Exploring the Potency of Computational Fluid Dynamics for Holistic Reconstruction of flow behavior in the NIST Neutron Design

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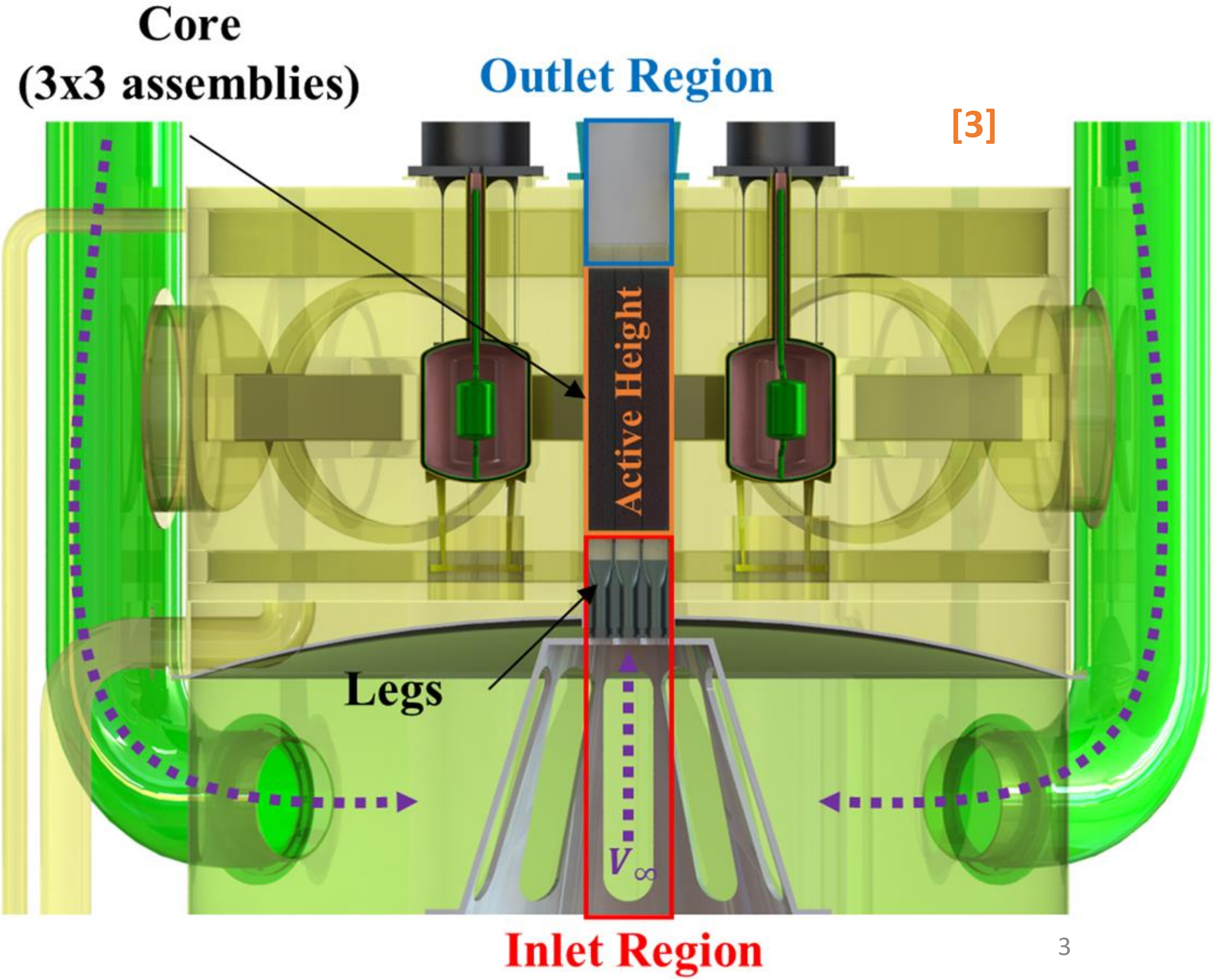
About me

- Evan Bures
- Senior at Texas A&M University
- Nuclear Engineering Major
- Worked in **T**hermal **H**ydraulics **V**erification and **V**alidation Group for almost 2 years under Dr. Mark Kimber
- Close to 2 years of experience in Computational Fluid dynamics (CFD)
- Most work done with highly transient turbulent flows with heat transfer

NNS Reactor Design

- NIST Neutron Source (NNS)
  - Planned replacement for current reactor (NBSR)
- High power density reactor meant for neutron generation
- Flow modelling centered around:
- Inlet region (lower plenum)
- Curved fuel plates with curved fuel channels separating them (Active Height)
- Outlet region (long stack)



Geometries of Interest

Fuel Channels (Curved Rectangular Channels)
Single-channel Studies

[1]

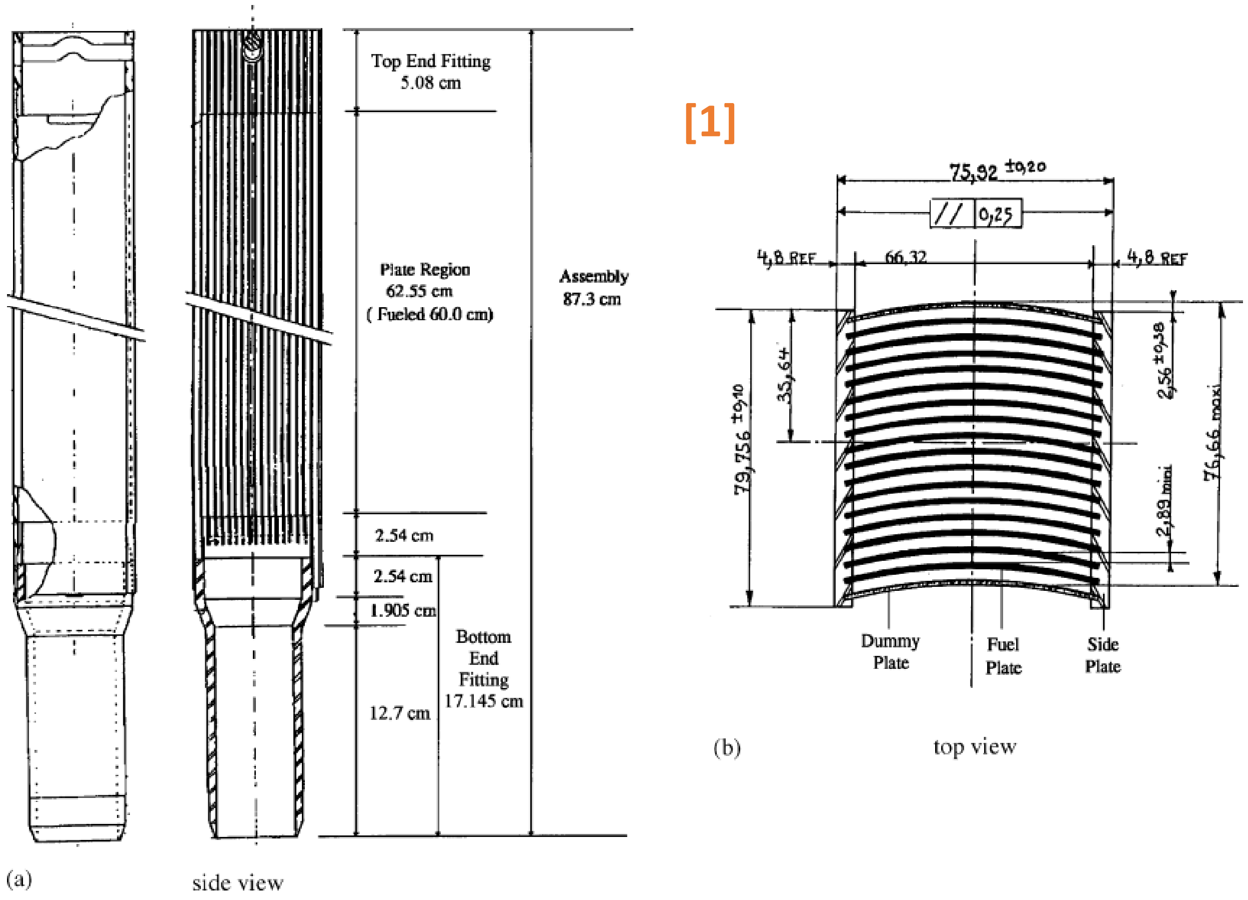
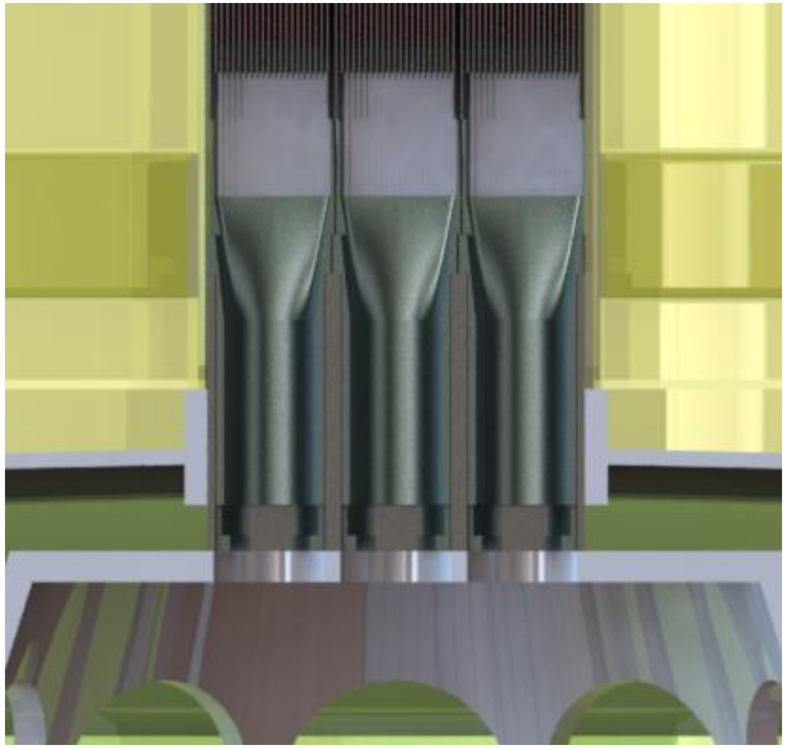


