The Role of COMSOL Toward a Low-Enriched Uranium Fuel Design for the High Flux Isotope Reactor

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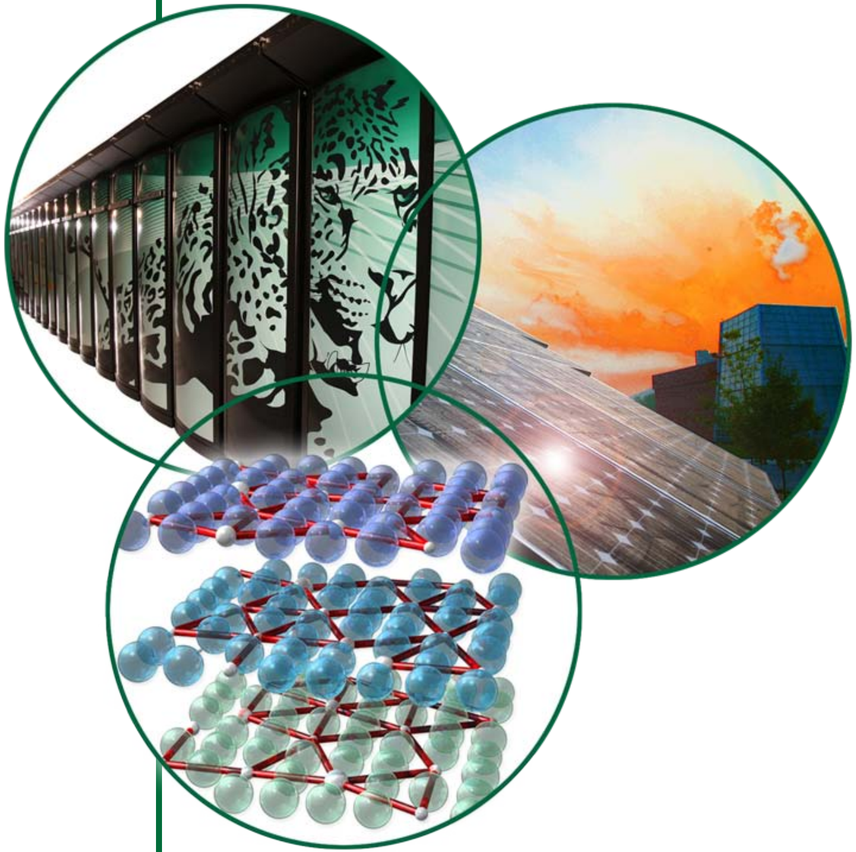

U.S. DEPARTMENT OF ENERGY

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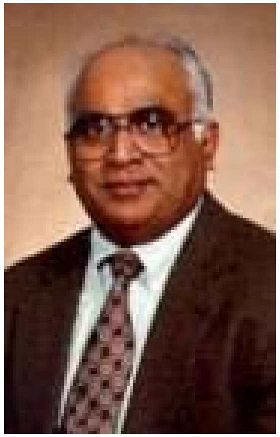
The following topics are discussed in this presentation

- very short introduction to HFIR
- research goals
- where we are in our research
- areas we expect intense activity
- current status
- some results

The current HFIR LEU project COMSOL team

Jim Freels, has been to this conference since the first one in 2005. Started with v3.0.



Professor Rao Arimilli was on Jim's PhD committee, a long-time COMSOL user, expert in applied ME, heat transfer, fluids, etc.

Kirk Lowe is nearing completion of his PhD in ME using COMSOL as a primary tool. We lose Kirk in December to full-time employment.

Isaac Bodey is qualified and early in the ME Ph.D. program, has already used COMSOL extensively, and is now making major contributions.

Fundamental goals for COMSOL on this project

- LEU fuel must fit in the existing fuel assembly, deliver the equivalent or enhanced {neutron flux and cycle time}.
- In order to achieve this LEU fuel design goal, modern analysis codes with increased accuracy and capabilities over the existing design-basis codes are required.
- The existing design and safety basis codes are limited to 1D conservative analysis using legacy FORTRAN.
- COMSOL provides 3D, multi-physics, high-accuracy, and enhanced analysis capabilities to meet these goals.

A unique design feature of the HFIR fuel element is the involute shape of the individual fuel plates

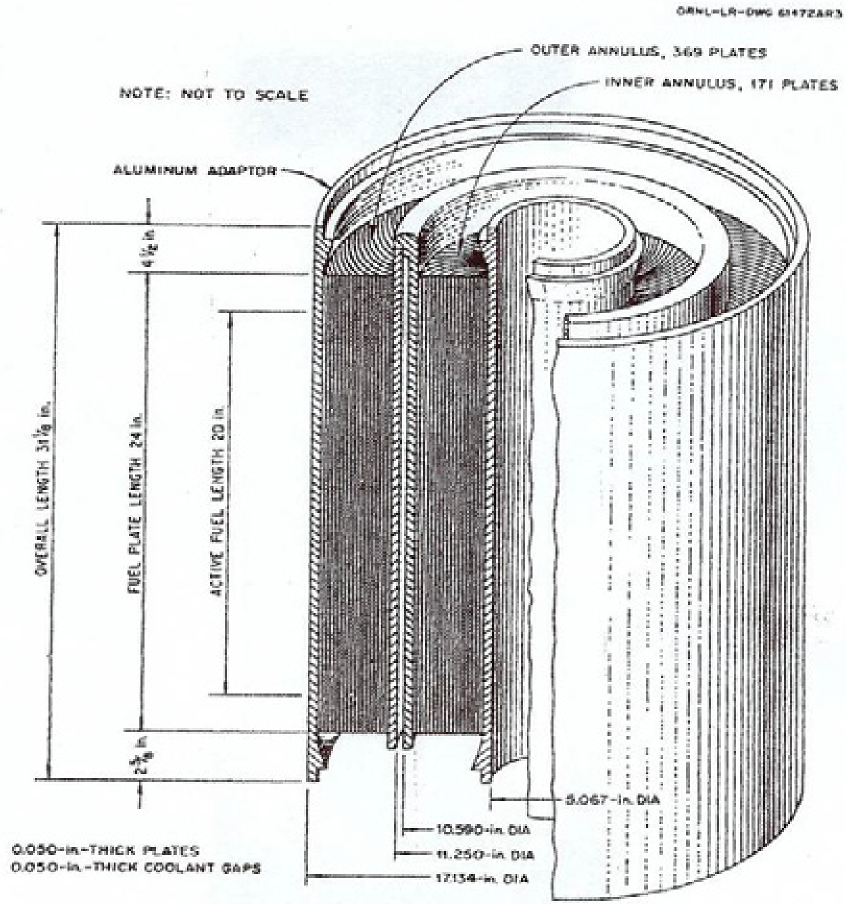


Fig. 3. HFIR Fuel Assembly.

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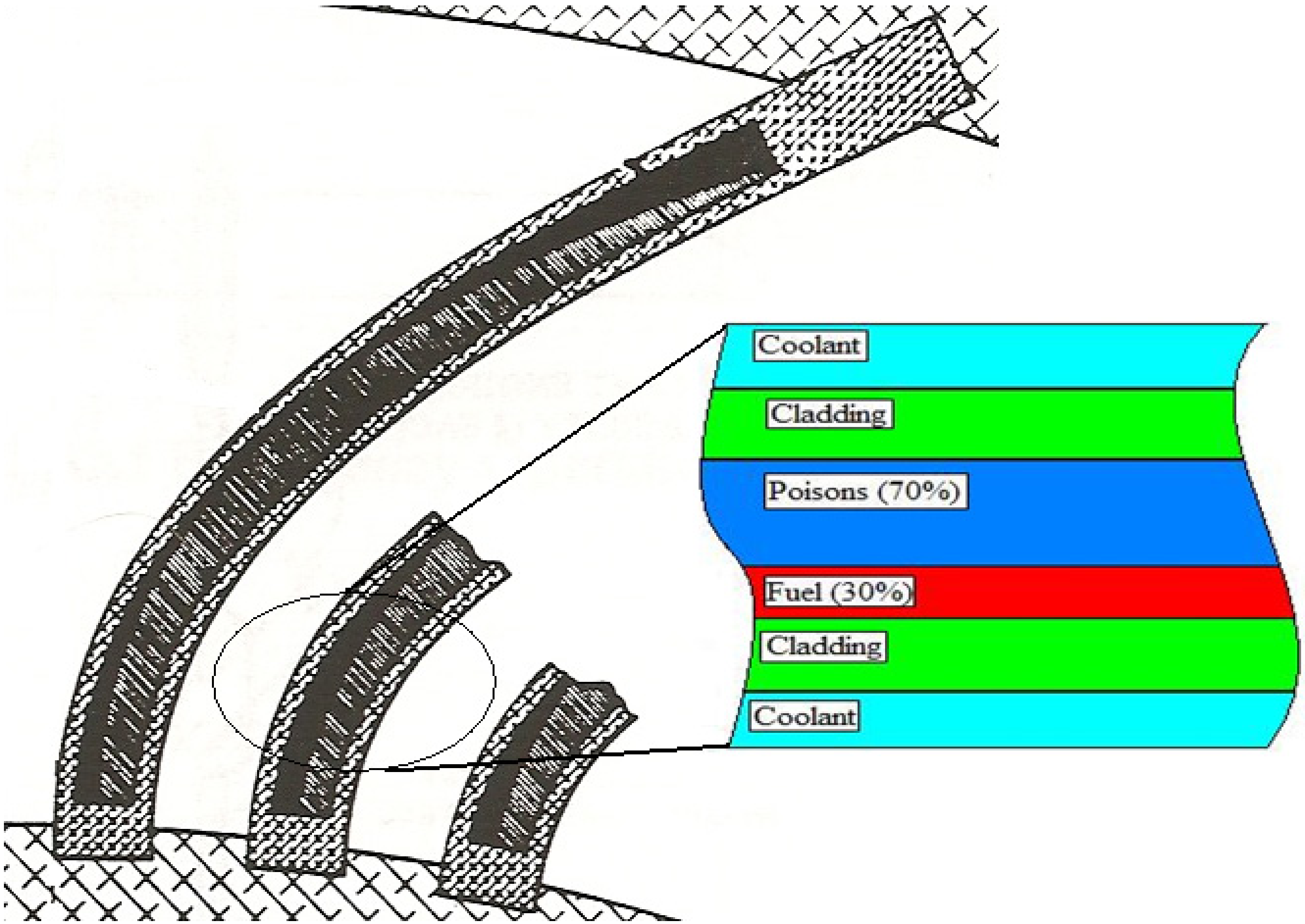
Large aspect ratios exist in both the axial (24/.05 or 480/1) and span-wise (~4/.05 or 80/1) directions



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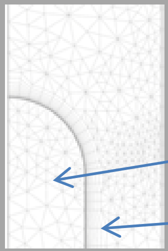
Input Material Properties into COMSOL Material Library

- **Several sources of HFIR fuel data have been compared and input into the COMSOL material library (a feature of the code).**
- **The COMSOL material library allows for direct comparison of data values, a straight-forward approach to establish the best-estimate basis, quality assurance, and convenience.**
- **Sources for data have included (thus far): 1) data from this project, 2) HFIR SSHTC, 3) HFIR RELAP5 model, 4) NIST (ASME) water properties package, 5) Thermophysical Properties of Matter (TPMD) database available through ORNL library, 6) COMSOL internal library (includes references).**
- **A new source not yet investigated is MATPRO database through RELAP5 and other codes from INL used for fuel performance analysis. This could also be incorporated.**
- **Properties established are k (W/m-K), ρ (kg/m^3), C_p(J/kg-K), and μ (Pa-s).**

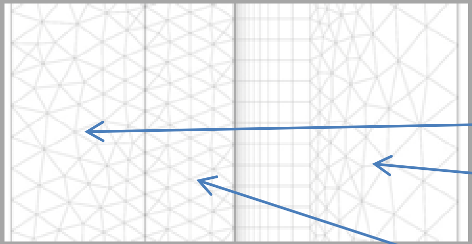
Use a 2D Model as a Test Bed for 3D -start with meshing (triangles)



entrance region is rounded

0.050”/2 symmetric clad width

0.050”/2 coolant channel width

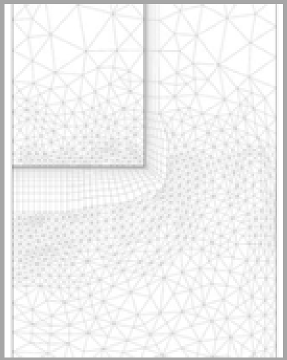


typical main channel section.

fuel (0.030”/2 symmetry)

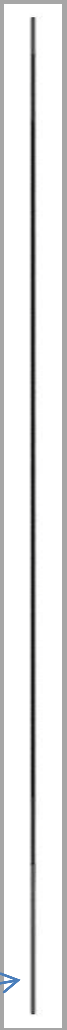
coolant with boundary layer mesh adjacent to the clad wall

clad (0.010” thick)



