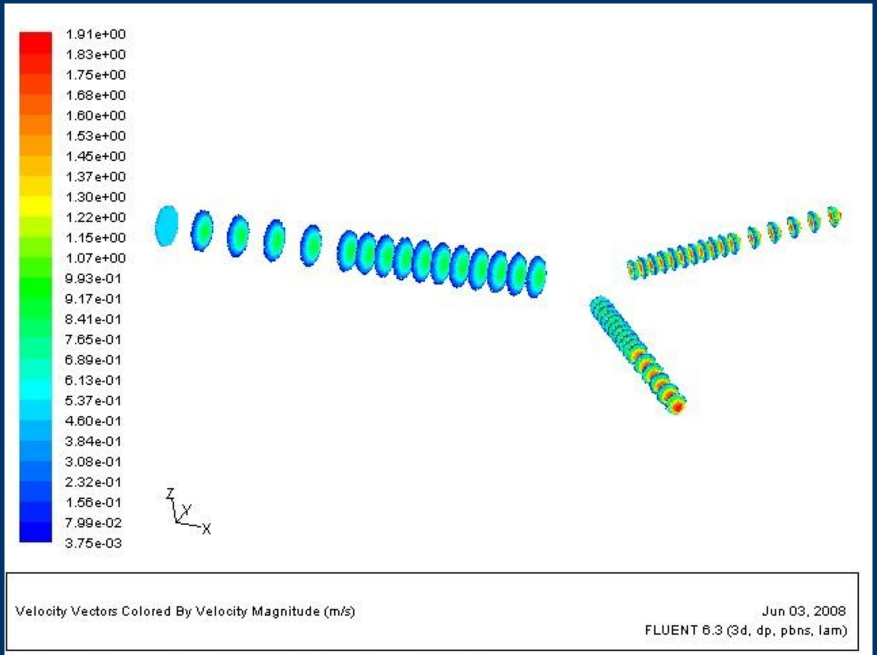
Junction With Surface Fills

Initial Simulations – 3D Mark II

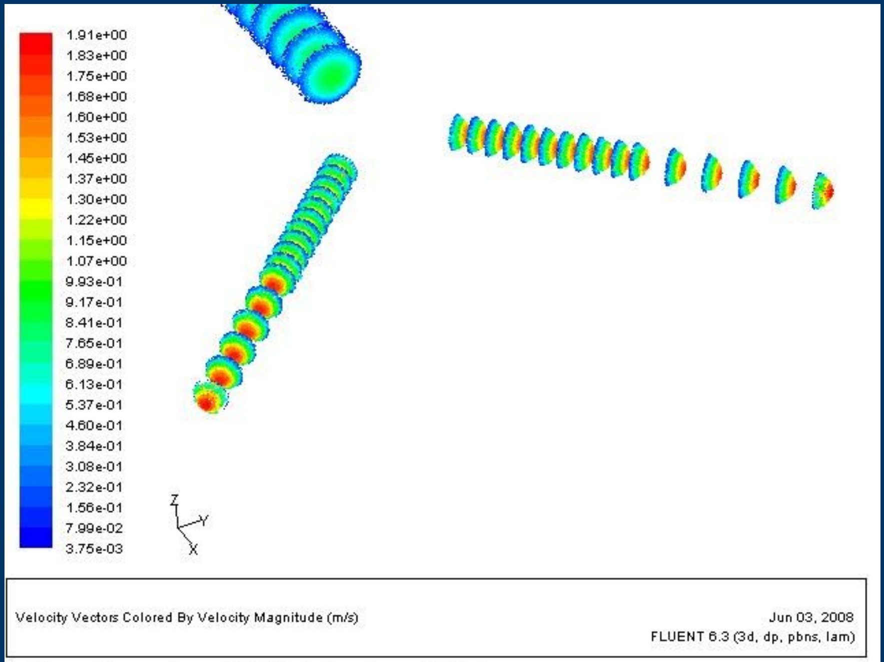
- Small batch
- Comparable results to original 3D runs



