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Code Verification Implications for Algebraic Equations

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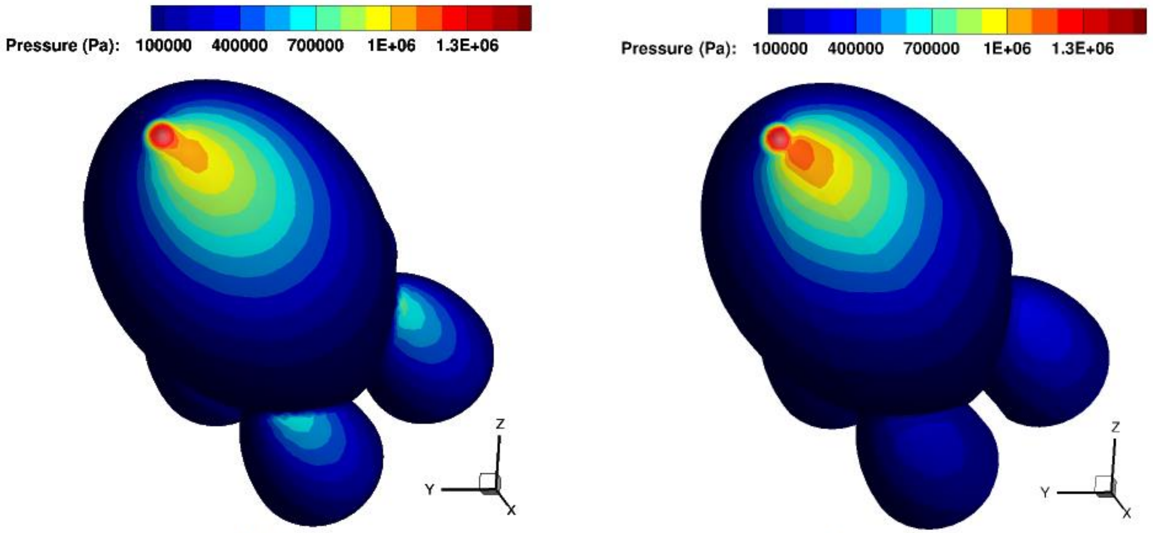
ASME VVUQ 2022 Symposium

Multifidelity background

- Algebraic models can often be found as part of multifidelity modeling
  - Uses a combination of high, medium, and low fidelity models to make predictions
  - The fidelity level refers to the relative level of physics captured by the model
  - Capturing more physics costs more computational time, so a balance must be reached
- When using multiple models, multiple code verification strategies might have to be leveraged
  - Specifically, how do we do code verification for algebraic models?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Pressure (Pa): 100000 400000 700000 1E+06 1.3E+06
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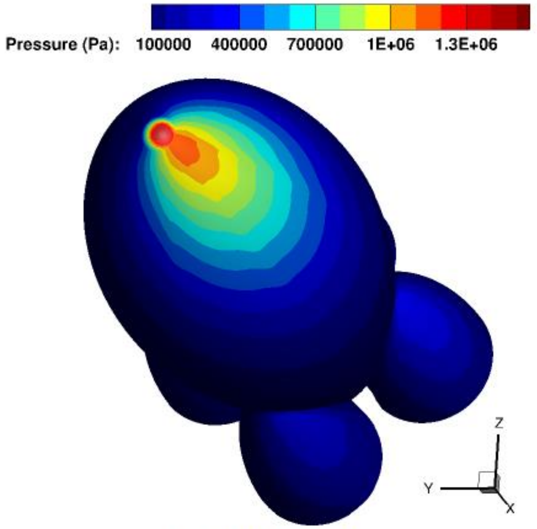
a) MNA solution

b) Euler solution



c) RANS solution

Figure 1: Example of Multifidelity Toolkit (MFTK) results for pressure[1]

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[1] Wagnild, R. M., Dinzl, D. J., Bopp, M. S., Dement, D. C., Robbins, B. A., Bruner, C.W. S., Grant, M. J., Murray, J., and Harper, J. M., "Development of a Multi-fidelity Toolkit for Rapid Aerothermal Model Development," Sandia Report SAND2019-13632, Sandia National Laboratories, Oct 2019.

What is code verification?