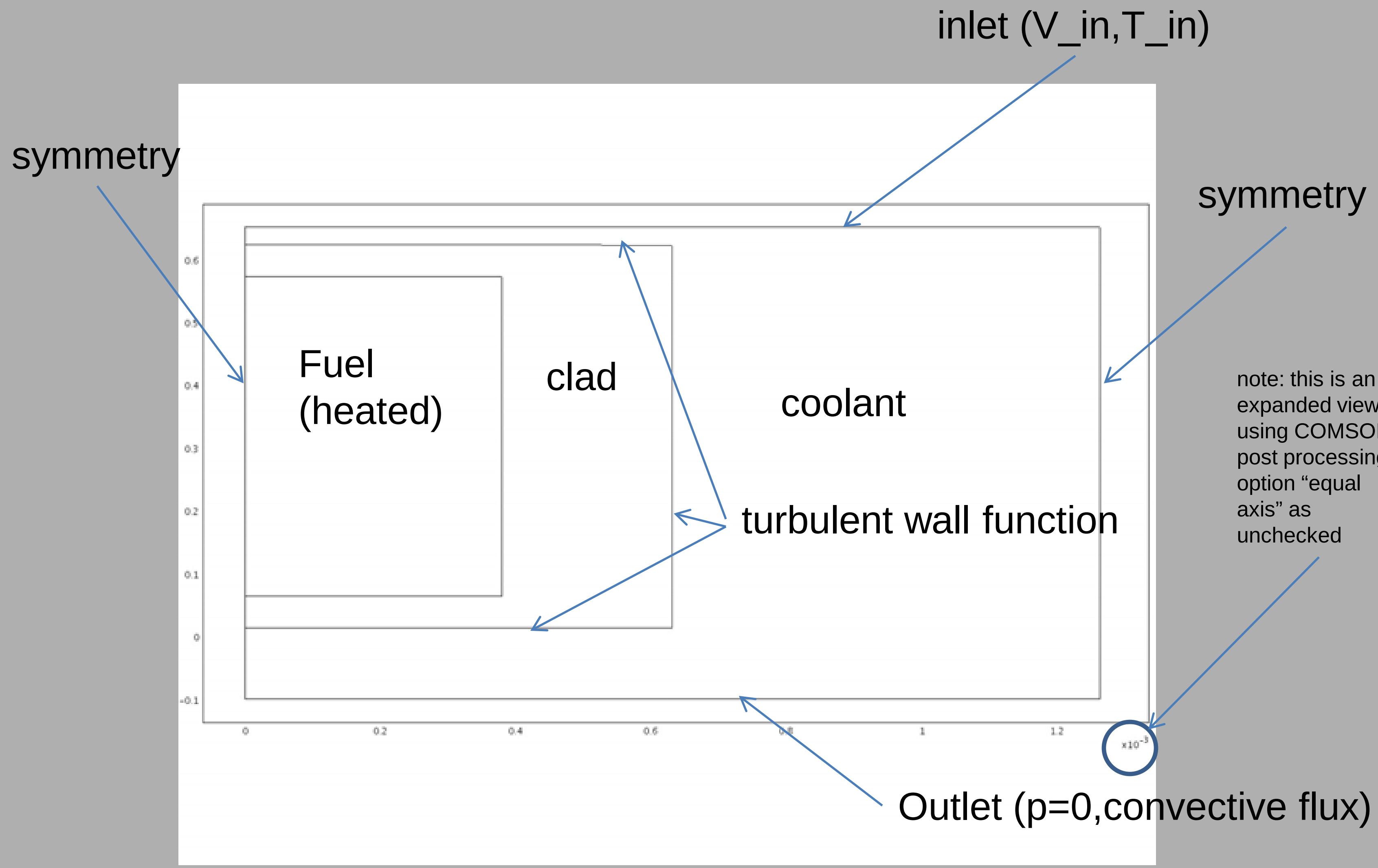
exit region is not rounded

extra mesh density in both the entrance and exit regions to capture the large changes in fluid velocity



overall length is > 24” causes the mesh to be difficult to view here due to the high-aspect ratio

Use a 2D Model as a Test Bed for 3D -establish proper boundary conditions



note: this is an expanded view using COMSOL post processing option “equal axis” as unchecked

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2D solutions:

- full power and flow

- Re ~ 1.8×10^4 based on channel half width of 0.025”

- Kays-Crawford expression for Pr_T used throughout

- V_in=7.945 m/s (26.07 ft/s), T_in=321.9 K (120 F), q’’’=5.316×10^9 W/m^3

- core exit pressure set to ~ 373 psia for water property evaluation

- solid properties are based on RELAP5 HFIR model and vary with temperature

-water properties are based on NIST/ASME Database 10 v2.21 and allowed to vary with temperature and pressure

- investigated y^+=30, 100, and 10 (and as related to boundary-layer mesh spacing at the wall) ***: graphics shown here for y^+=10***.

- investigated linear and quadratic finite-element basis

- investigated triangles and quadrilateral finite-elements ***: graphics shown here for triangles***.

2D solutions: COMSOL options

- k-ε turbulent, non-isothermal (weakly compressible) model

- GLS dissipation on Navier-Stokes, turbulence, and coolant temperature

- cross-flow dissipation on Navier-Stokes, and coolant temperature

- NO additional isotropic dissipation used !

- realizability constraint on turbulence model is used

- corner smoothing *not* used in 2D solutions, may be needed in 3D

- included optional surface heating from pressure and viscosity terms

- use manual scaling in advanced solution options

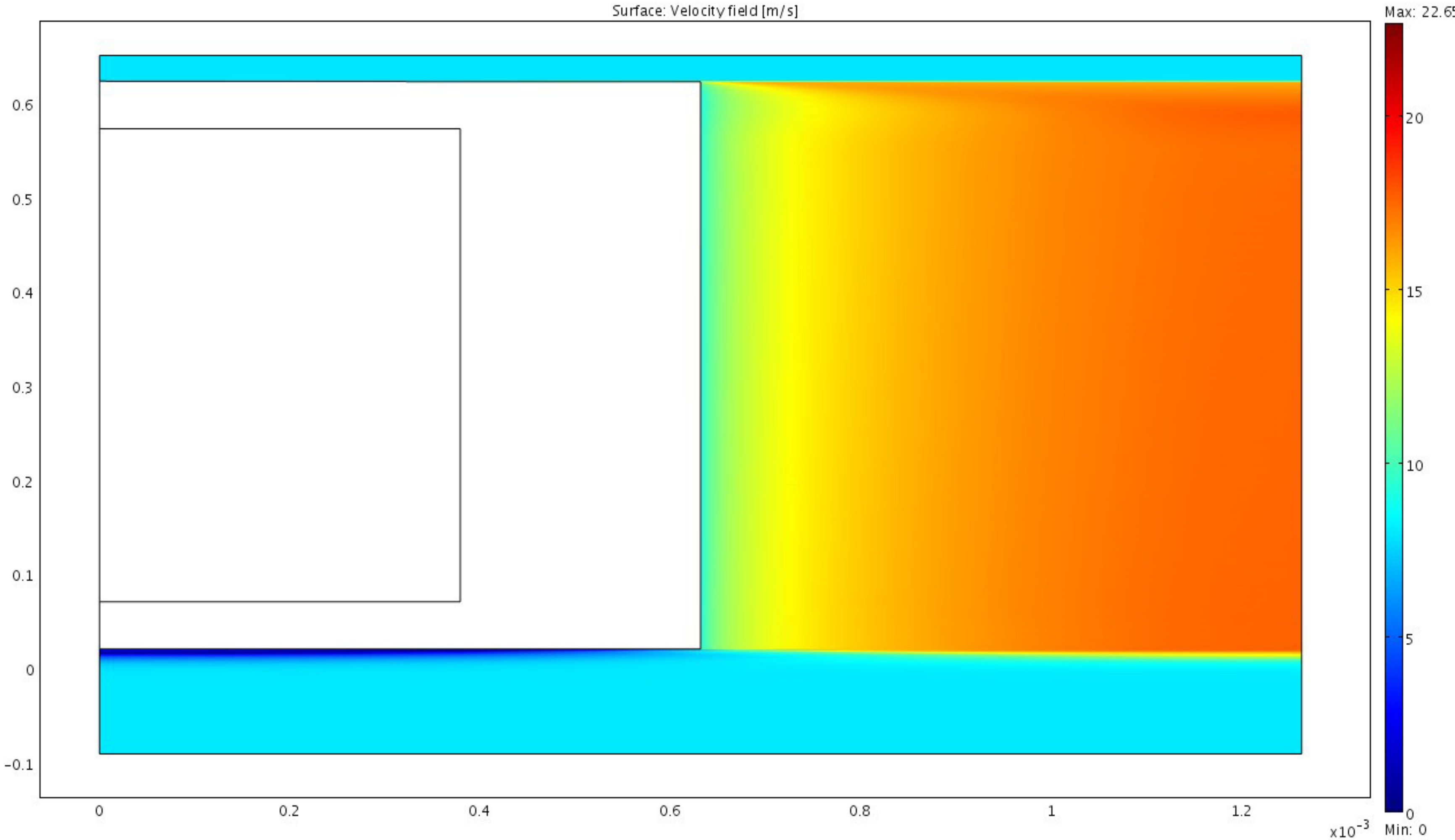
- use parametric solver on power level to get to full power

- used segregated solver to get to final solution

- final 2D solution is fully-coupled direct solver

- iterative solver in 3D (see full paper for discussion)

2D solutions: U_chns, quad elements, 4671216 dof



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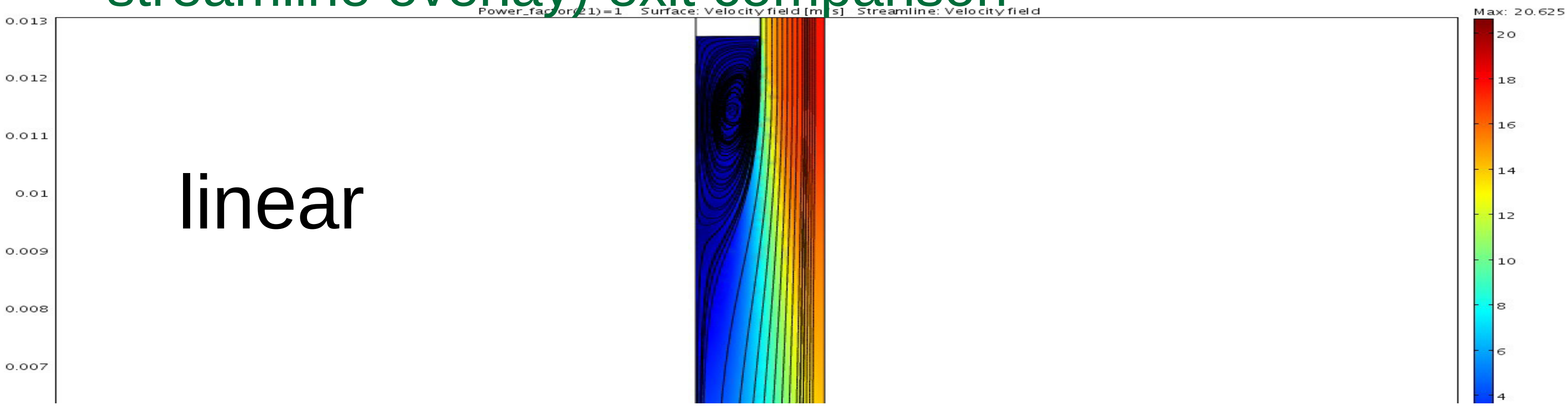
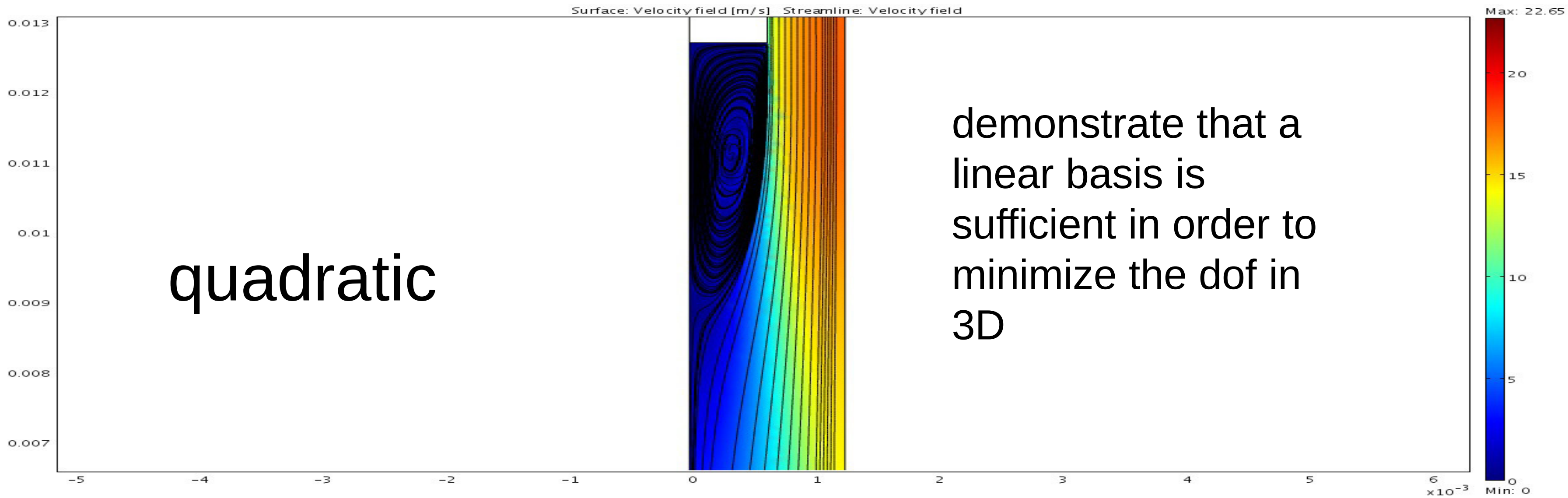
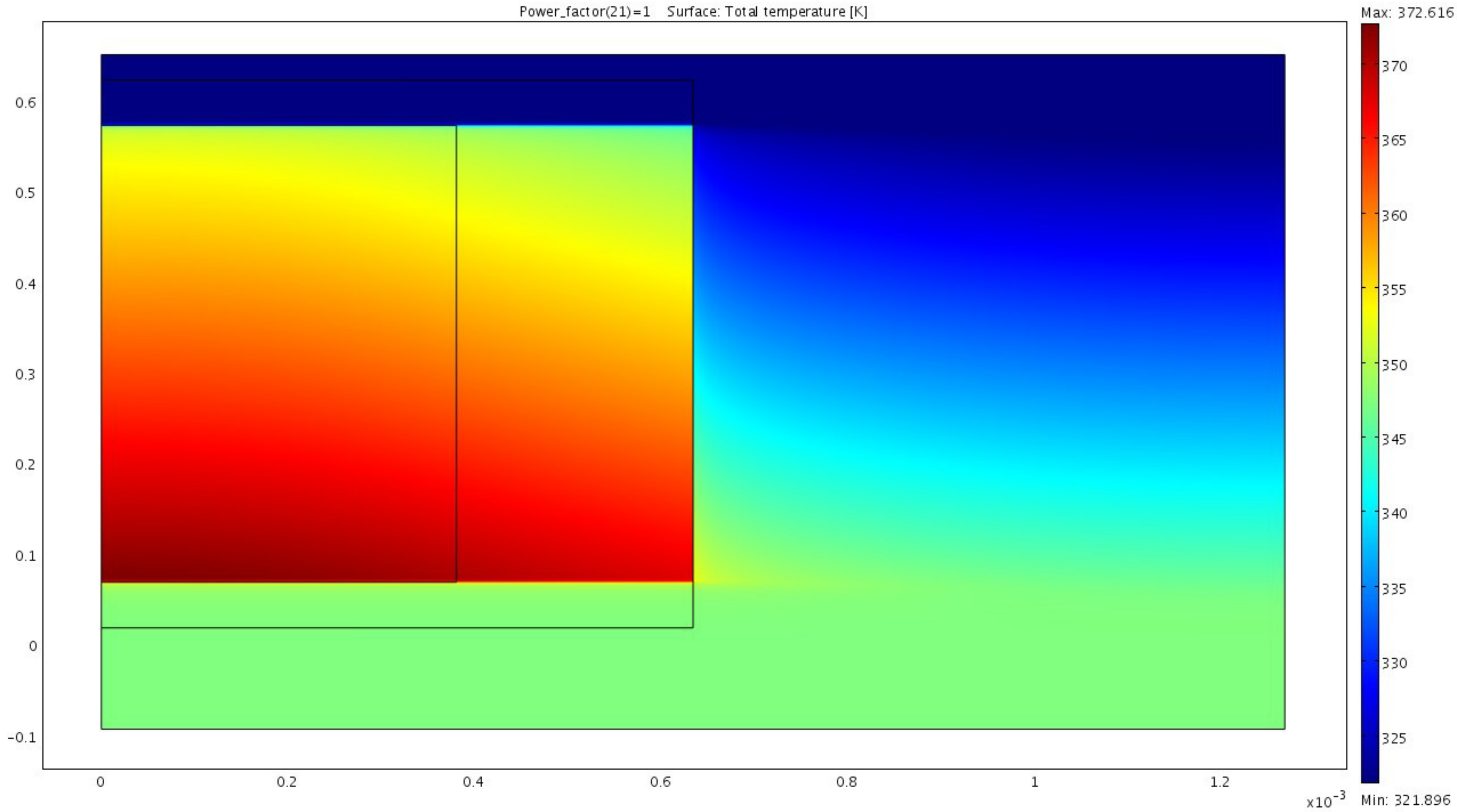
2D solutions: U_chns (velocity magnitude with streamline overlay) exit comparison