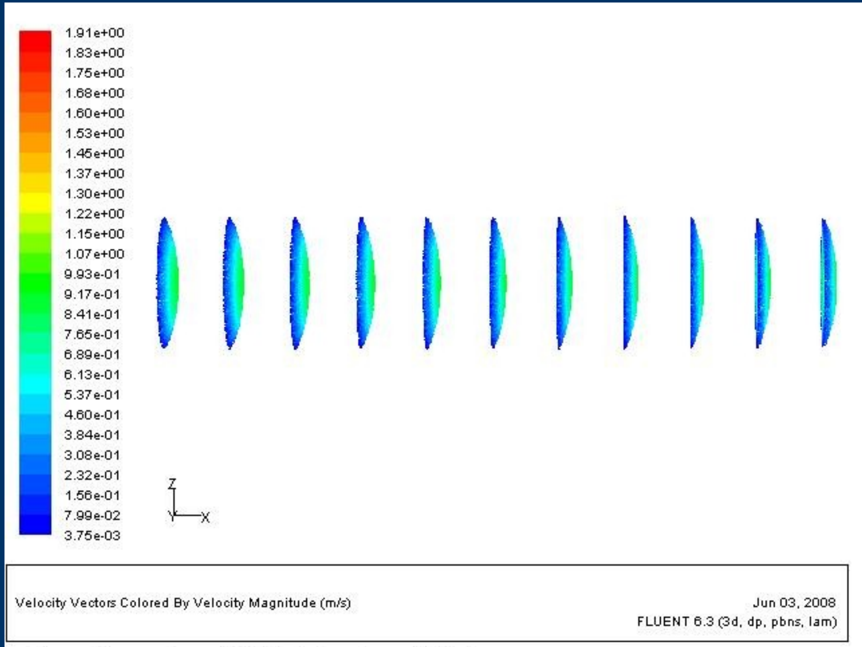
Reynolds number of 14 Inlet diameter of 30microns



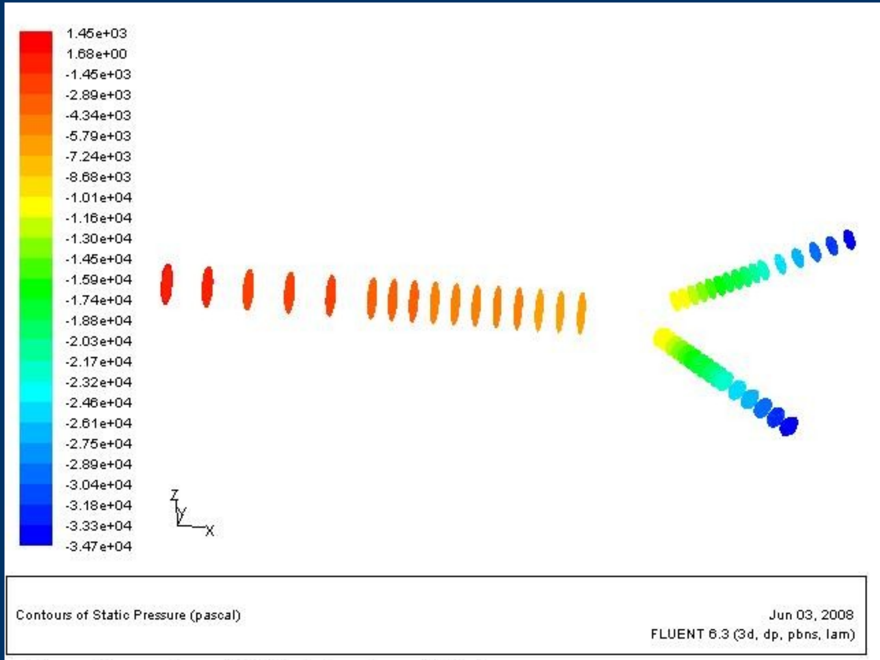
Reynolds number of 14 Inlet diameter of 30microns