Fig. 2. 18-Plate fuel assembly in MNR.

Intermediate Mixing Plenum (3-channel mixing)
Parallel Mixing Studies

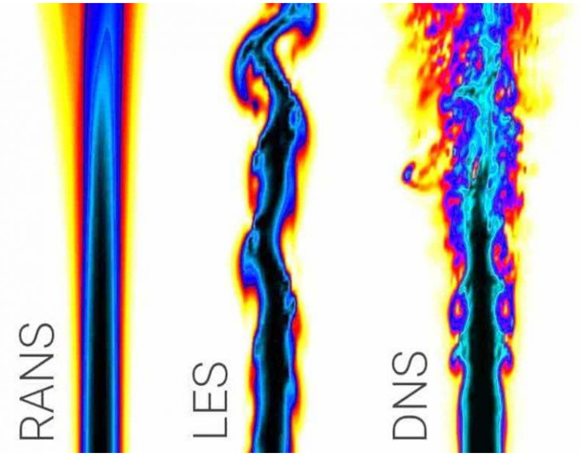


What is Computational Fluid Dynamics?

- We discretize fluid systems into multiple smaller elements known as cells to generate what is known as a “mesh”.
- Once we have our mesh we can attempt to model the Navier stokes equations in each individual cell to create one larger picture to represent the entire system
- In order to do this efficiently we employ multiple simplifications such as the Reynolds Averaged Navier Stokes (RANS) equations, Large Eddy decomposition equations (LES), or even in some cases attempting to directly solve the Navier Stokes equations in what's known as “Direct Numerical Simulation” (DNS)
- Furthermore, turbulent effects must be solved using a separate subset of models known as “turbulence models”.

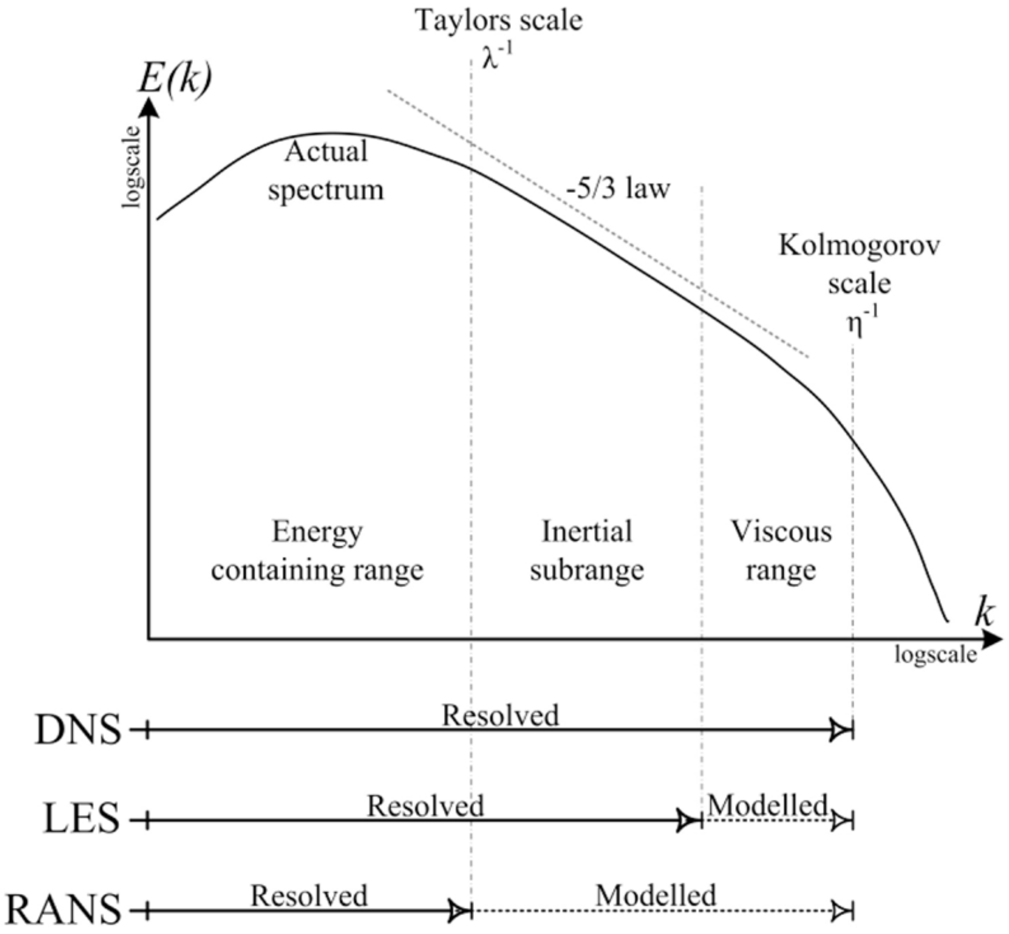
Navier-Stokes Equation

$$\underbrace{\frac{\partial U_i}{\partial t} + U_j \frac{\partial U_i}{\partial x_j}}_{\textit{Gas Pedal}} = - \underbrace{\frac{\partial P}{\partial x_i}}_{\substack{\textit{Steering}\\ \textit{Wheel}}} + \nu \underbrace{\frac{\partial^2 U_i}{\partial x_j \partial x_i}}_{\textit{Brakes}}$$



Reynolds Averaged Navier Stokes (RANS)

- Rans Resolves turbulence by creating large, averaged, general approximations for turbulent effects in regions.
- We can use RANS to model simple flows or flows that we want a general idea of how the flow will behave (no super specific values of velocity or pressure)
- RANS is fast!!! Work horse of CFD



Large Eddy Simulation (LES)

- Resolves turbulence at much smaller scales by seperating and directly solving large, more influential turbulence scales while modelling smaller scales.
- Much more accurate than RANS
- Significantly more computationally expensive
- Note: as models increase in order of fidelity, more refined meshes of higher cell counts are required so not only are your models becoming more expensive on just an equation basis, but your meshes are needing to increase in size too.