- According to ASME V&V 20, “ Code verification establishes that the code accurately solves the mathematical model incorporated in the code (i.e., that the code is free of mistakes for the simulations of interest)”.
- ASME V&V 20 also says “Code verification, establishing the correctness of the code itself, can only be done by systematic discretization convergence tests and monitoring the convergence of the solutions towards a known “benchmark” solution (i.e., a standard of comparison).”
- What if a computational model doesn’t have any discretization error? How do we do code verification?

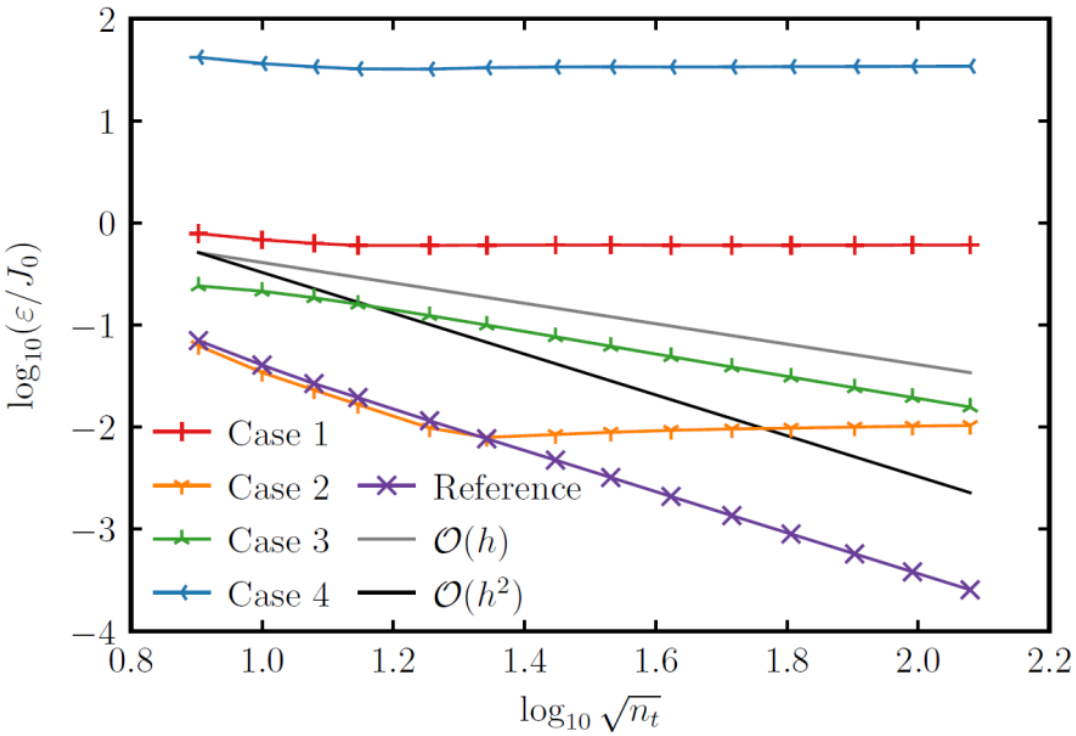

Figure 2: Convergence example with and without coding errors[2]