demonstrate that a linear basis is sufficient in order to minimize the dof in 3D

2D solutions: Ttot, linear elements, 1346998 dof



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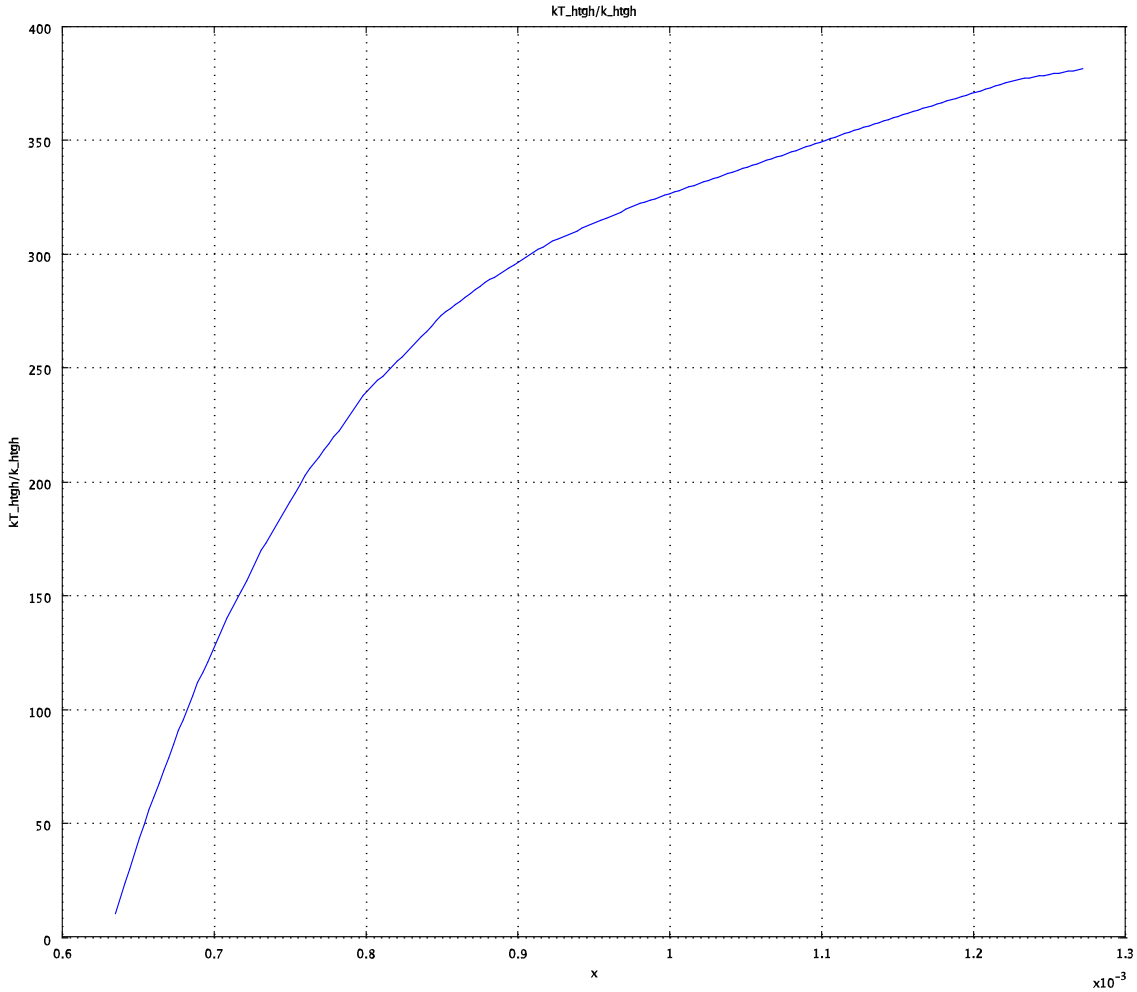
2D solution details: k_T/k 0.1m upstream from the exit

wall boundary



symmetry boundary

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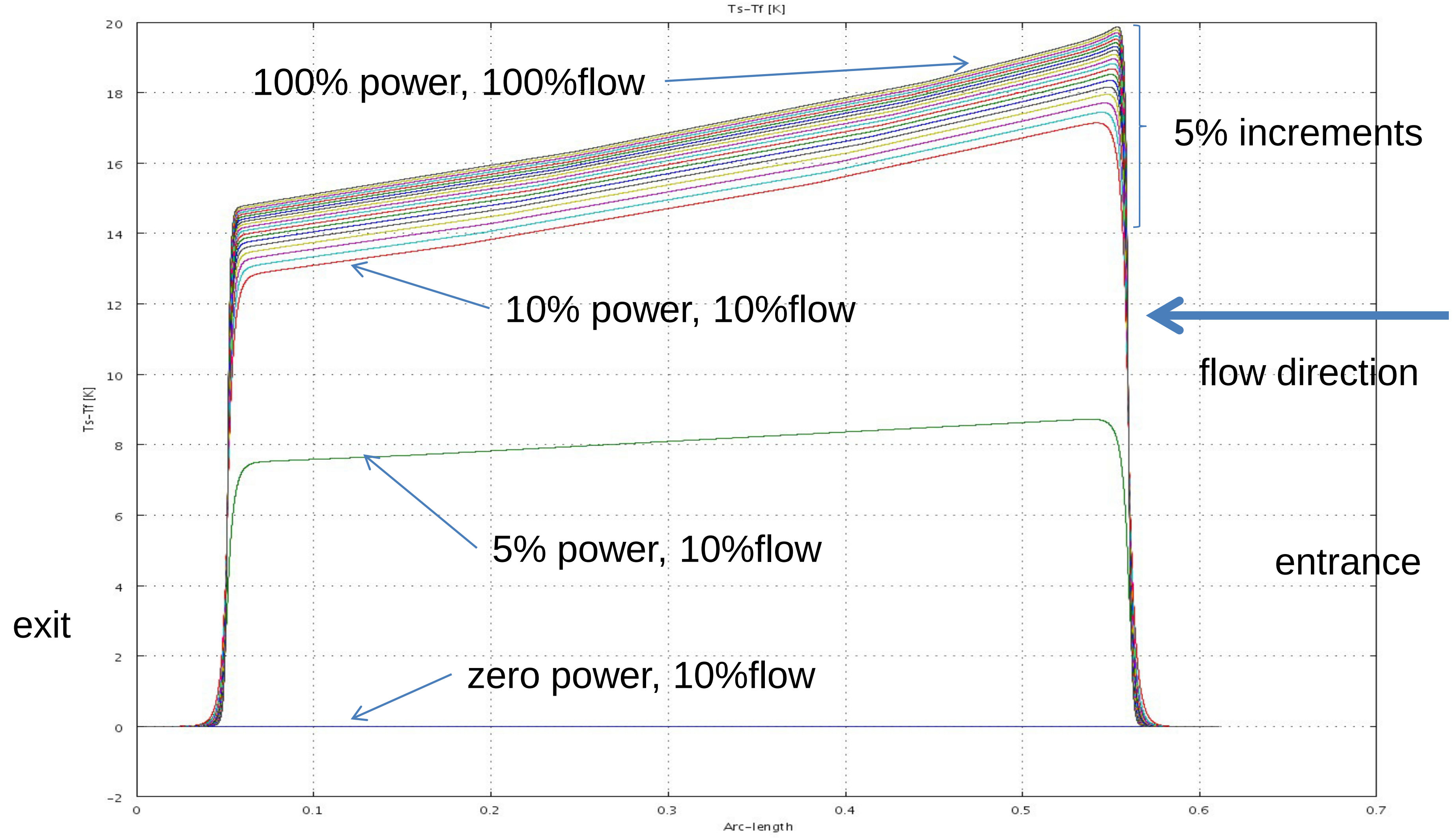
2D solution details:ΔT along the wall as a function of power & flow level (0:.05:1.0)



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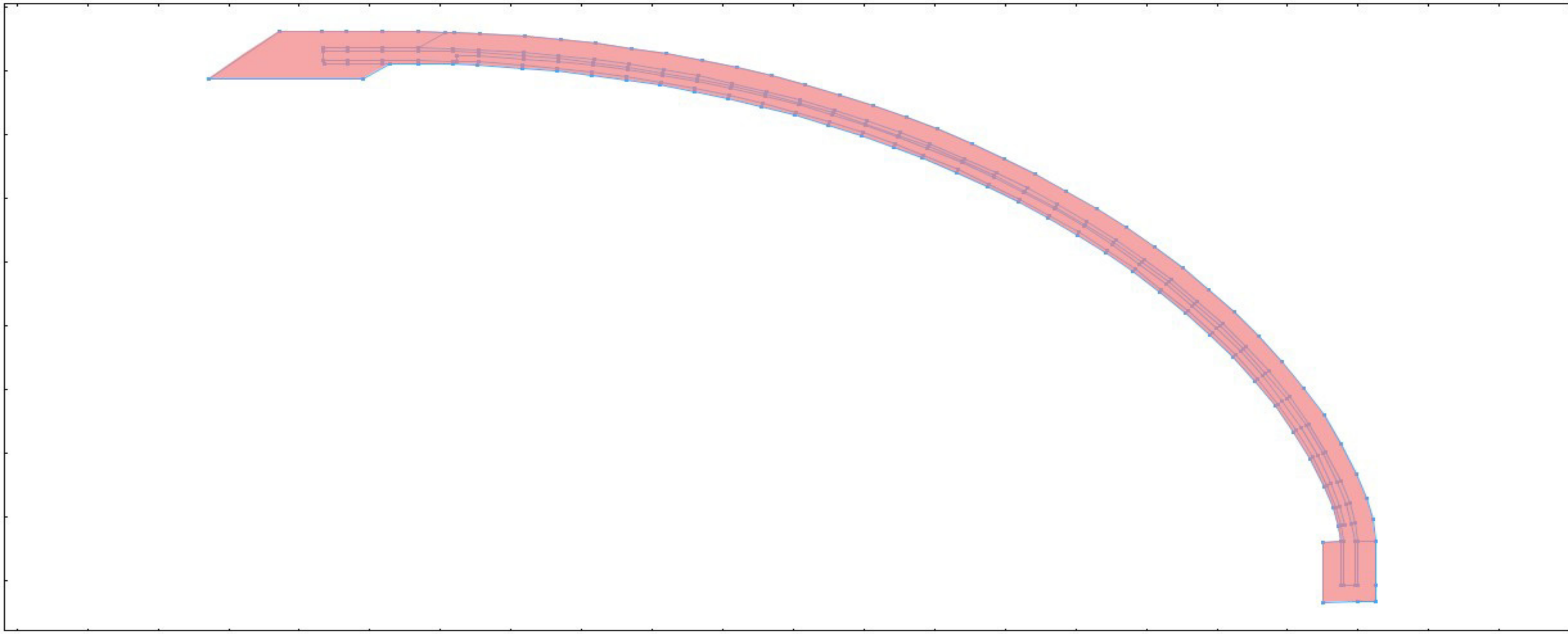
entrance