OpenFOAM (for CFD simulations)

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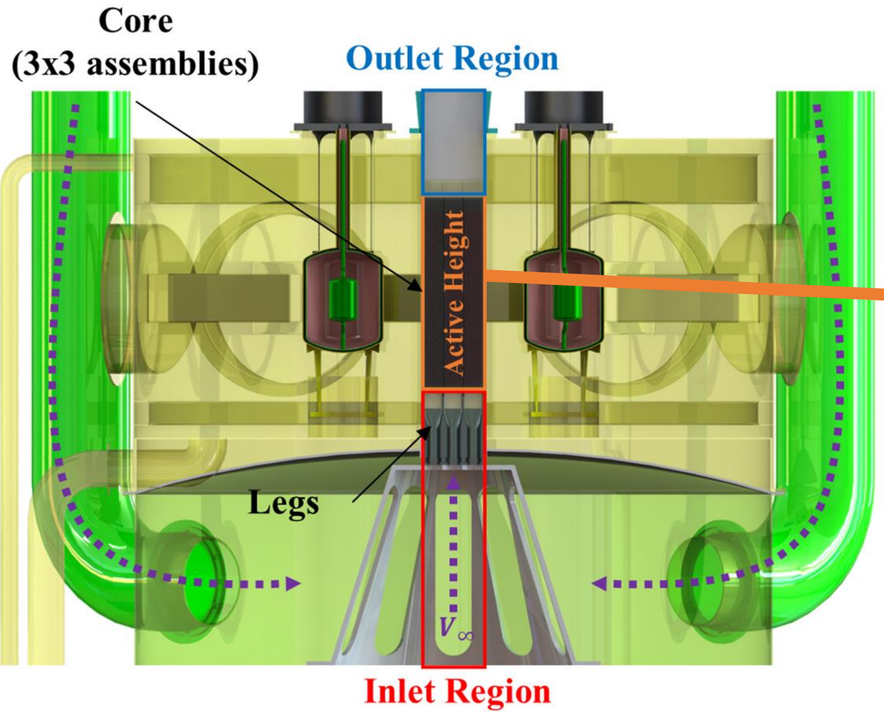
- OpenFOAM is the most popular and commercially standard open source CFD software.
- Provides unequalled amounts of customization due to it being opensource
- Effectively a CFD sandbox.

OpenFOAM [4]

ANSYS ICEM (for meshing)

- Commercial Meshing software
- Universal meshing software for all range of transport problems
- Entirely structured meshing (meshes that are hand crafted and not automatically generated)

Single Channel Studies



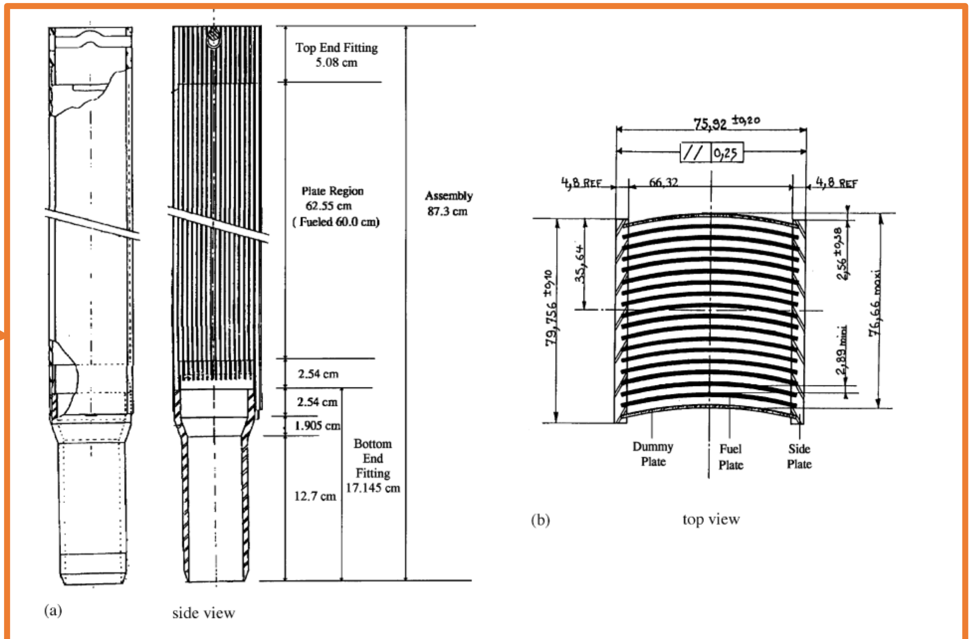


Fig. 2. 18-Plate fuel assembly in MNR.

Models

For the purpose of this work, we will focus around 3 models:

1. k-ϵ Realizable (2-equation model) (A more complex K-epsilon that adds constraints to ensure predictions adhere to physics more closely)
2. Spalart Almaras (1-equation model)
3. k-ω SST (2 equation model)

Example of K-Omega-SST from OpenFOAM User Guide:

The turbulence specific dissipation rate equation is given by:

$$\frac{D}{Dt}(\rho\omega) = \nabla \cdot (\rho D_\omega \nabla\omega) + \frac{\rho\gamma G}{\nu} - \frac{2}{3}\rho\gamma\omega(\nabla \cdot \mathbf{u}) - \rho\beta\omega^2 - \rho(F_1 - 1)CD_{k\omega} + S_\omega,$$ [4]

and the turbulence kinetic energy by:

$$\frac{D}{Dt}(\rho k) = \nabla \cdot (\rho D_k \nabla k) + \rho G - \frac{2}{3}\rho k(\nabla \cdot \mathbf{u}) - \rho\beta^* \omega k + S_k.$$

The turbulence viscosity is obtained using:

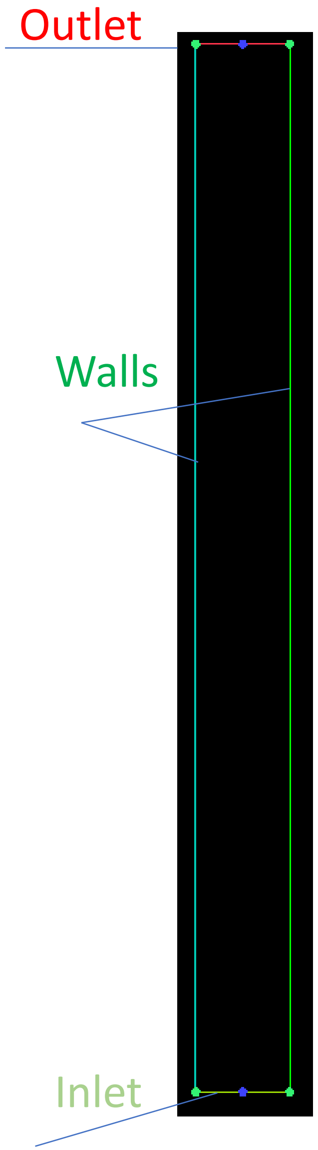
$$\nu_t = a_1 \frac{k}{\max(a_1\omega, b_1 F_{23}\mathbf{S})}$$