Reynolds number of 14 Inlet diameter of 30microns



Reynolds number of 14 Inlet diameter of 30microns



Reynolds number of 14 Inlet diameter of 30microns

Pipe Mesh Testing

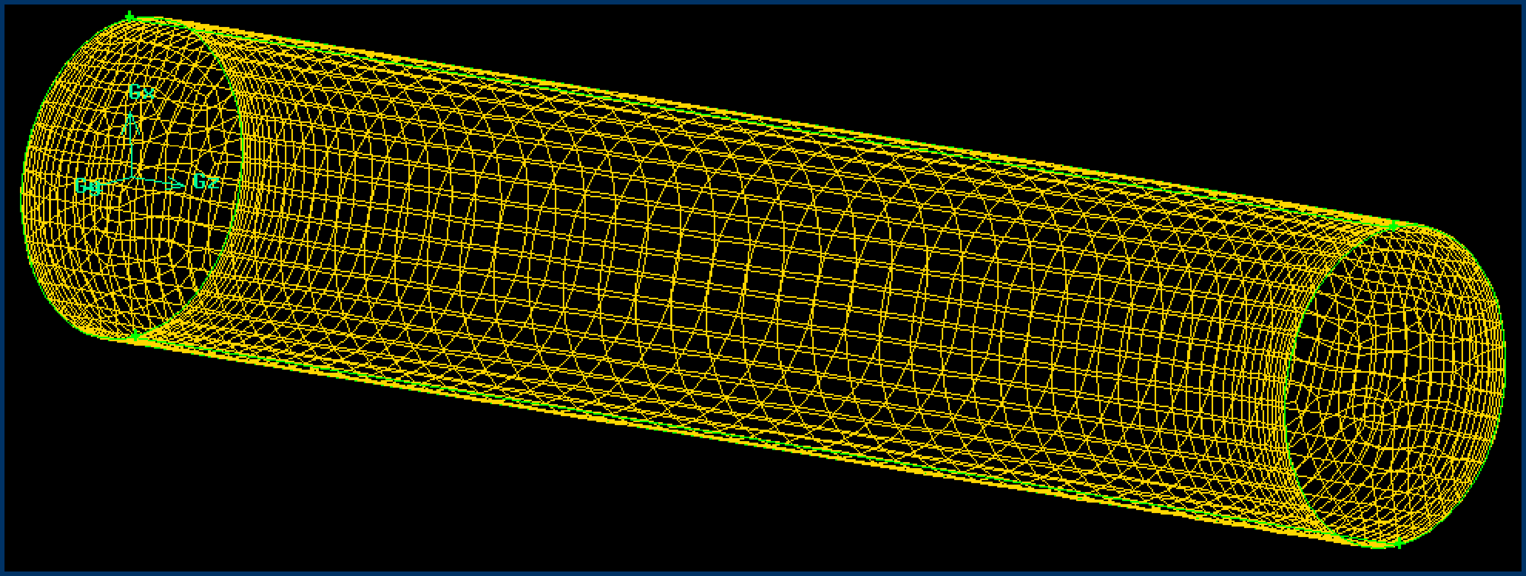
Flow-aligned hex core