Involute plate geometry yields an asymmetry of the coolant channel at the element sidewalls

- **The 3D model was expanded to include a full single flow channel and a full fuel plate on one side**
- **A COMSOL extrusion coupling variable allows for this configuration to be used**
- **This option was investigated along with several additional options**
- **Most important is the asymmetry of the fuel plate itself due to the non-symmetric fuel loading**
- **Also investigating Solidworks interface for more consistent user interface to the boundary conditions**
- **A final configuration has been established for detailed, best-estimate single plate model of the HFIR**

one full coolant channel with extruded coupling variables to couple opposite side,
one full best-estimate fuel plate including separate fuel, filler, and clad regions,
accurate side-plate representation



this is the only design that preserves physical symmetries correctly !!

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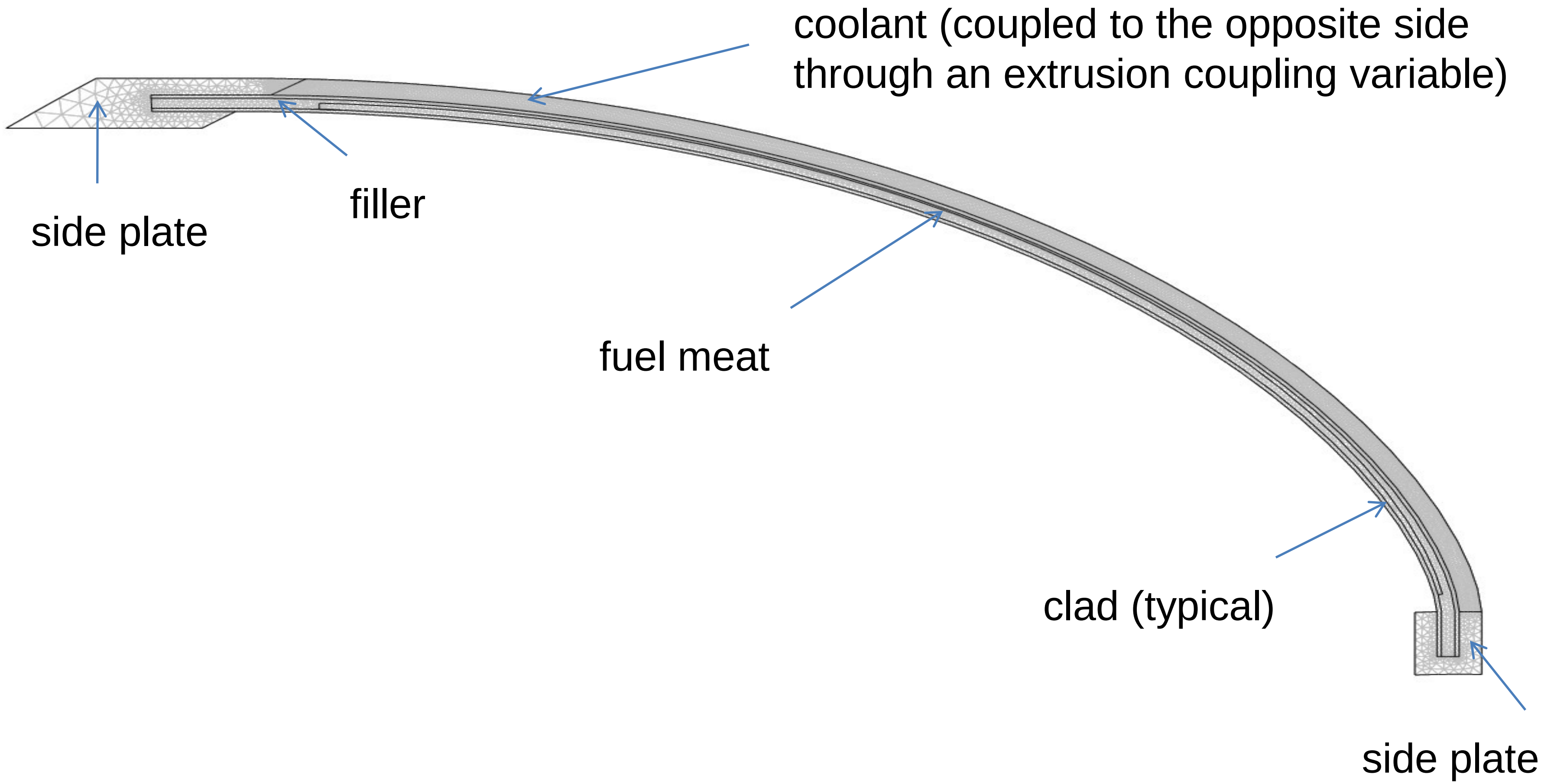
3D meshing starts with a 2D working plane of the involute plate to be extruded in the axial direction



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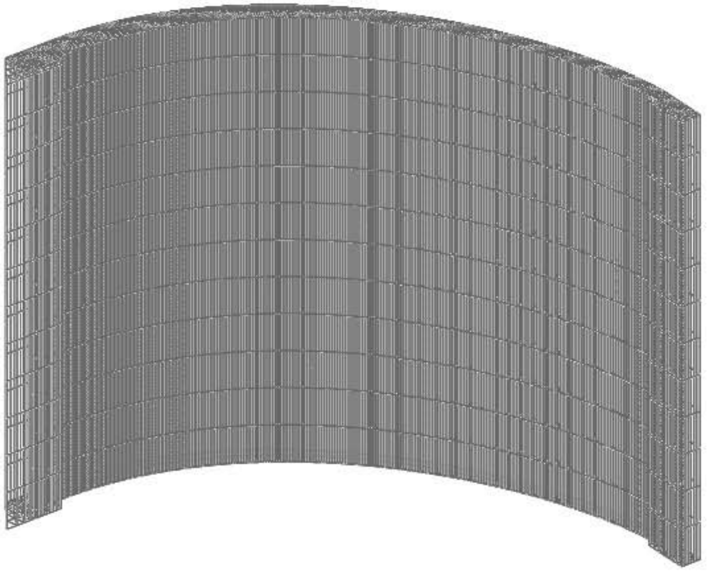
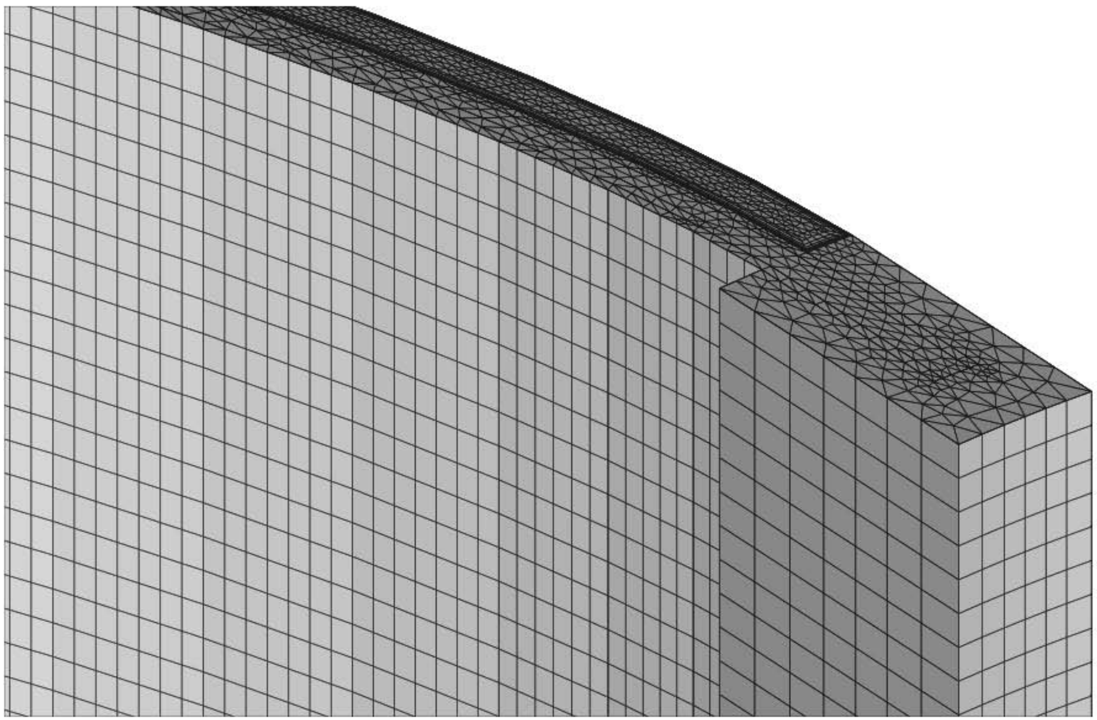
the extruded 3D mesh density depends on the specified number of axial mesh spacing

boundary condition specification similar to 2D, just more to worry about !



note: we are also investigating the Solidworks CAD interface which provides for fewer surfaces that need to be specified as boundary conditions as well as other benefits

Magnified right side extruded 3D mesh



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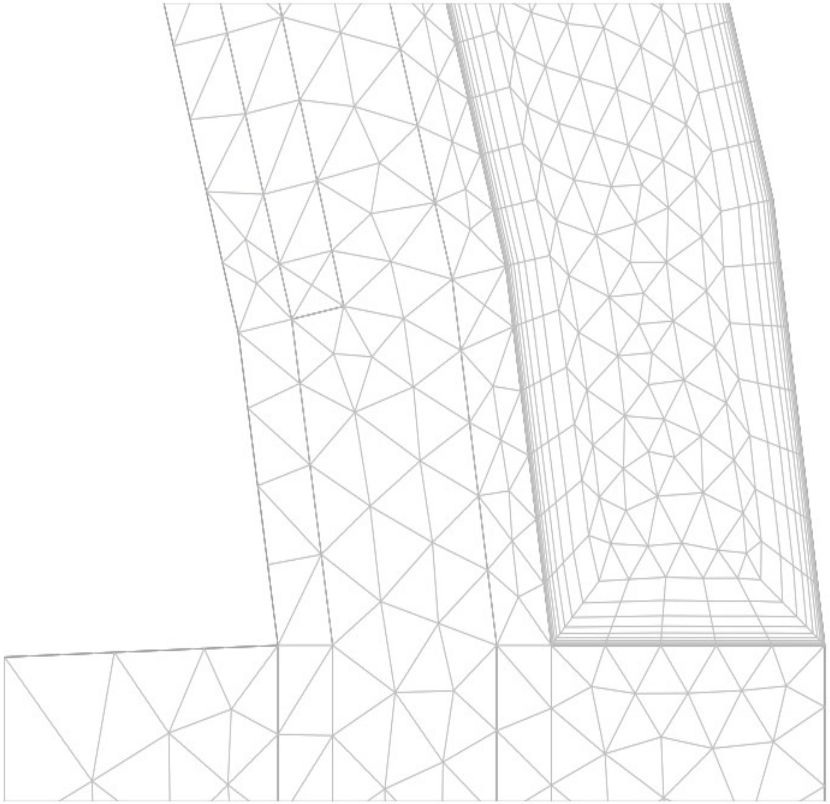
Magnified right side 2D mesh



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Confirm or modify the turbulence model (p1/2)

- **The k-ε and k-ω turbulence models are the most common turbulence models used in the world and these are what are preloaded into COMSOL for general application.**