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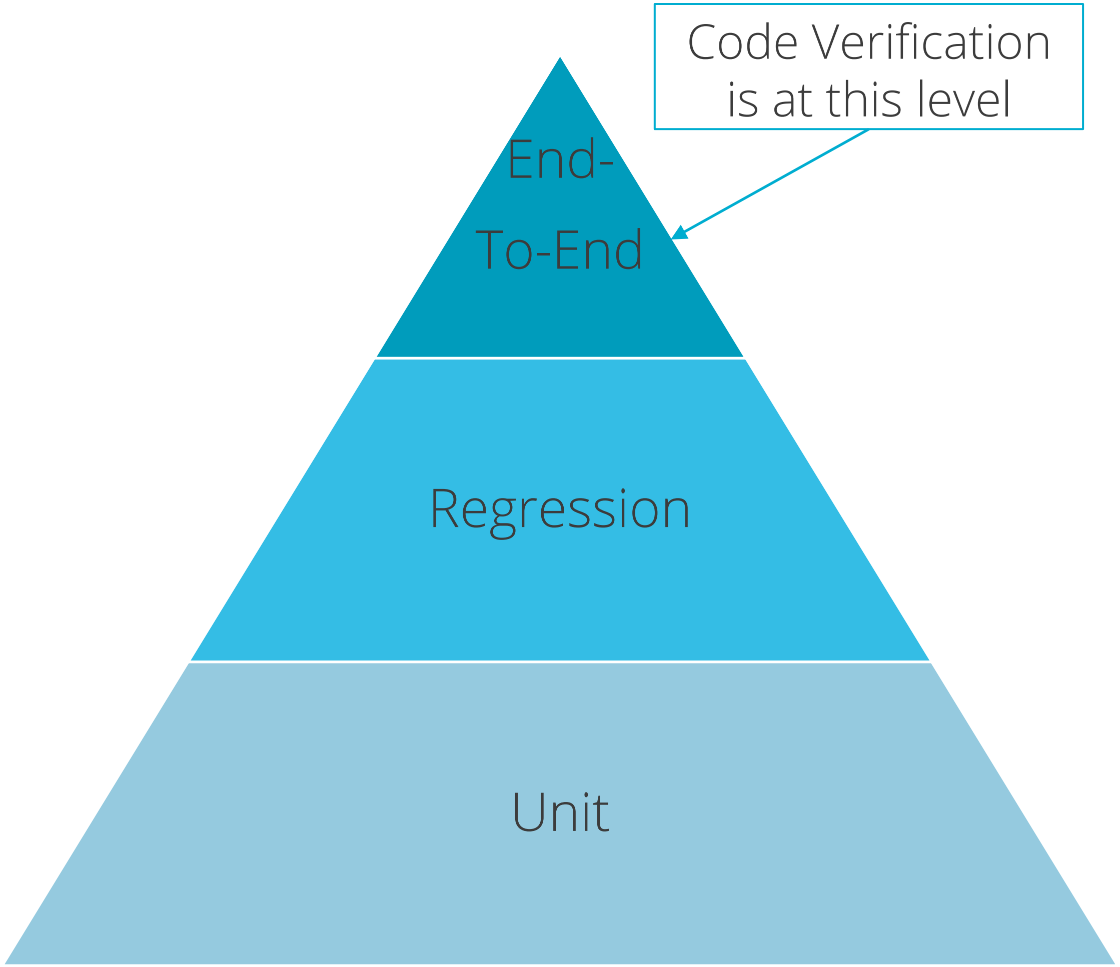
[2] Freno, Brian A., Carnes, Brian R., and Weirs, V. Gregory. “Code-verification techniques for hypersonic reacting flows in thermochemical nonequilibrium.” *Journal of Computational Physics*, Vol. 425, Jan. 2021.

What should the testing strategy be for algebraic models?

- Is it a regression test?
  - Regression testing is "Selective retesting of a system or component to verify that modifications have not caused unintended effects and that the system or component still complies with its specified requirements."[3]
  - This is typically an automated relative test that compares today's result with yesterday's result, rather than comparing with some known true solution
- Is it a unit test?
  - Unit testing is "Testing of individual hardware or software units or groups of related units." [3]
  - This is testing of individual functions rather than a large portion of the code
- We need a test that covers a large portion of the code and compares to a true solution
  - This type of testing is with the spirit of code verification, but different in which metric to measure



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[3] IEEE StD 610.12-1990, "IEEE Standard Glossary of Software Engineering Terminology

Using analytic solutions for algebraic models

- Since an analytic solution is readily available for algebraic models, comparing the code solution to the analytic solution is straight forward
  - This comparison should match exactly up to round-off precision
  - Since we are comparing the solutions directly, only one mesh is required (more refinements confirm results)
  - Unlike the method of manufactured solutions (MMS), no right hand side term is needed

- To test out this strategy, we'll apply this code verification technique to a low-fidelity model in a high-speed compressible flow code
- Testing will start simple with additional complexity added later
- Complete a validation assessment before and after code verification testing