Varied axial and radial spacing

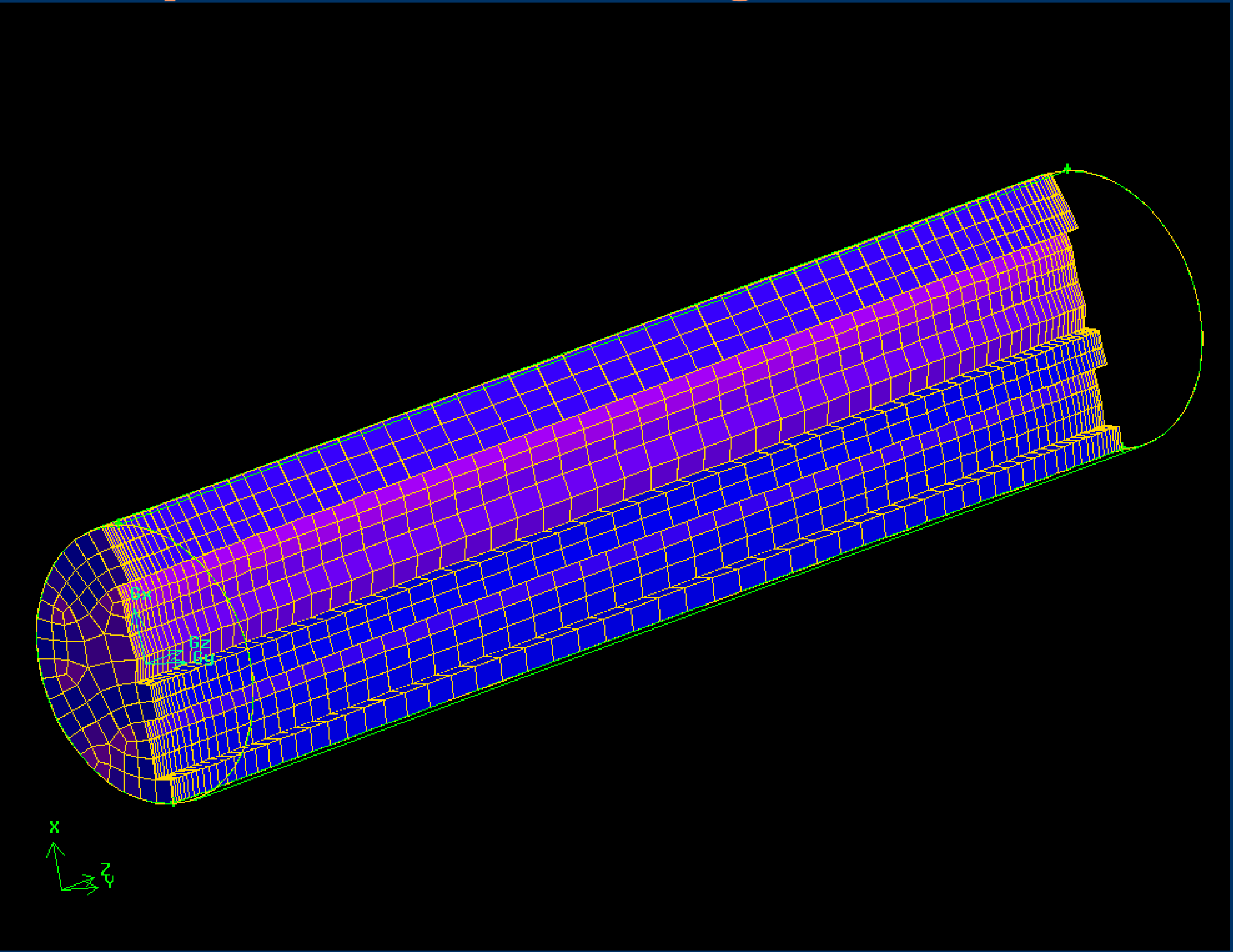
MySQL results database

Automated

Results database easy to setup for junction runs



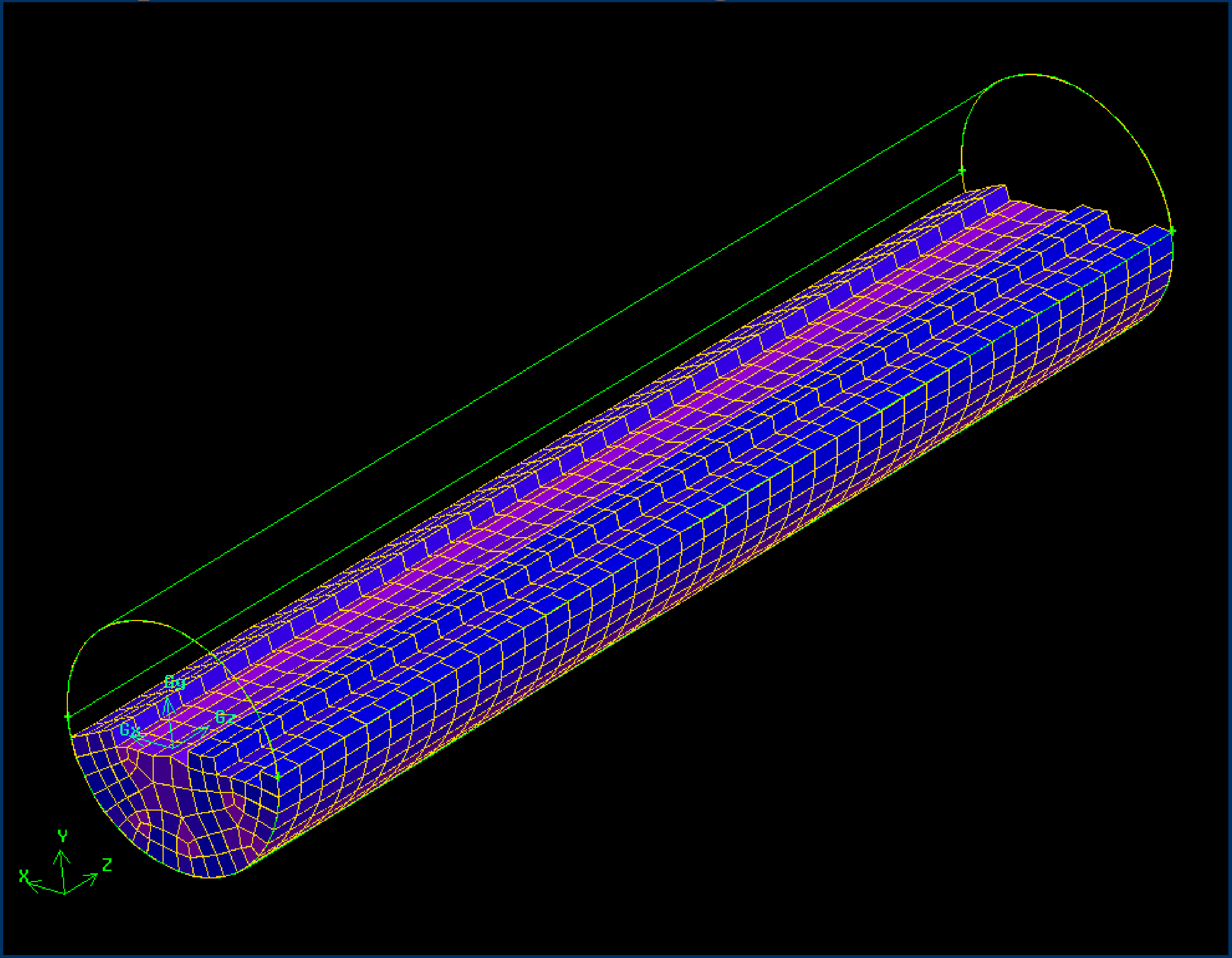
Pipe Mesh Testing



"Bell Shaped"