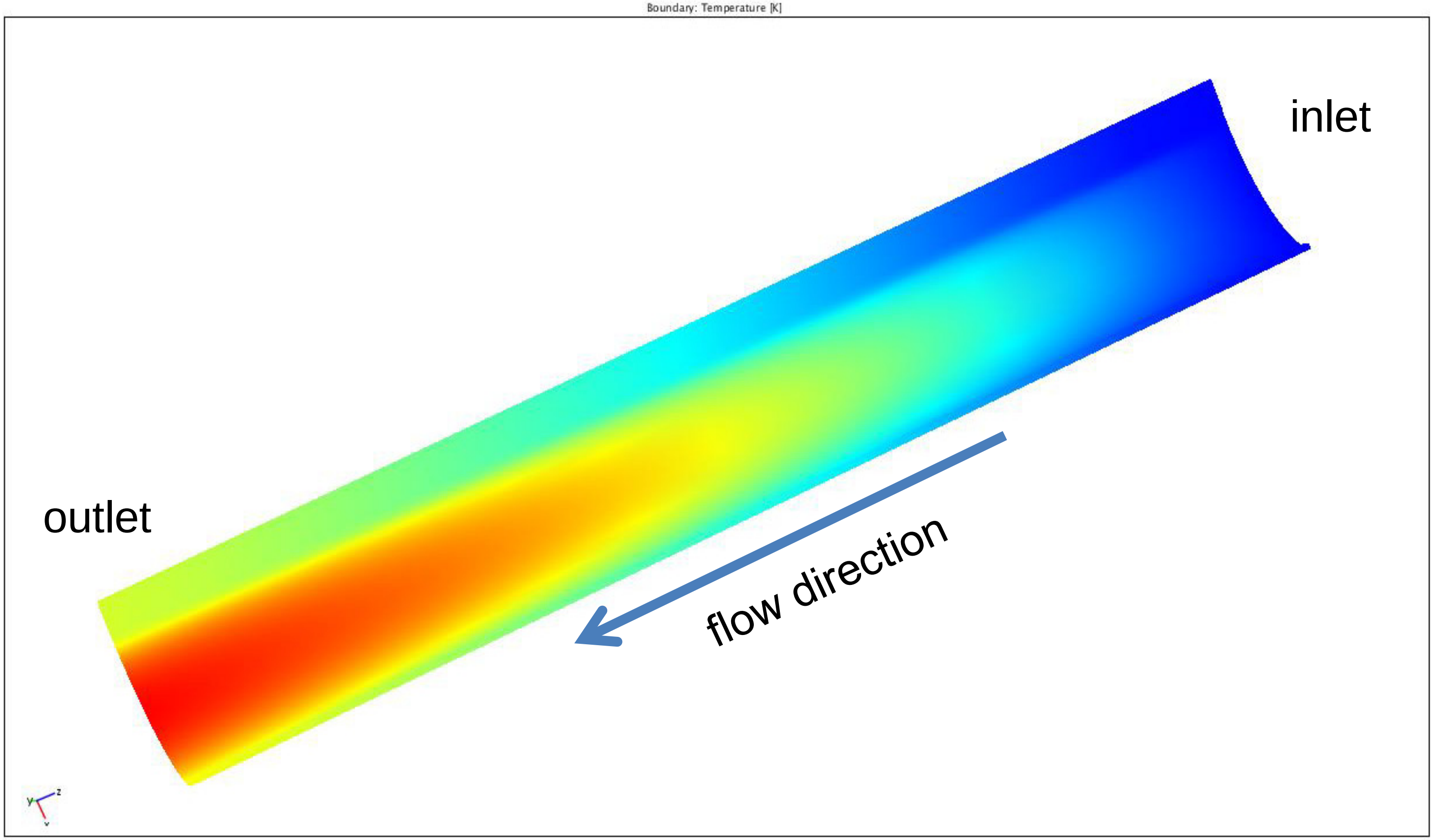
- **In our utilization of the k-ε model with COMSOL, it has been observed that the wall-offset parameter (δw) has a noticeable effect on the fluid temperature close to the wall.**

- **The applicable value of δw will be determined by matching the predicted fluid temperatures near the wall with measured values during startup testing of the reactor.**

Confirm or modify the turbulence model (p 2/2)

- **We need to investigate the literature for the application of turbulence models in similar situations (high heat flux, high mass flux, turbulent forced convection, heat generation, etc.).**
- **Should it become necessary to derive, invent, or modify the turbulence model, COMSOL provides this capability in a straight-forward manner by modifying inputs, not developing new code.**
- **This is perhaps the most important reason to be using COMSOL for this project.**

Typical 3D result: metal surface temperature



shown is the clad surface temperature adjacent to the turbulent-wall of the coolant

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Structural mechanics will be coupled to account for buckling effects caused by thermal expansion

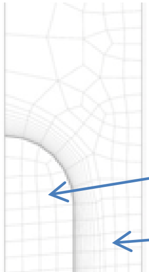
- **This task has not started.**
- **Addition of structural mechanics effects using COMSOL is a routine task (COMSOL multiphysics).**
- **Many examples of how to do this are in the COMSOL manuals.**
- **Do not anticipate any issues or problems with incorporating this.**
- **Anticipate starting this before end of the fiscal year.**

Conclusions and Current Status

- **COMSOL is providing a modern simulation tool for the design of LEU fuel and analysis of present HEU fuel.**
- **The COMSOL analysis provides details and accuracy heretofore not possible, and allows for precise margin estimates.**
- **The 2D analysis provides a test bed for the 3D analysis to establish consistent parameter set (wall offset, mesh density, solution procedure, etc.)**
- **2D results demonstrate methods that yield accurate benchmarks with established data base (work ongoing).**
- **3D computational requirements have been demonstrated on a representative model. 3D results are not completed yet.**

extra slides not presented at the conference

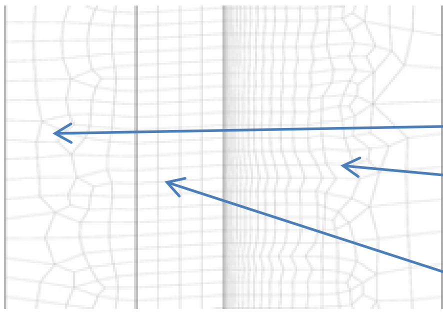
Use a 2D Model as a Test Bed for 3D -also investigated quad meshing



entrance region is rounded.

0.050”/2 symmetric clad width

0.050”/2 coolant channel width



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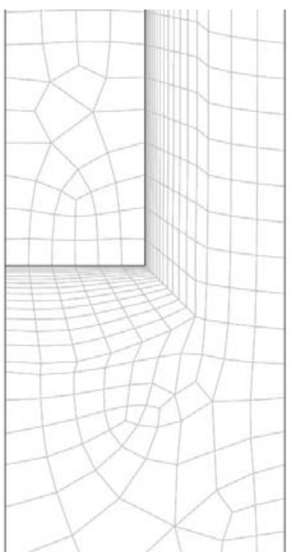

exit region is not rounded. note extra mesh density in both the entrance and exit regions is not possible for the quad meshing

quad meshing may help establish axial mesh criteria for the 3D extension

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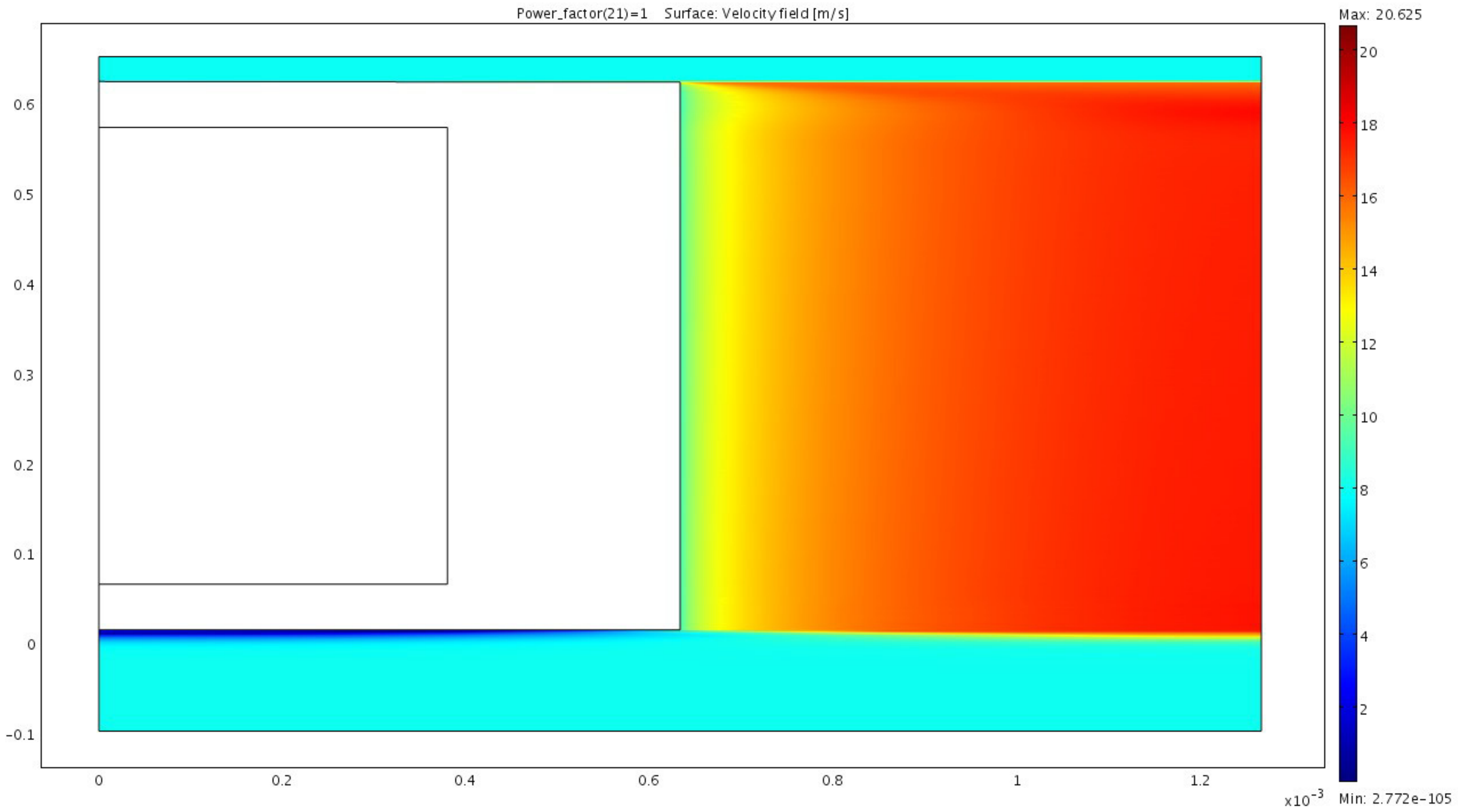
2D solutions: U_chns, linear elements, 1346998 dof



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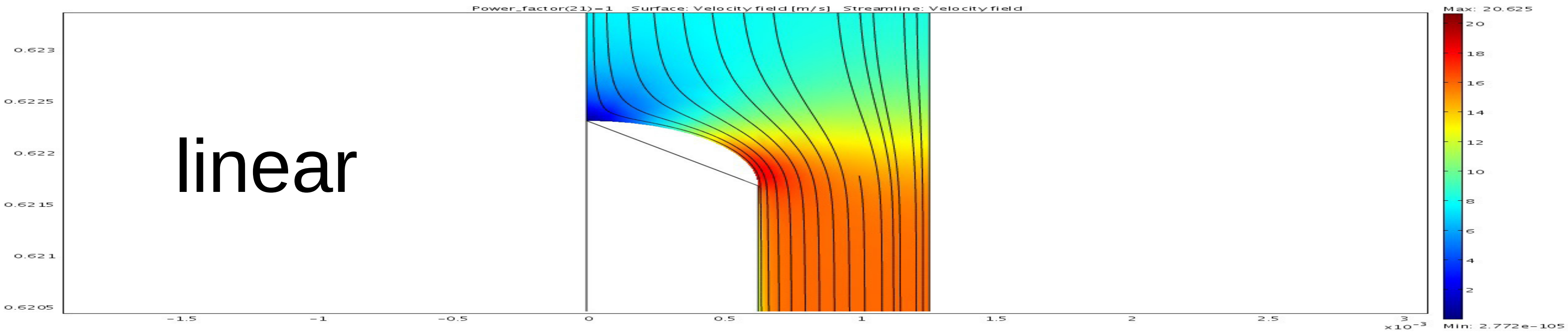
2D solutions: U_chns (velocity magnitude with streamline overlay), entrance comparison



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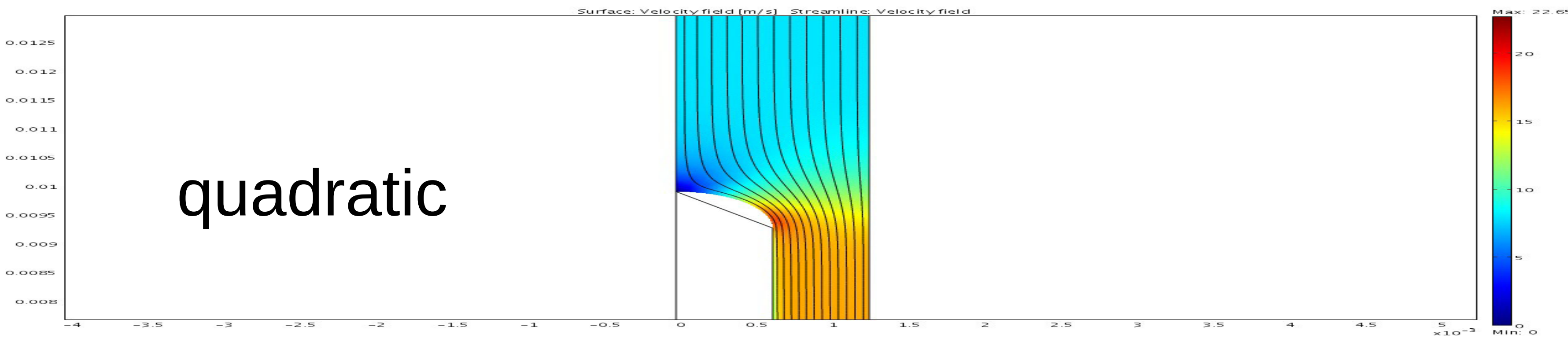
in order to minimize the dof in 3D