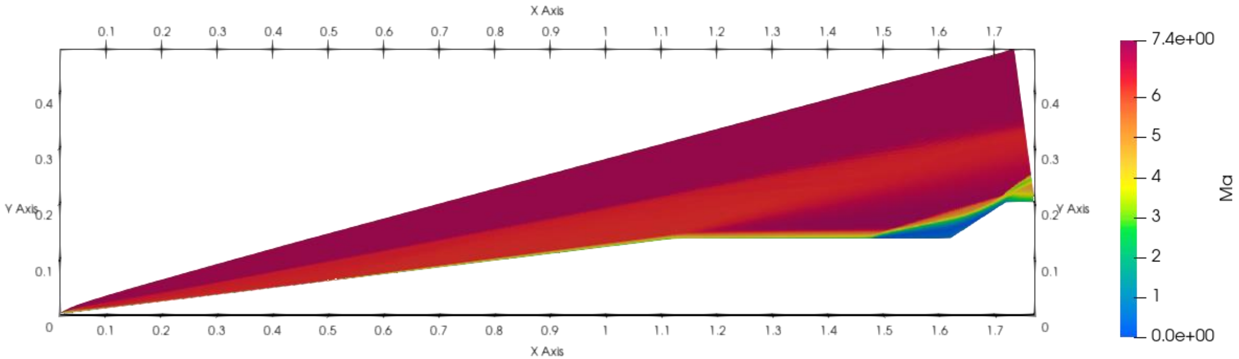

Figure 3: HIFiRE-1 wind tunnel simulation Mach number predictions for RANS-SST[4]

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[4] B. W. Lance, A. M. Krueger, B. A. Freno, R. M. Wagnild, Verification and Validation Activities for the Multi-Fidelity Toolkit, Tech. Rep. SAND2022-1479, Sandia National Laboratories, Albuquerque, NM, Feb 2022.

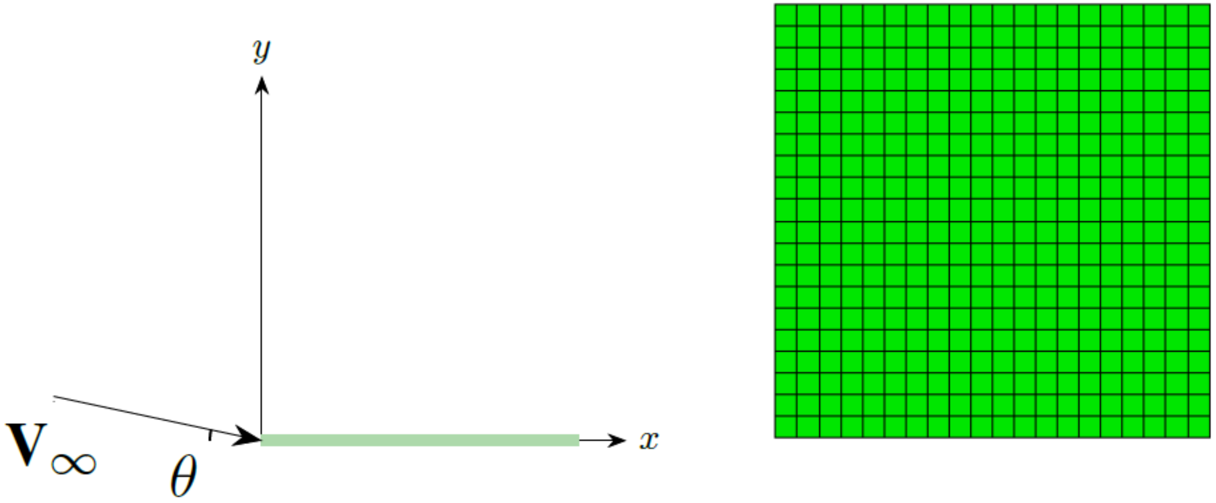
High-speed compressible flow problem set up

- Two separate problems in MFTK were analyzed
  - Flat plate
  - Inclined plate
- Only one mesh was required since discretization errors were not present
- Using analytical solutions, the maximum relative error is identified