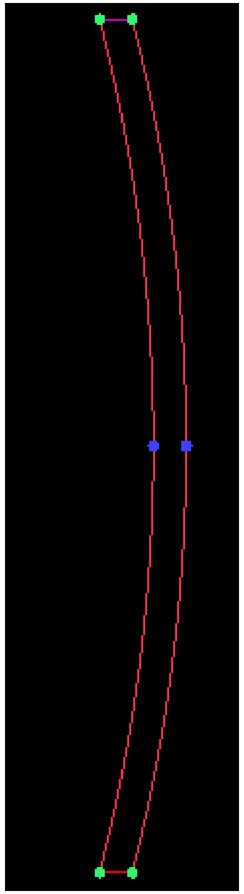
Goals

- Are 2D simulations enough to approximate the channel flow?
- Comparing 1 channel models before scaling up to multi channel
- If the 2D models are in a comfortable range to find a tuning factor too, we can use 2D models for multi channel approach.
- A comparison of separate turbulence models is also done for similar reason.
- Experimental data from Ha et al. is used as a baseline for determining model accuracy

Design parameters

- FP channel design is used
- Height of 780 mm
- Width of 69.757 mm
- Inlet velocity of 12.78 m/s is prescribed at a fixed value across the whole length
- Pressure set to fixed value of 0 at the outlet
- Velocity is assumed to be 0 at all walls





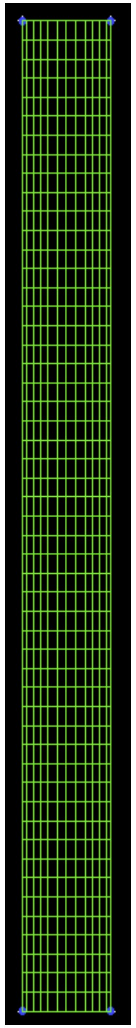
About y^+

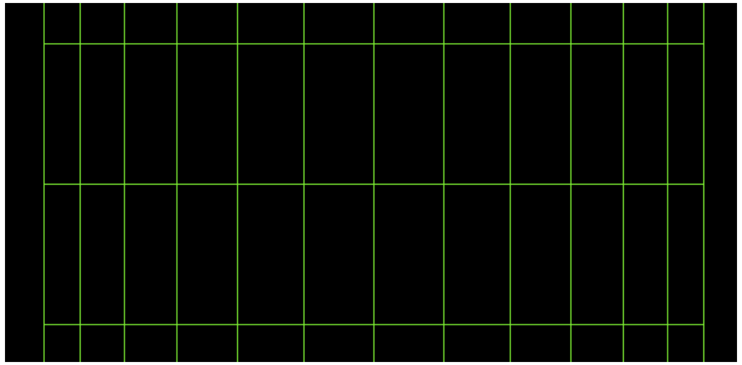
- y^+ is a non-dimensional parameter we use in CFD to represent the ratio of inertial to viscous forces for a fluid near a wall boundary.
- We essentially use this term in grid dependence studies to help determine how much resolution is needed near the wall
- Think of it as just parameter of how many cells need to be near the wall to ensure we are modelling all the effects of that wall.
- So, if y^+ is close to 1 and there's not a lot of cells near the wall, that means the wall functions the model is using are pretty good at modelling the walls
- A high y+ that has a lot of cells near the wall means wall effects are quite strong and large amounts of cells will be needed near the wall to model the flow accurately

$$y^+ = \frac{u^* y}{\nu}$$

2D Mesh design

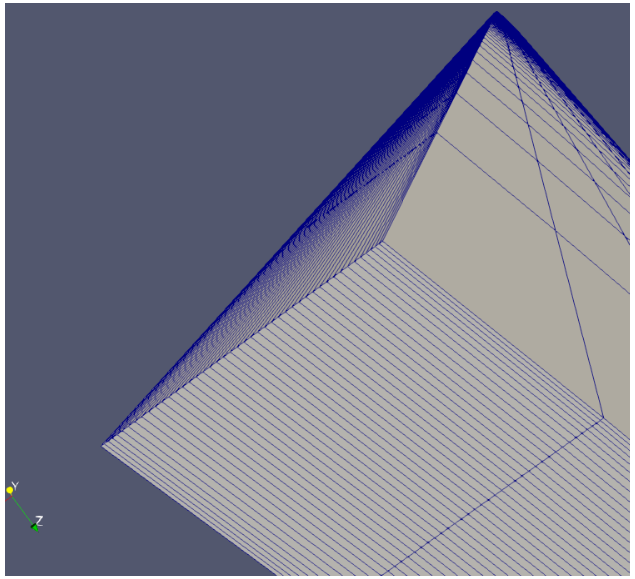
- To the right is shown the full mesh and zoom in of 1 layer to show inflation layer.
- Due to the simplicity of the flow, we can employ wall functions and a very coarse gradient from the wall distance to the center of the channel.
- A comparison of multiple boundary layer thicknesses were tested and it was found to be negligible when $y^+ < 5$.
- Mesh contains 752 elements
- y^+ was generally found to be around 2.

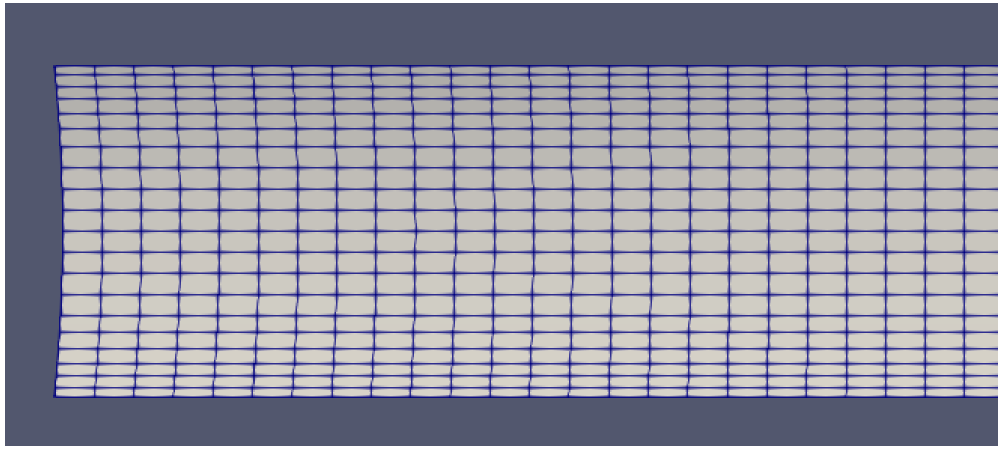




3D Mesh Design

- Same setup as 2D Mesh
- A high z direction partition is employed in order to catch the 3D effects of the model as much as possible.
- While a study was conducted to see if lower z partitions could capture the same amount of physics, ultimately- even though the results maintained low variance, the higher z was chosen due to the simple computational nature of the model.
- X and Y partitions are also greatly increased to maintain y^+ ~2
- Total elements 99262