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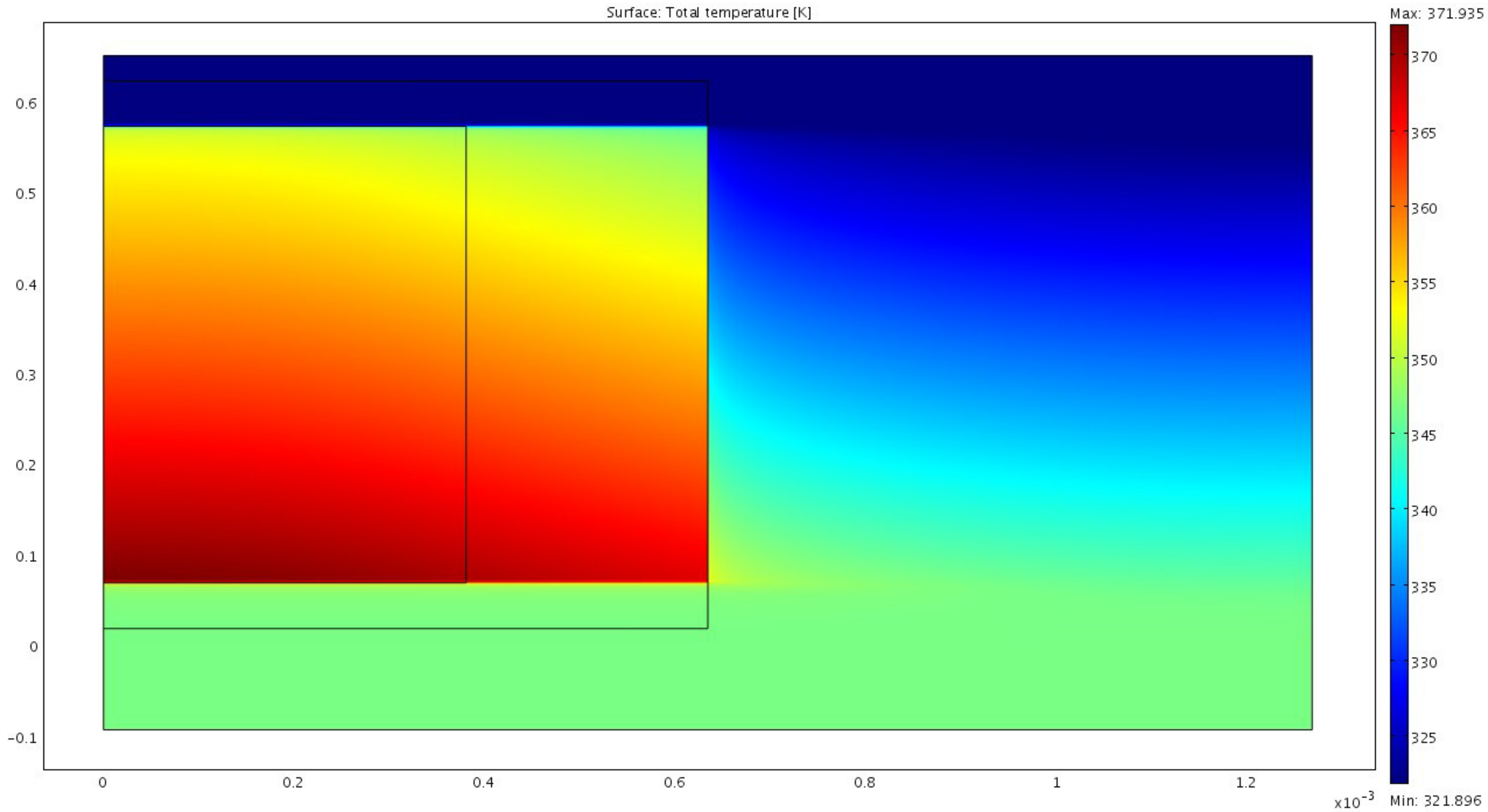
2D solutions: Ttot, quad elements, 4671216 dof



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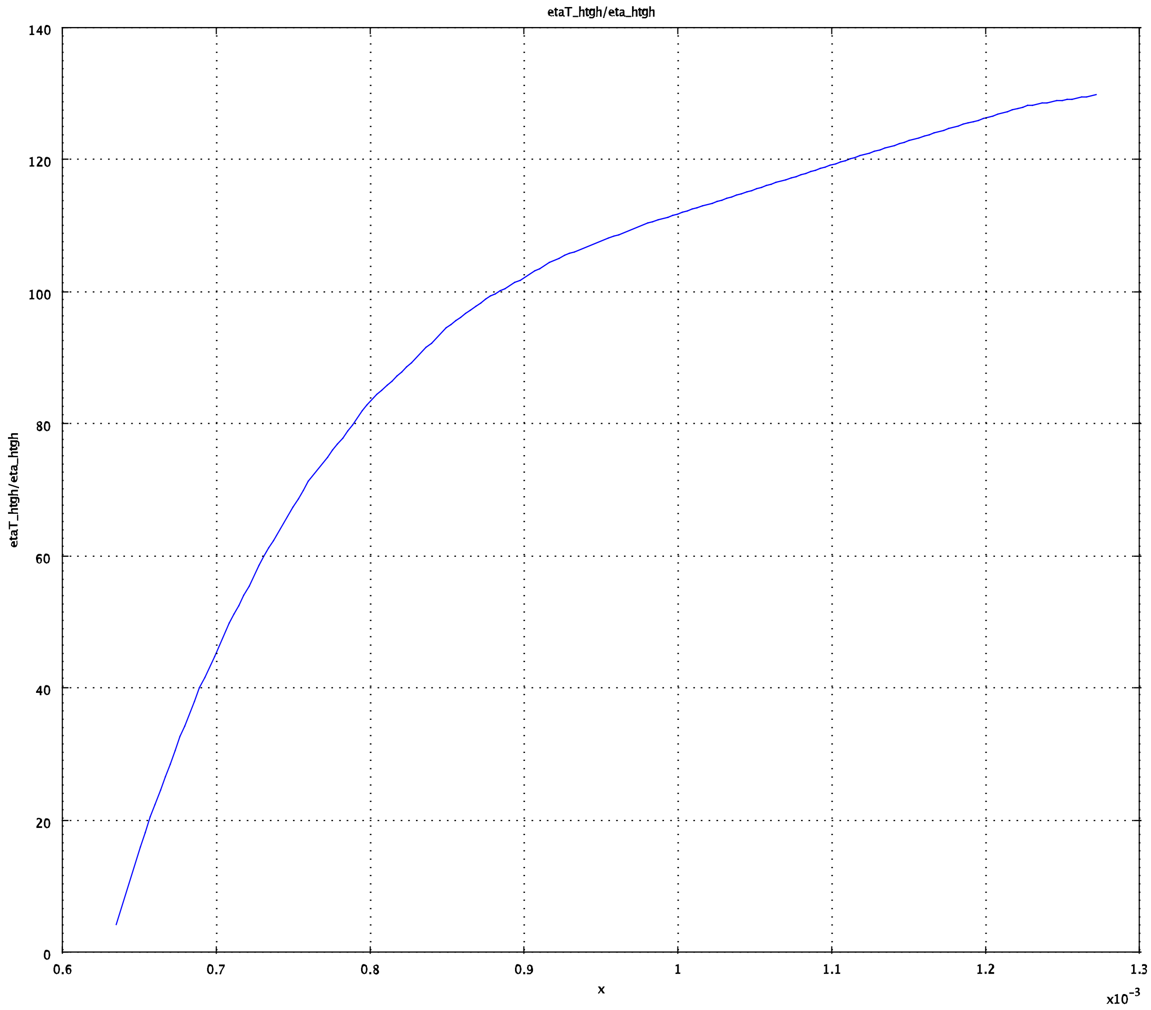
2D solution details: μ_T/μ 0.1m upstream from the exit

wall boundary



symmetry boundary

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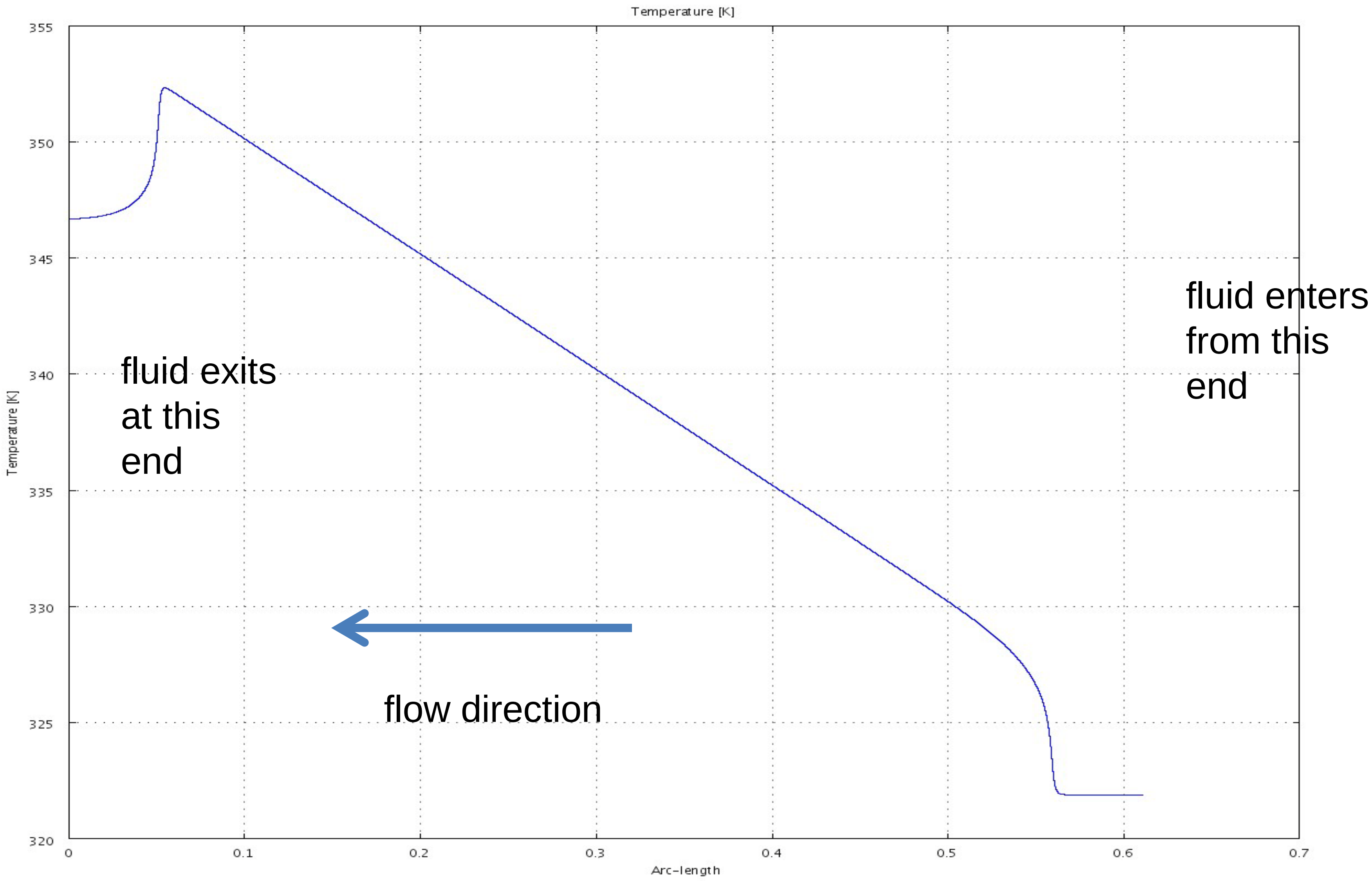
2D solution details:Tf along the wall