Axial Spacing

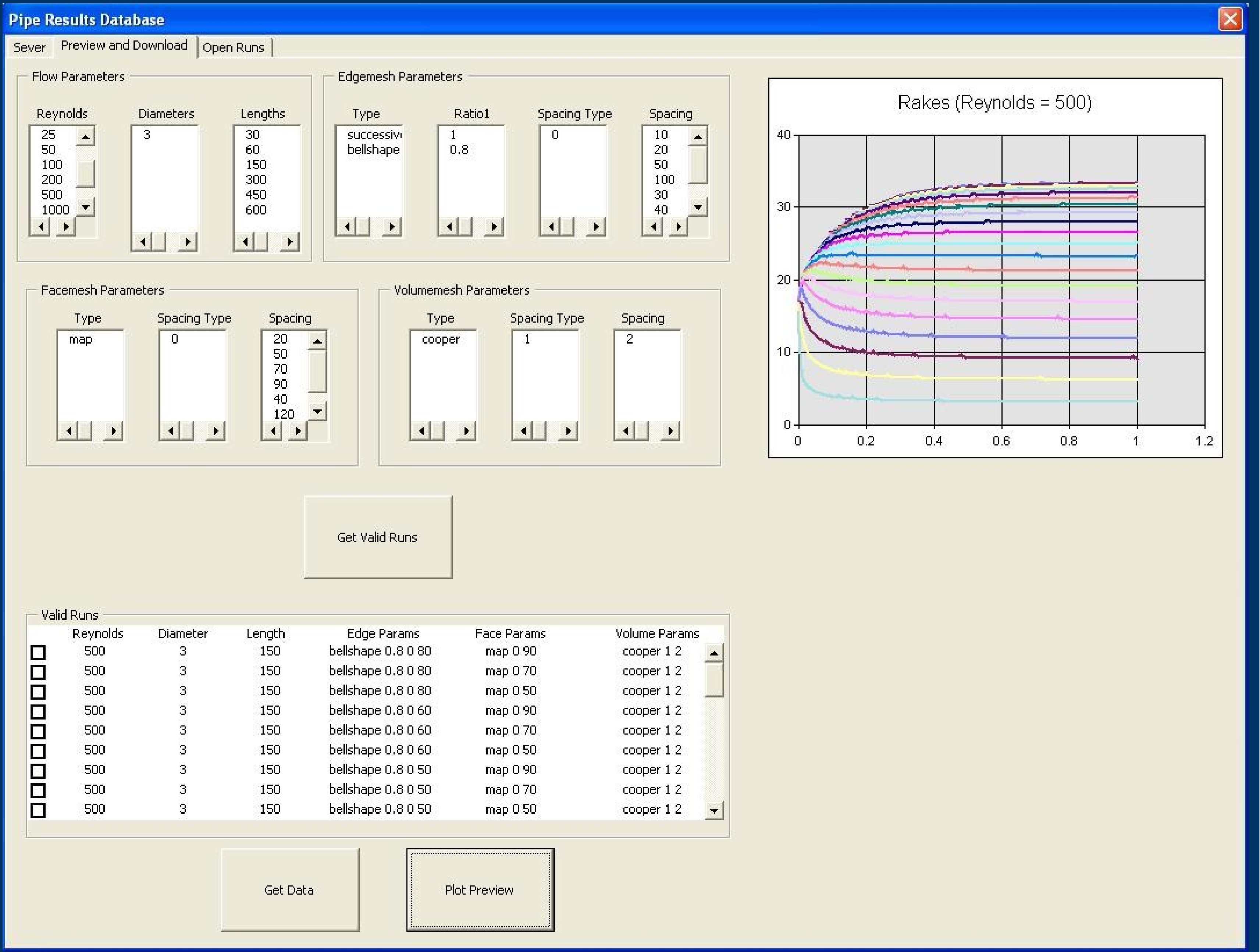
Pipe Mesh Testing