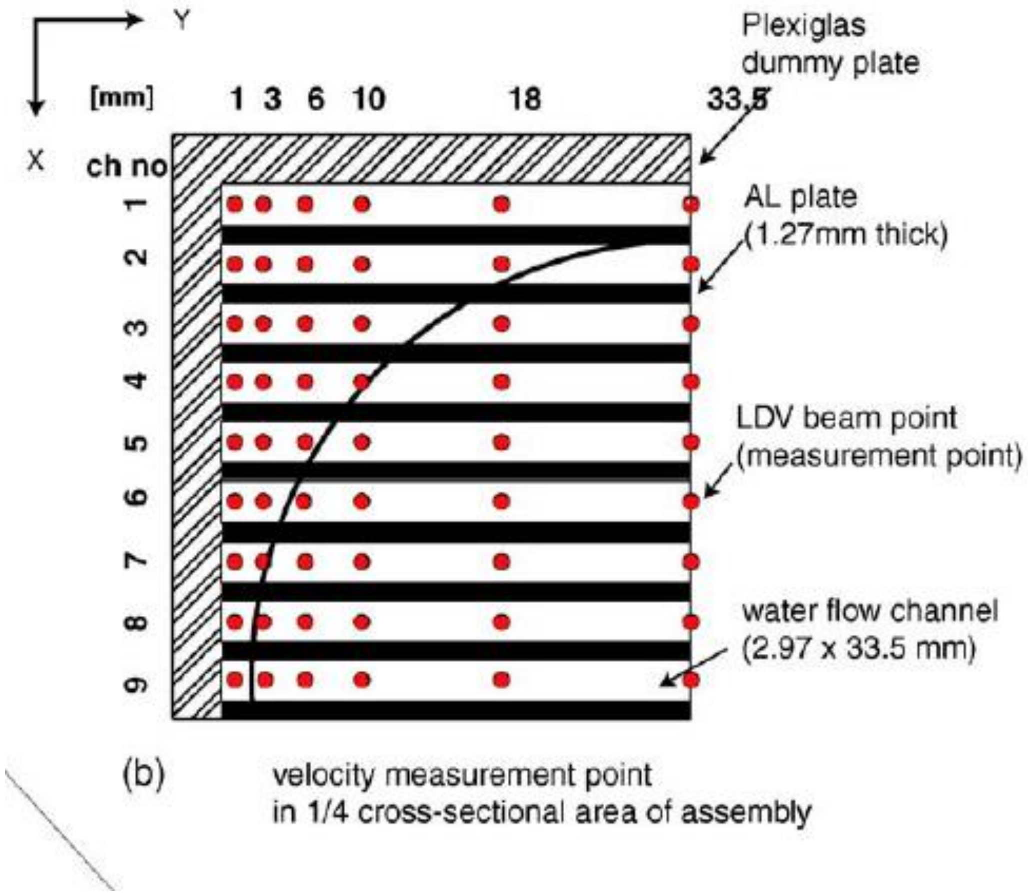


Turbulence Models

- 3 Turbulence models were tested.
- Spalart Almaras was chosen due to its computational efficiency and its ability to model confined flow.
- k-ϵ is chosen as a standard, generally works well for everything.
- k-ϵ Realizable model is used to analyze if wall effects are greatly varying the flow.

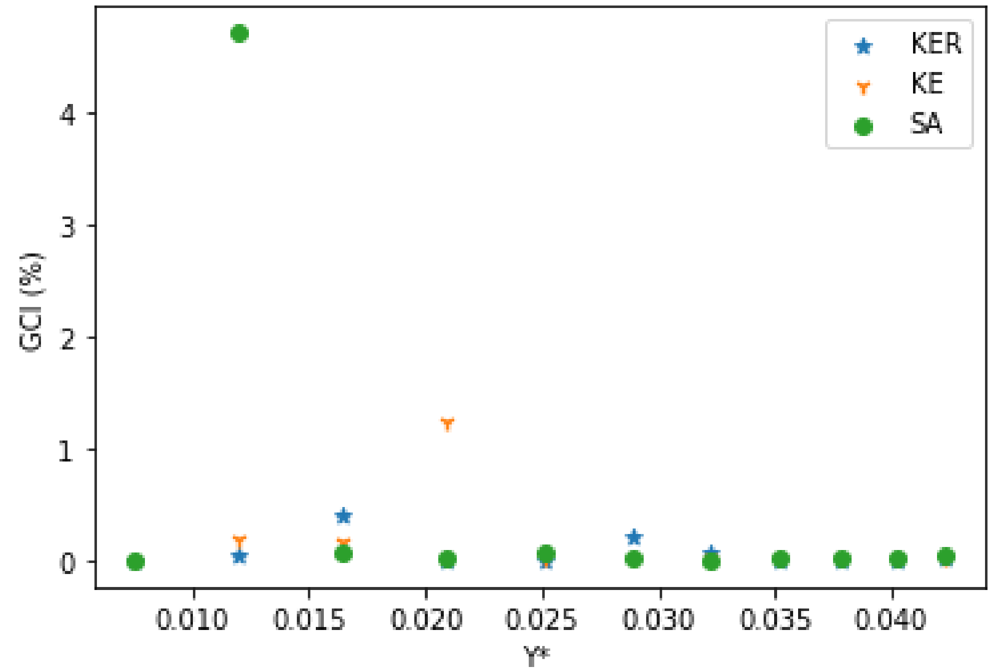
Points of interest

- For this study, the center of the channel along the y axis will be studied in order to validate with works of Ha et al.
- A visualization of these points of interest are shown below from a visual from Ha et al. [1]



Grid Convergence Study

- 3 meshes are created for each mesh, each with a refinement factor of 1.25 the size of the coarser mesh
- A GCI study is conducted on the points of interest. This is done by taking 3 meshes and comparing them to each other at each cell center.
- Error bounds are found to be at a maximum of around 4% in Spalart Almaras



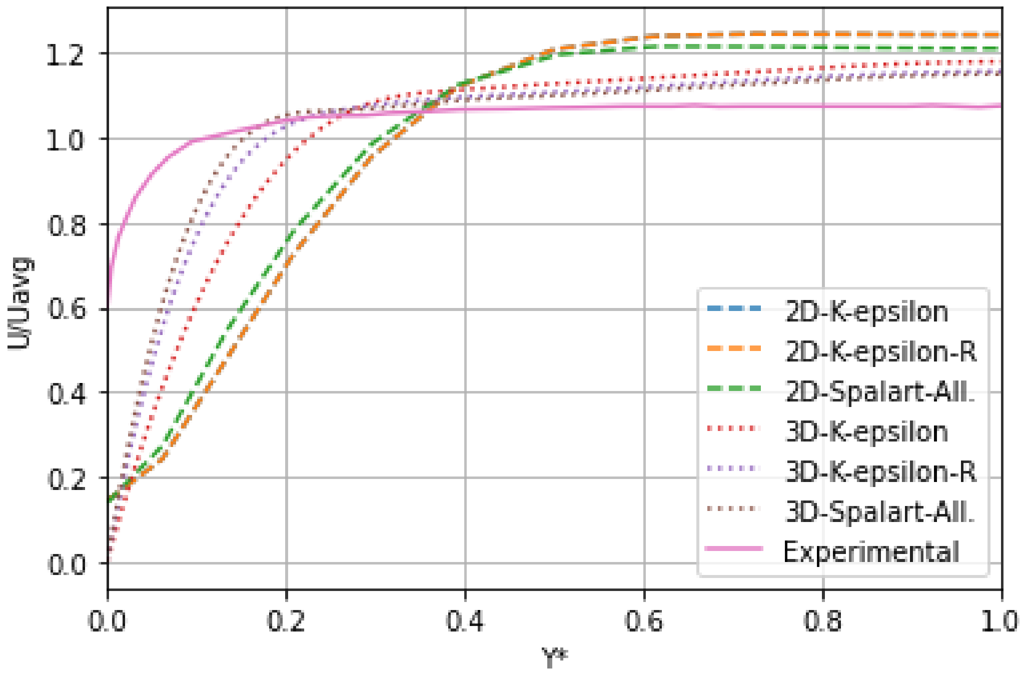
$$F_s \approx 1.25, \qquad r = \frac{h_2}{h_1} = \frac{h_3}{h_2}, \qquad p \approx \frac{\ln\left(\frac{U_3 - U_2}{U_2 - U_1}\right)}{\ln(r)}$$

$$\boldsymbol{\delta_{num} \equiv GCI} = \frac{F_s}{r^p - 1}|U_2 - U_1|$$

Numerical Uncertainty!