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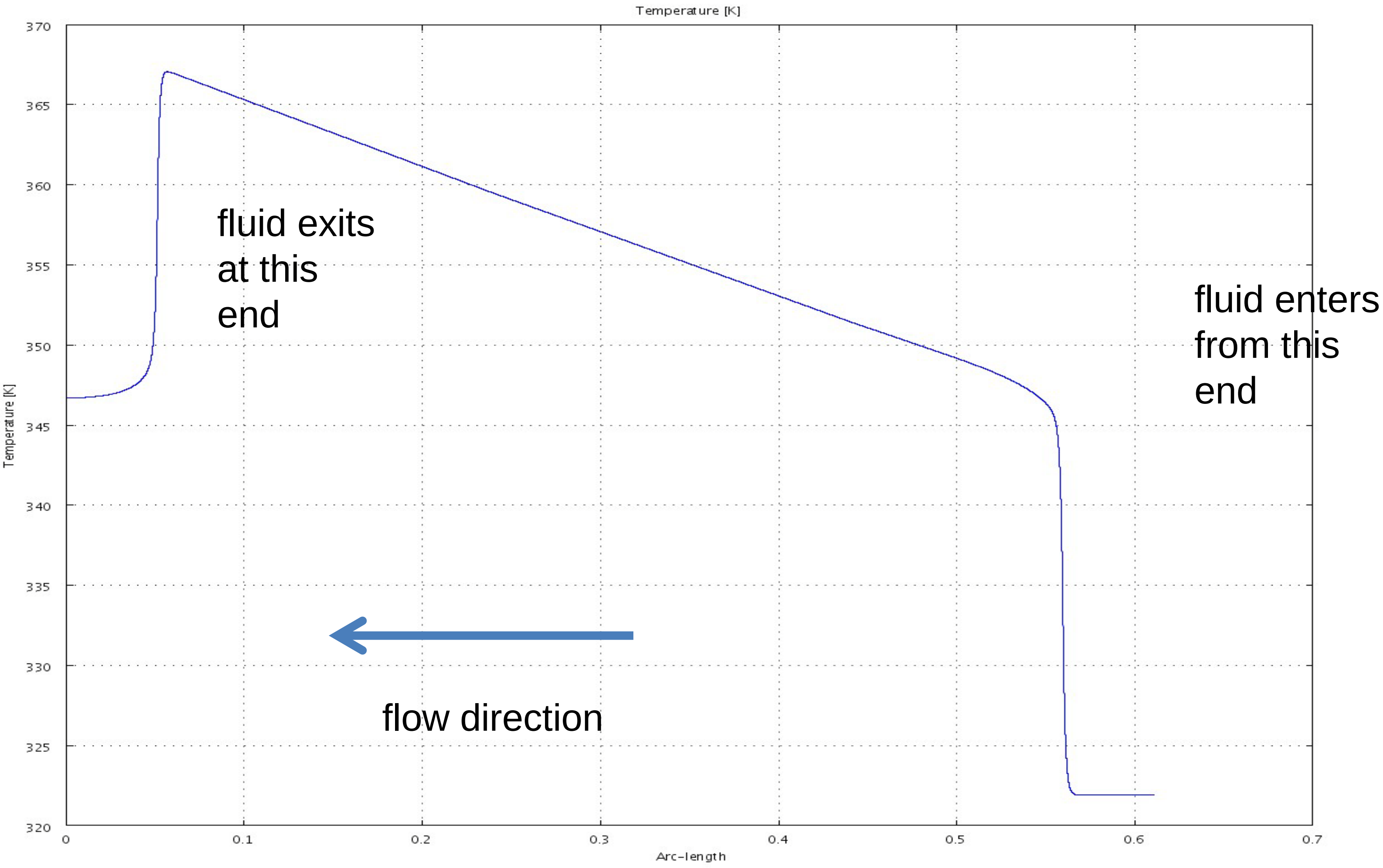
2D solution details:Ts along the wall



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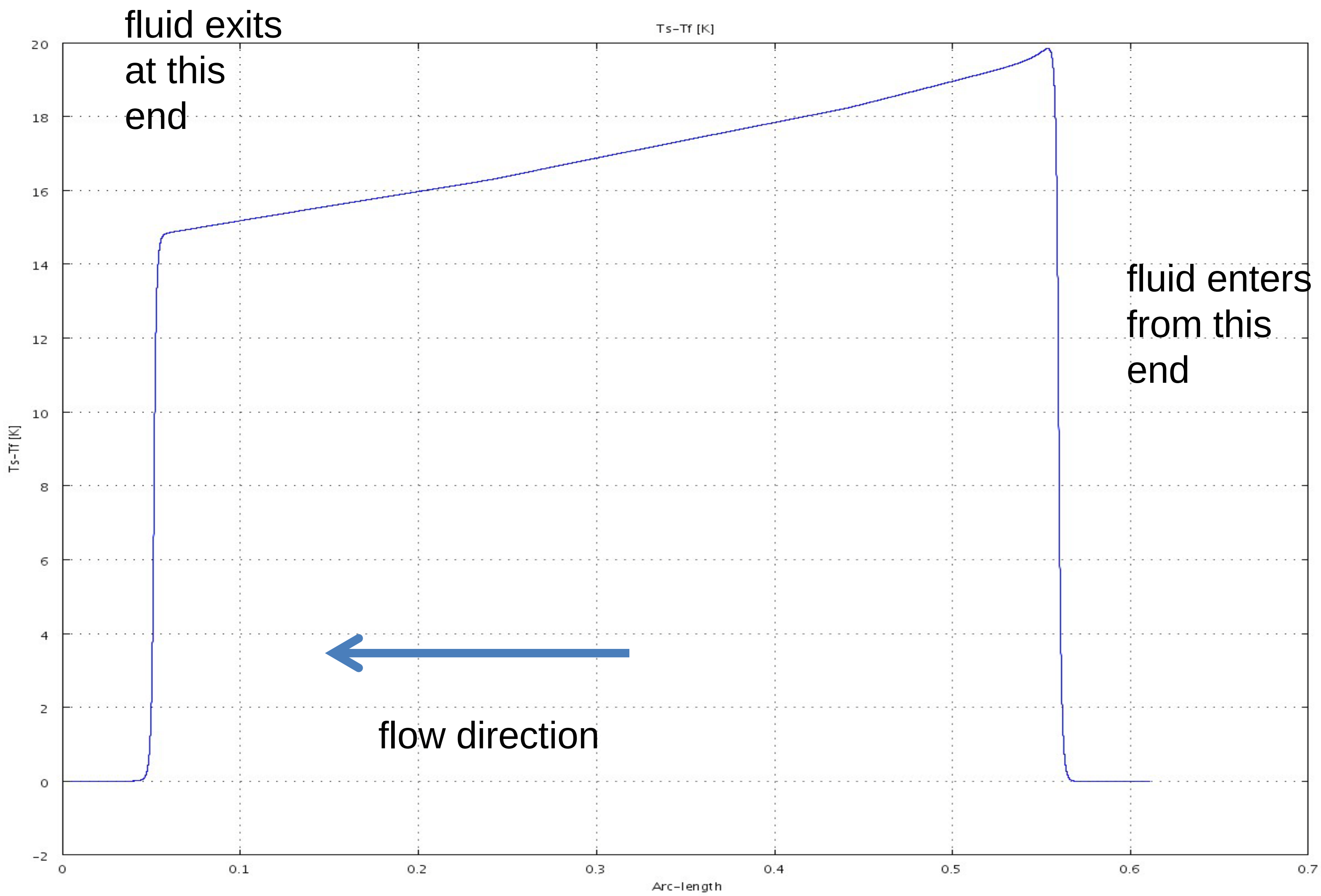
2D solution details:ΔT along the wall



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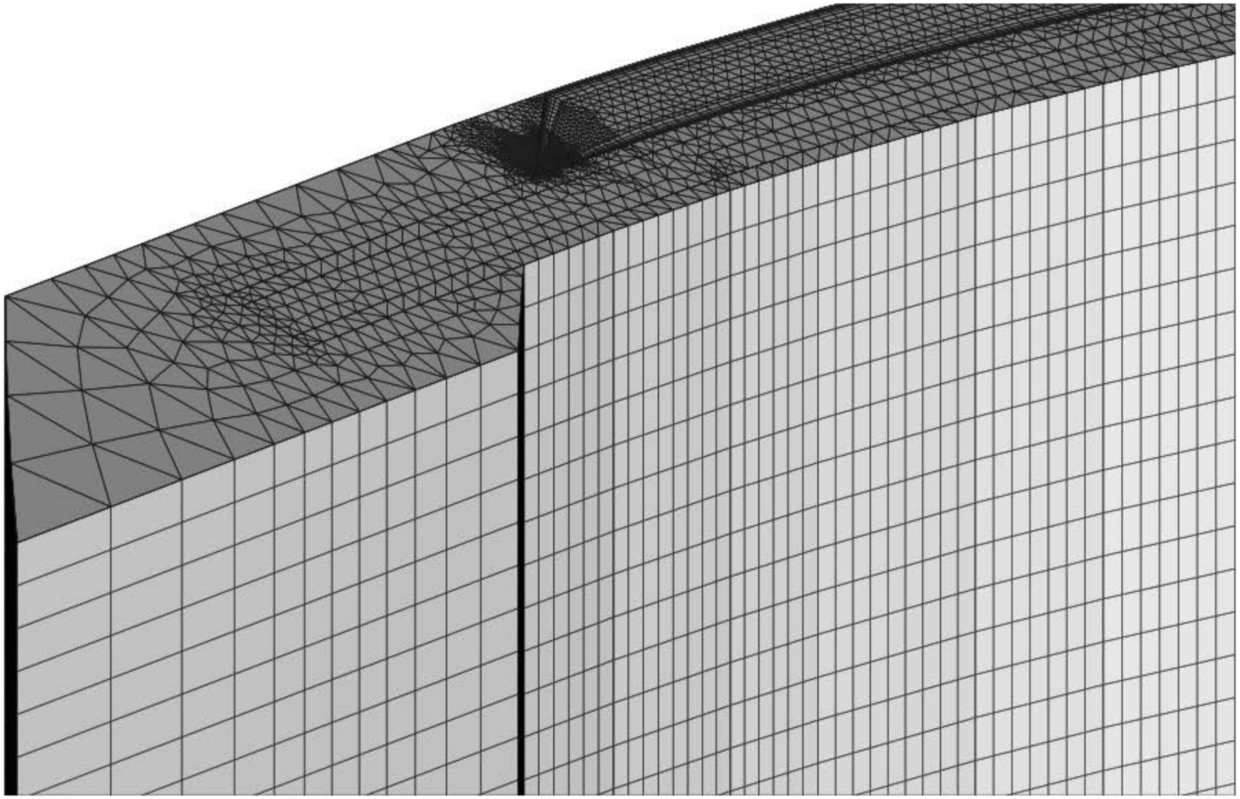
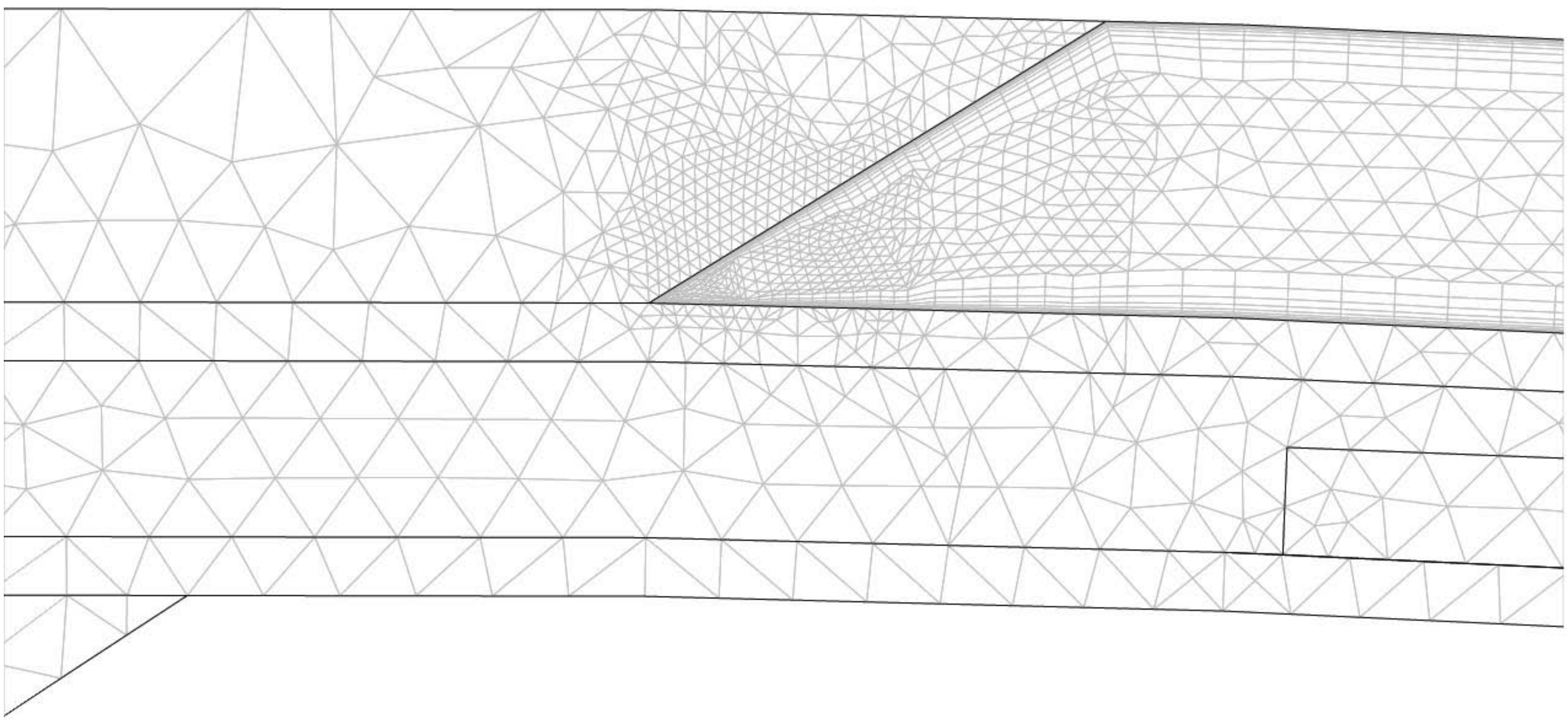
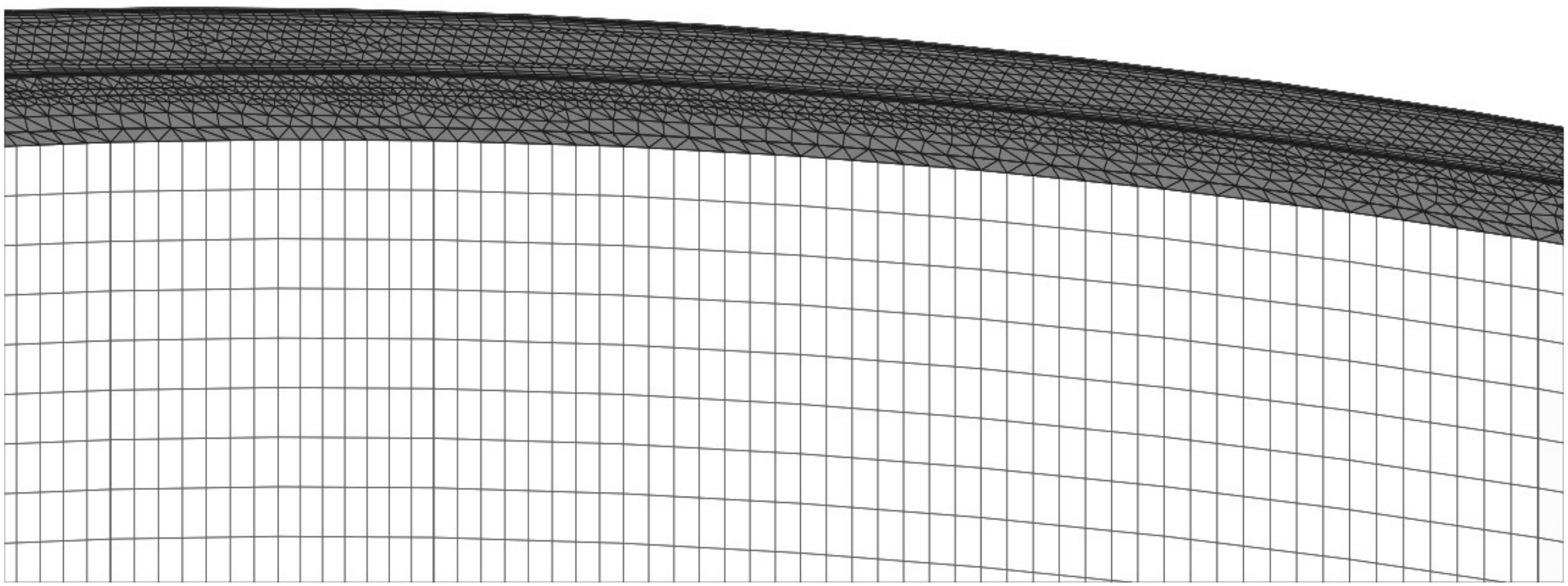
Magnified left side extruded 3D mesh