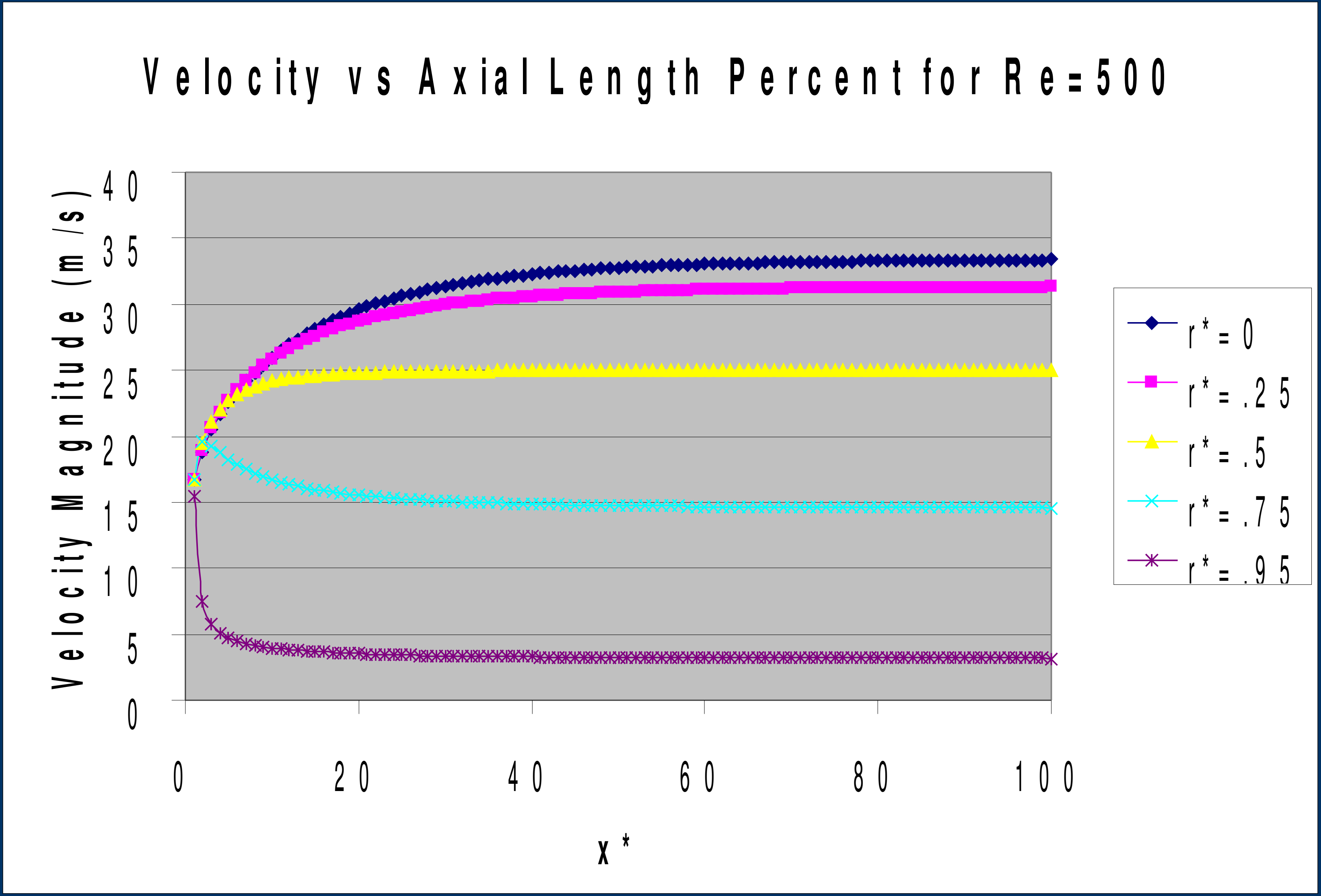
Uniform Axial Spacing

Pipe Mesh Testing

Database Interface