Comparison of models

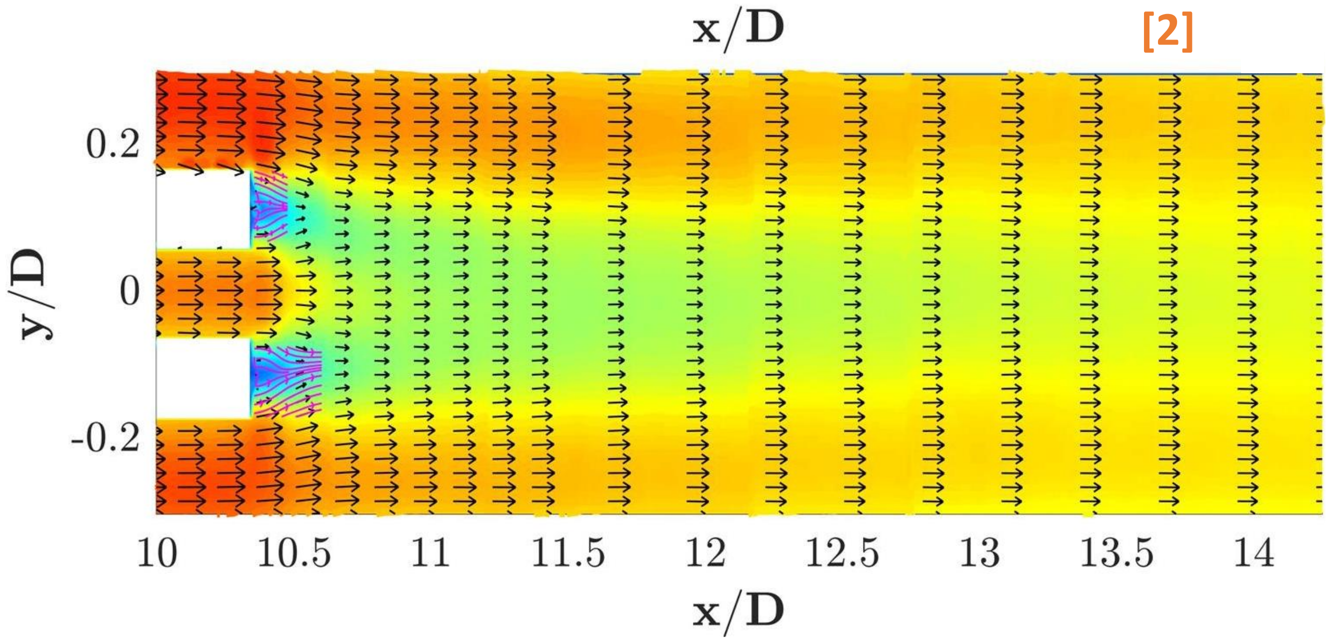
- Data is taken from Ha et al. shown on the pink solid line
- 2D meshes are shown with dashed lines
- 3D meshes are shown with dotted lines
- It is found that for the central flow portion of the channel, the 2D model overapproximates by roughly 20% of the original velocity
- It is also found that velocity ramps slower in the 2D mesh coming off the walls, however this could be attributed to significantly larger inflation layers
- 3D data mostly agrees with the experimental data, slightly slower ramp with a larger approximation of central flow by about a max of 10%
- Furthermore, it is seen that K-epsilon-Resizable is marginally closer to experimental data than other turbulence models
- Since error is in range of 0-4% (most of the time less than 1%), error bars were deemed not necessary to showcase the data

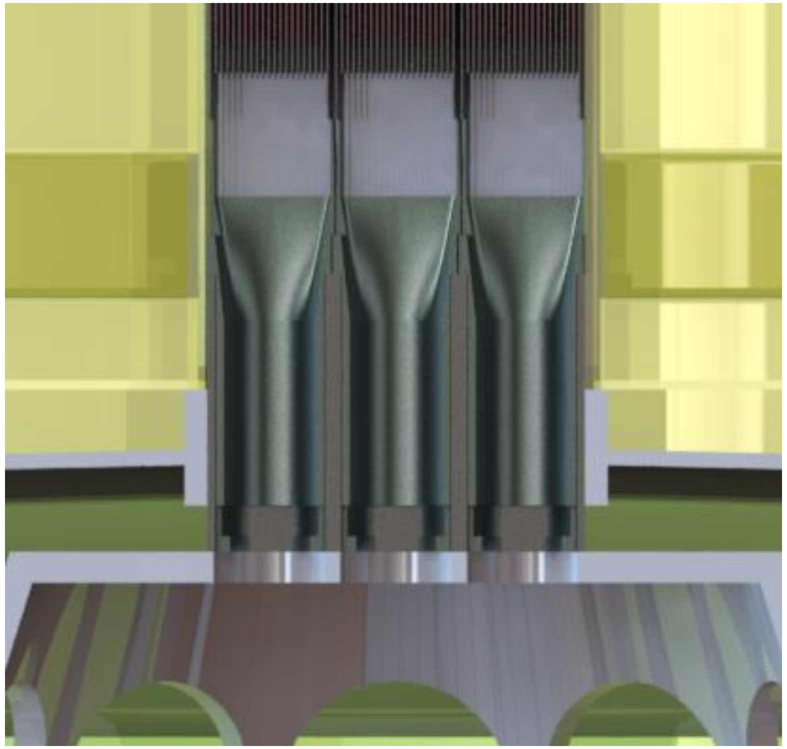


Conclusions so far

- Flow can be modeled by 2D if attempting to estimate center velocity however struggles around walls.
- K-Epsilon-resizable seems to best align with experimental data, only overestimating by 1-2% on center velocity.
- Very Coarse mesh sizes can be used to model channels if just attempting to find center velocity

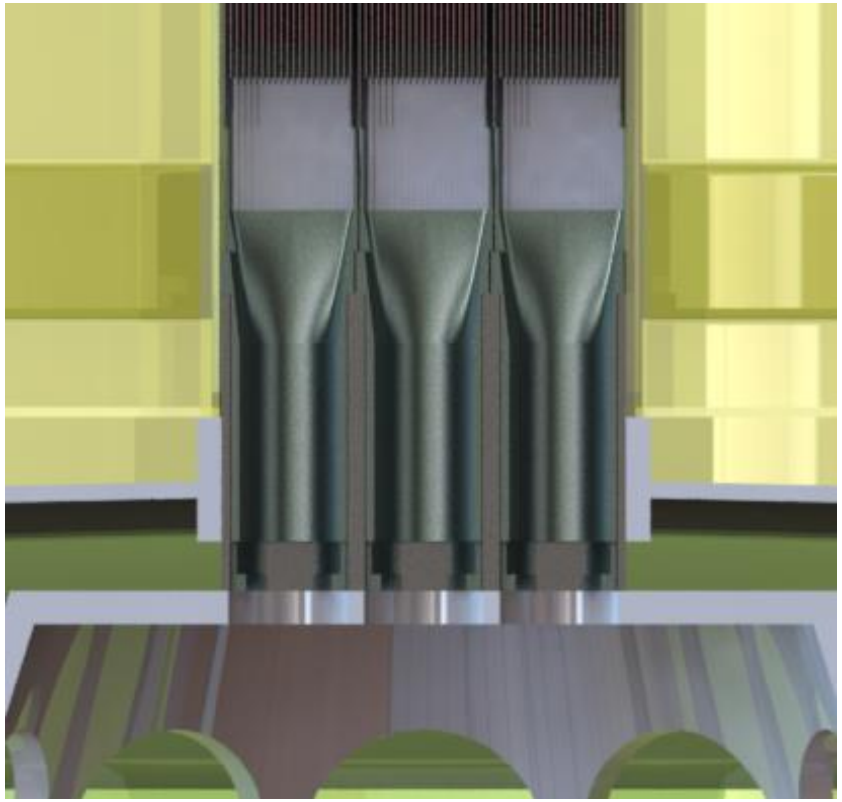
Preliminary Parallel Mixing Studies





Goals

- Recall the geometry from before:
- Inside this geometry we have a mixing region that comes from 3 parallel channels opening into an empty lower plenum.
- We are interested in determining how much mixing and if the flow will be fully developed by the time it reaches the active height.