Magnified left side 2D



Magnified Middle, extruded 3D mesh



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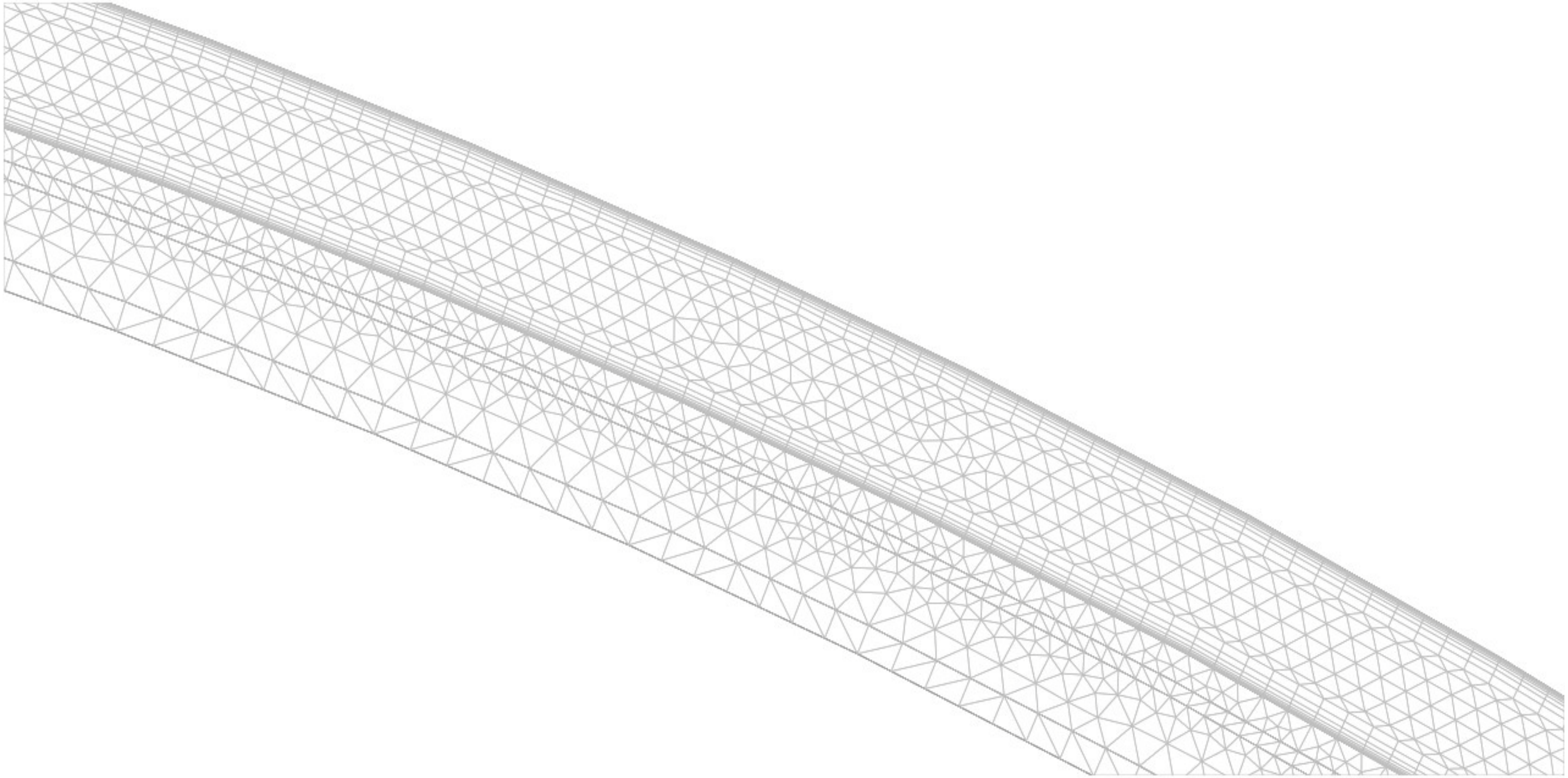
Middle, 2D mesh



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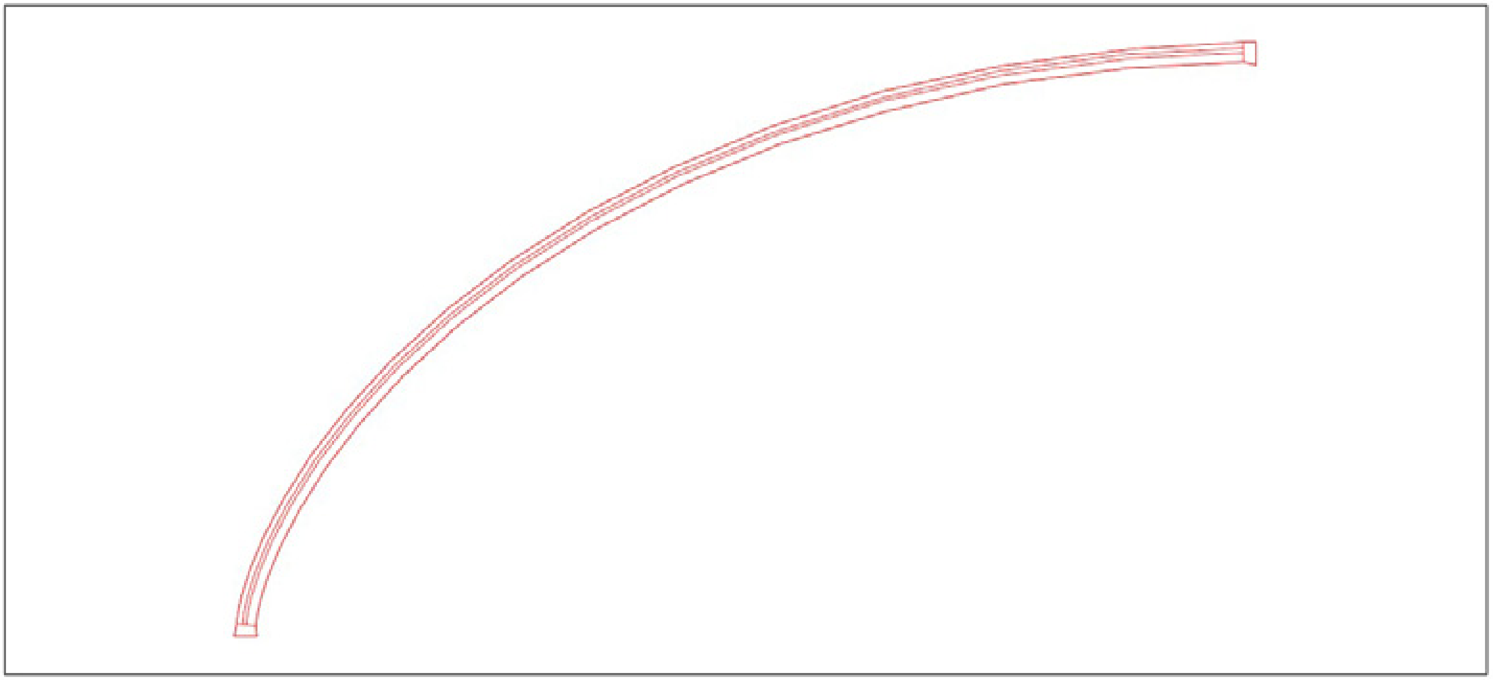
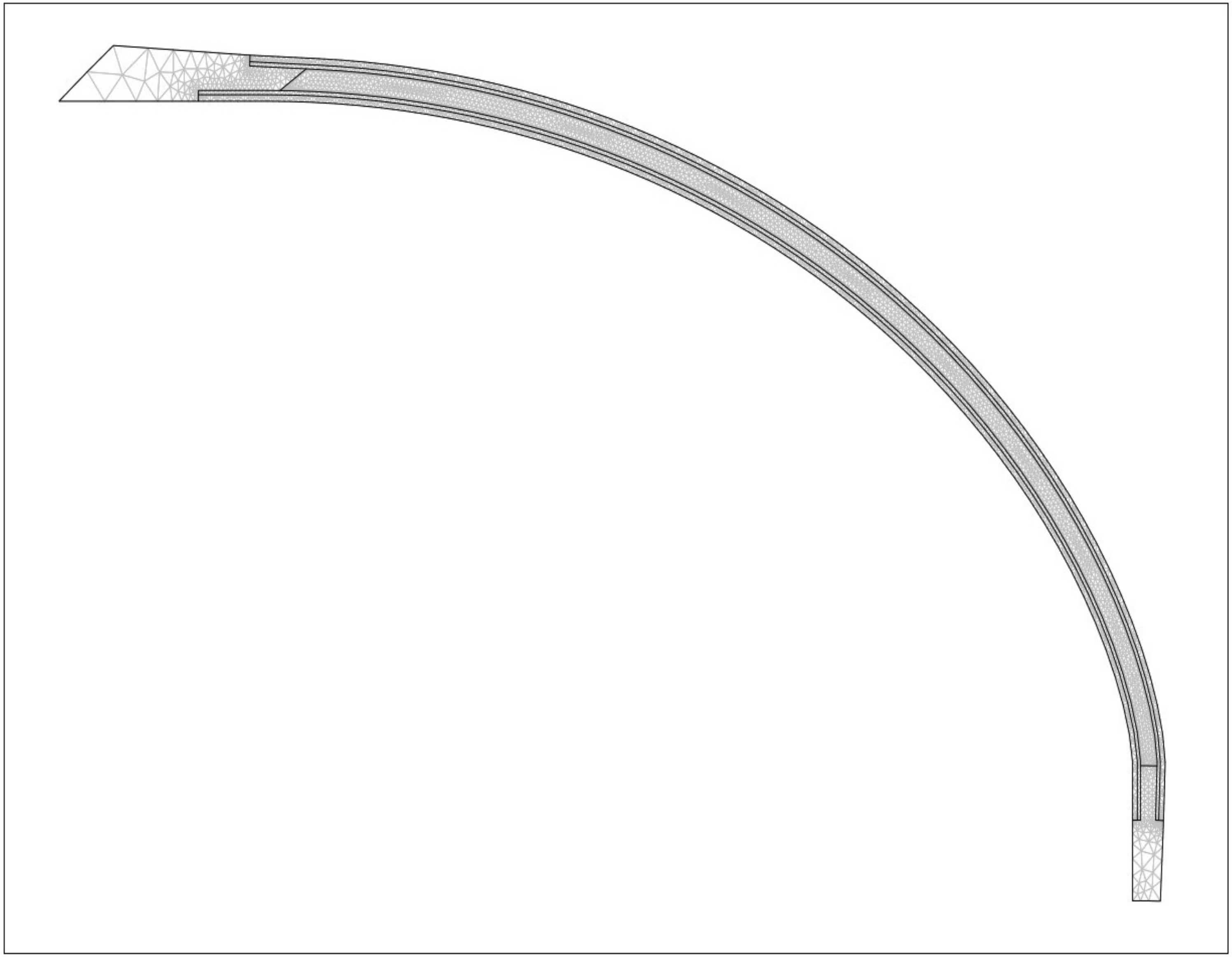
½ fuel plate, ½ coolant channel, simple side plate, uniform fuel



two ½ fuel plates, one full coolant channel, uniform fuel, representative side plates



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two ½ coolant channels, accurate side plate representation, full fuel plate including separate fuel and filler regions