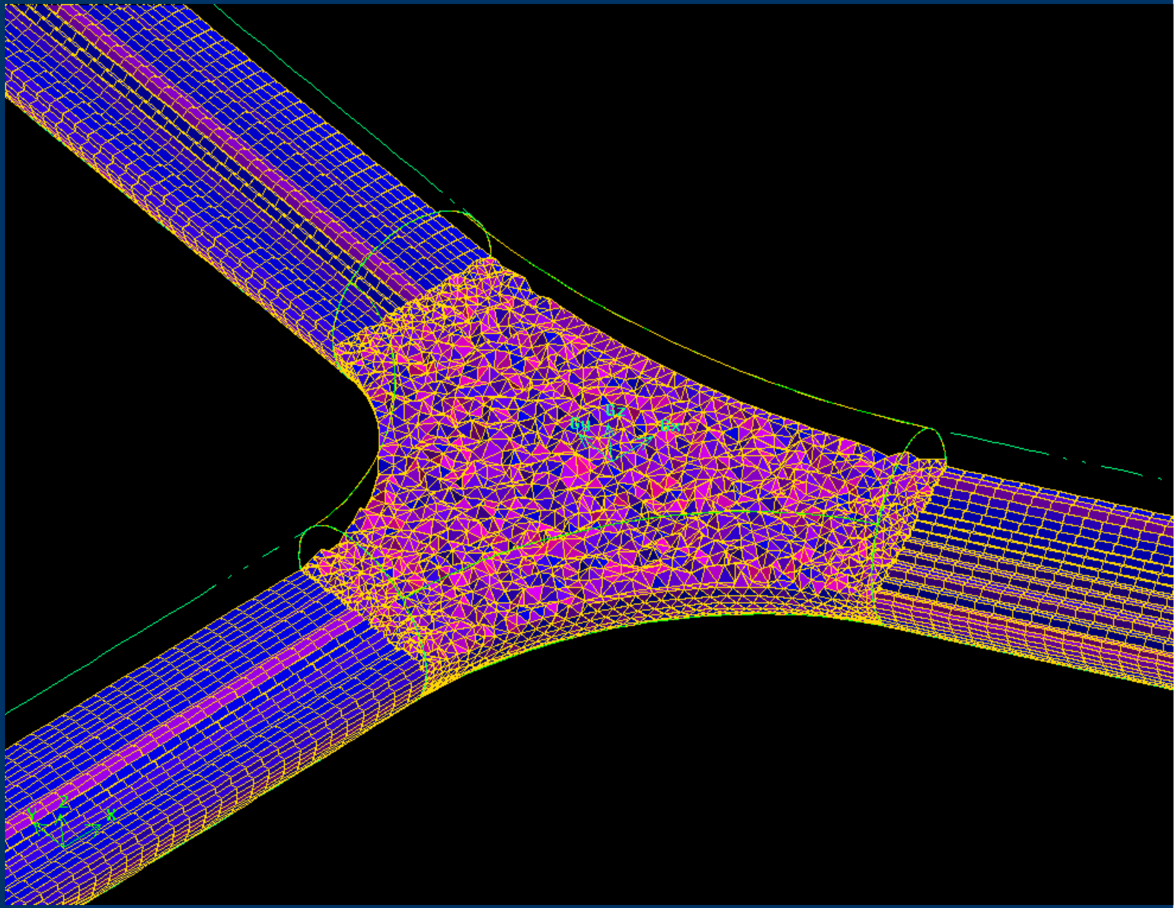


Single Tube Results for Entry Length (Re = 500)