Goals

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- Fortunately for us, we have experimental data extracted by Weiss et al. , this allows us to validate multiple turbulence models to help find a group/set of models we can use to model the mixing region in the NNS.
- We are primarily looking to see just how much fidelity we will need to get an accurate representation of the mixing regions at the bottom of the core. (do we need 3d models? Wall resolved (explained later)? LES?)

ELSEVIER

Experimental Thermal and Fluid Science

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[2]

Flow regime and Reynolds number variation effects on the mixing behavior of parallel flows

Abdullah G. Weiss [a], Paul J. Kristo [b], Juan R. Gonzalez [a], Mark L. Kimber [a b]

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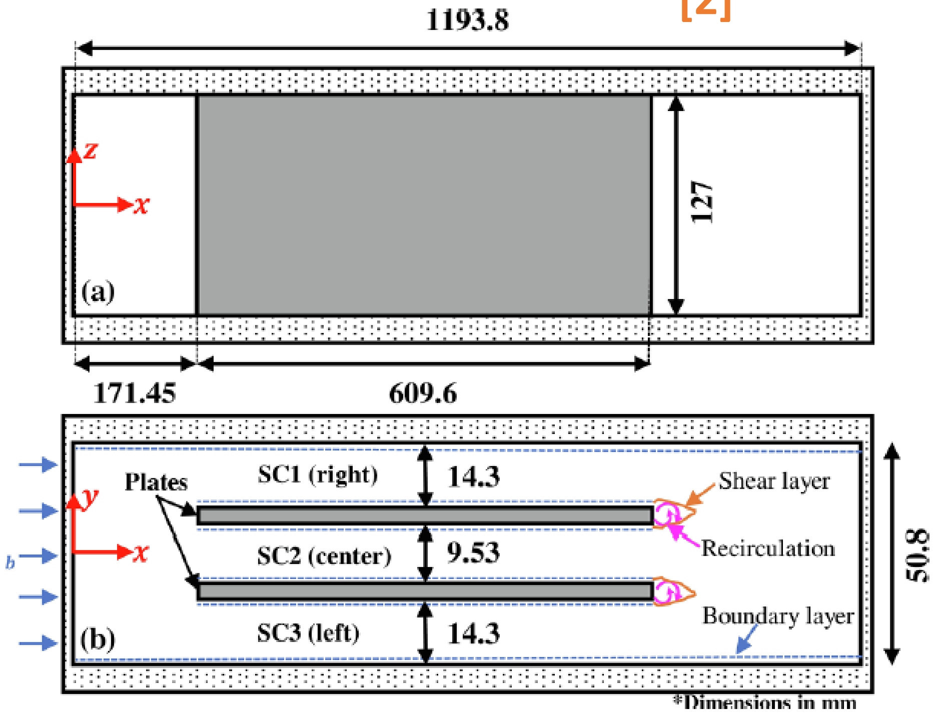
Design Parameters

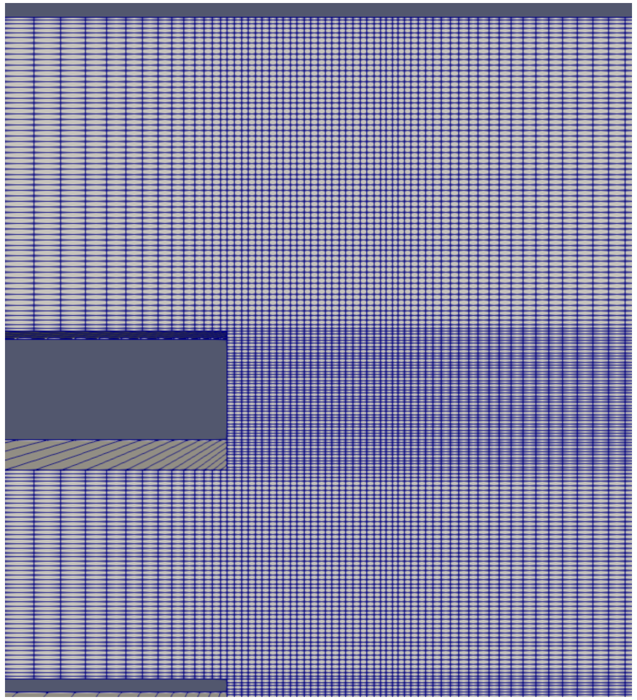
- Models remain 2d for now
- Case for preliminary study of an inlet velocity of 6.69 m/s is chosen
- Pressure set to fixed value of 0 at the outlet
- Velocity is assumed to be 0 at all walls
- ANSYS ICEM is used for Meshing
- OpenFOAM v2206 is used for simulation
- All preliminary models are tested at x/D = 10.35

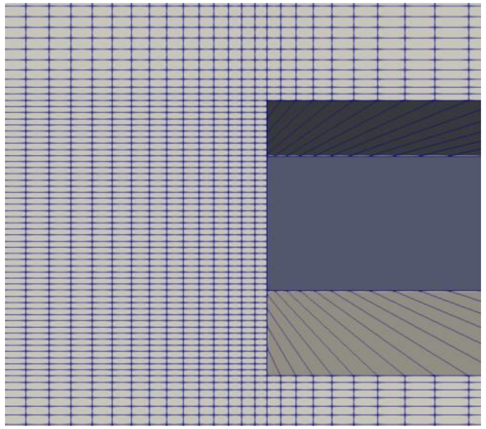
[2]