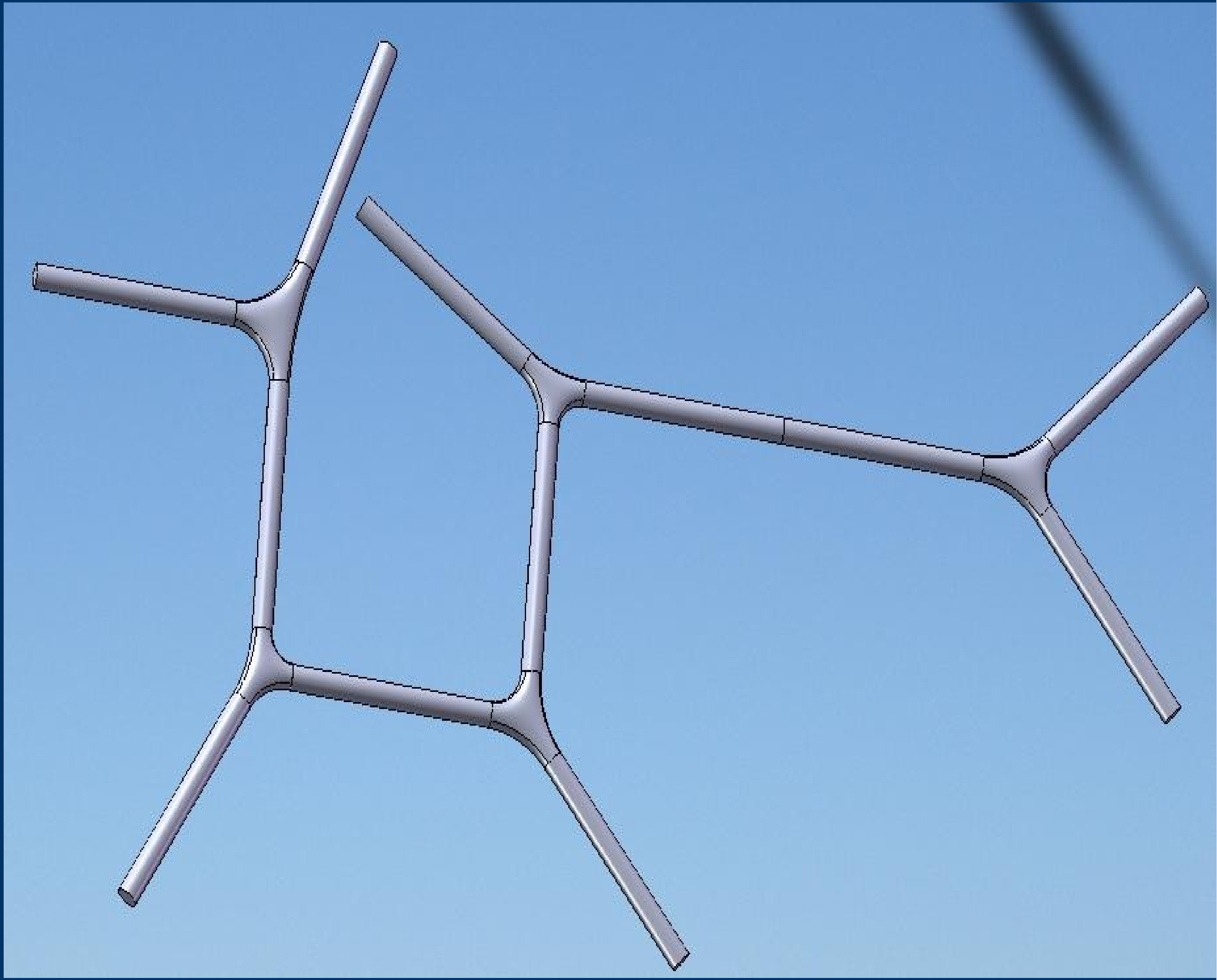
New Junction Simulations

- Combination of previous methods to allow for complete control and automation from geometry creation to data analysis
- Flow-aligned hex core in pipes
- Tetrahedral elements in junction region – do not want to "guide" flow by using hex core
- Use of HPC Solution to speed up cases and higher order meshing.



Future Work

- Immediately able to plug into porous networks from Flow Through Porous Media (FTPM)
- Non-planar micro-bifurcations
- "N-furcations"
- Out of plane junctions (for use in porous media code)
- Effects of Roughness
- Experiments to establish laminar loss coefficients for number of configurations (in progress)



Acknowledgments

The Office of Research and Grants at the University of Central Oklahoma is acknowledged for support of this research.

The Donors of The Petroleum Research Fund, administered by the American Chemical Society, are also be acknowledged for support of this research through grant PRF# 47193-B9.

National Science Foundation EPSCoR Research Opportunity Award Program

Dimitrios Papavassiliou and Henry Neeman