2D Mesh design

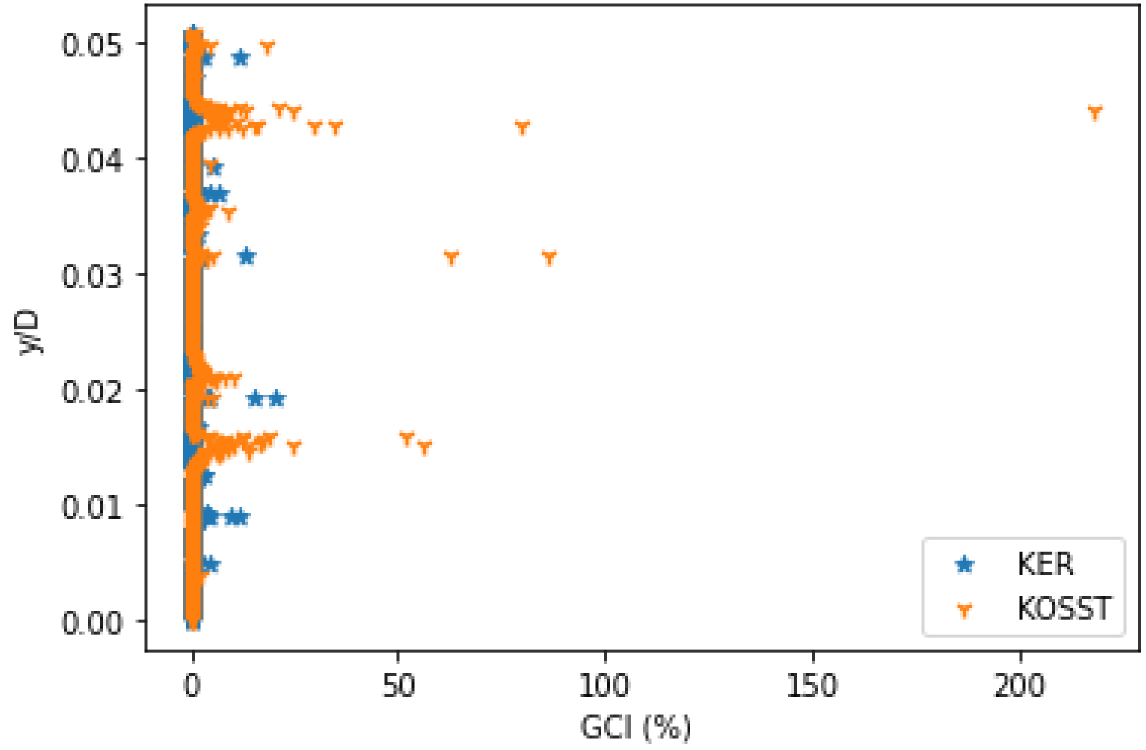
- For the purpose of the preliminary models, wall functions are being used but a close refinement is still kept near the walls to help determine the effectiveness of certain wall functions and varying y^+
- 8 meshes were tested for each turbulence model to determine grid dependence.
- After study was conducted, 3 meshes of sizes (~8,000),(~20,000),(~40,000) cells were chosen for uncertainty analysis and validation ($\boldsymbol{r = 1.5}$)
- y^+ floats around 1.1 with a minimum of 1.02 and a maximum of 1.5





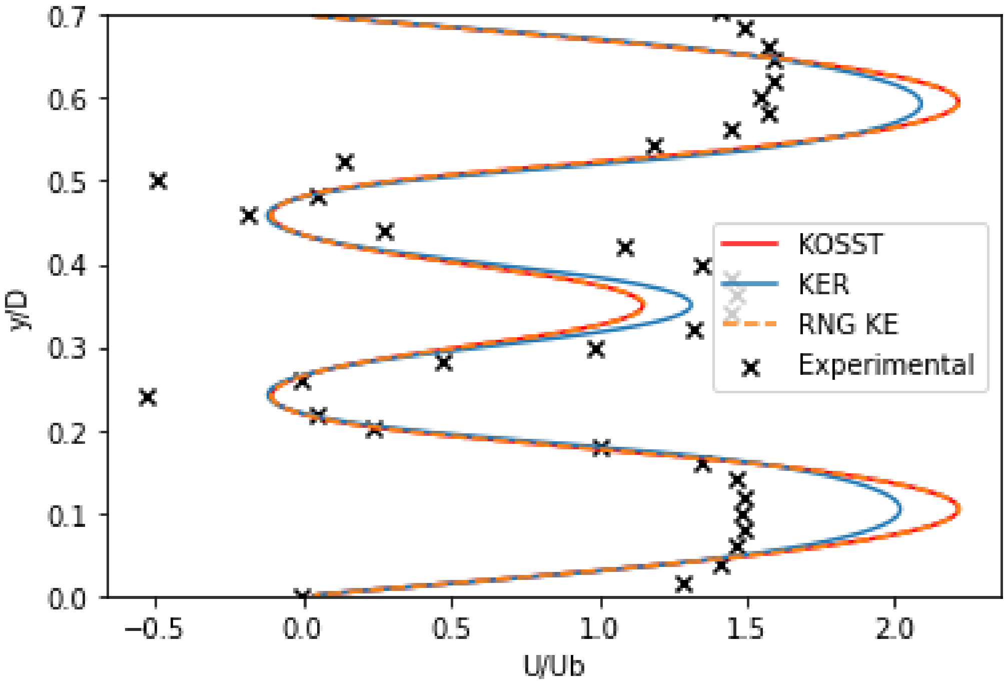
Grid Convergence Study

- At **x/D = 10.35**
- GCI points near walls reflective of a need for increased grid refinement for wall resolved models. (200% error at the highest case)
- Indicates a need for higher fidelity models



Comparison of models

- Data is taken at **x/D = 10.35**
- Mix of under and over approximation of experimental data
- Under approximating center channel
- Over approximating outer channels
- Failing to model extent of circulation in mixing regions
- Likely 3D fluctuations are necessary and potentially wall resolved.



Conclusions

- More complex models required, most likely starting with 3D wall resolved (y+ < 1 with no wall functions).
- Will likely need to work up to LES which will drastically increase computational cost
- 2D models and standard RANS deemed mostly ineffective

Citations

1. Ha, Taesung, and William J. Garland. "Hydraulic study of turbulent flow in MTR-type nuclear fuel assembly." *Nuclear Engineering and Design* 236.9 (2006): 975-984.
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4. Weller, H. G., Tabor, G., Jasak, H., and Fureby, C., 1998, “A Tensorial Approach to Computational Continuum Mechanics Using Object-Oriented Techniques,” Comput. Phys., 12(6), pp. 620–631.

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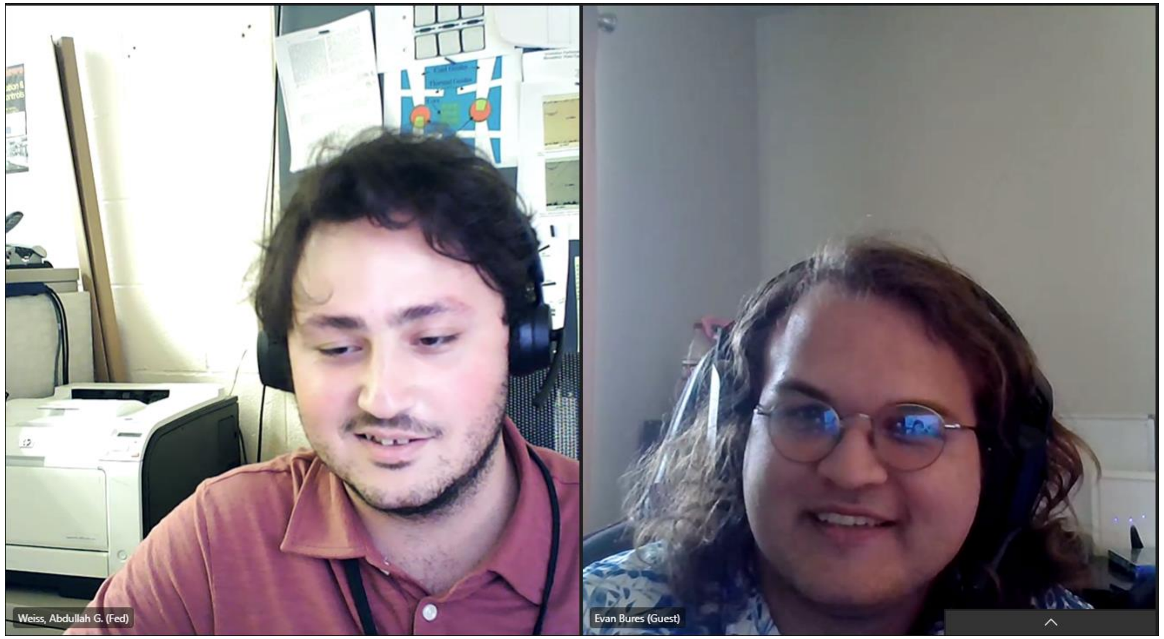

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