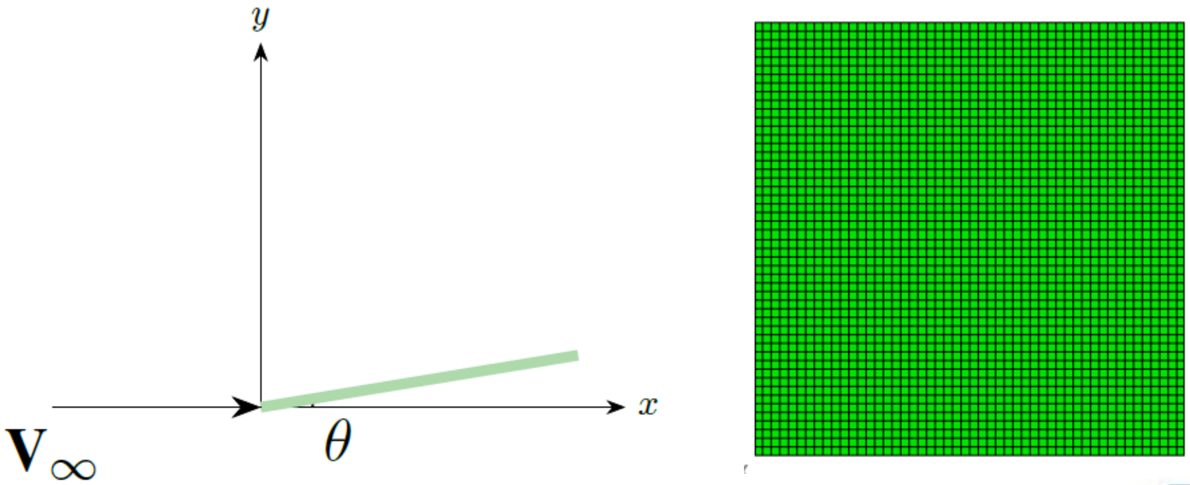
$$\varepsilon_\infty = \max_i \left| \frac{QoI_{i_{exact}} - QoI_{i_{SPARC}}}{QoI_{i_{exact}}} \right|$$

- For problems without discretization errors, ε_∞ should be on the order of round-off error (10^{-10})
- $C_p, P_e, \boldsymbol{V}_e, M_e, T_e, \rho_e, \boldsymbol{n}_v$, Dist, τ, and q_w are tested

Flat Plate Problem

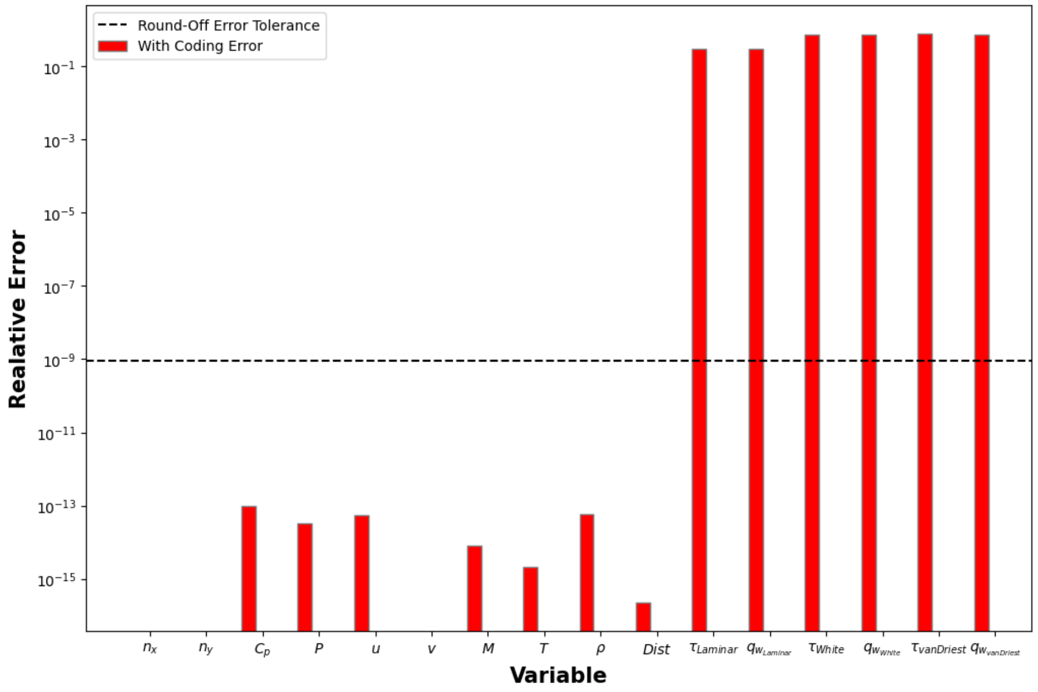


Inclined Plate Problem

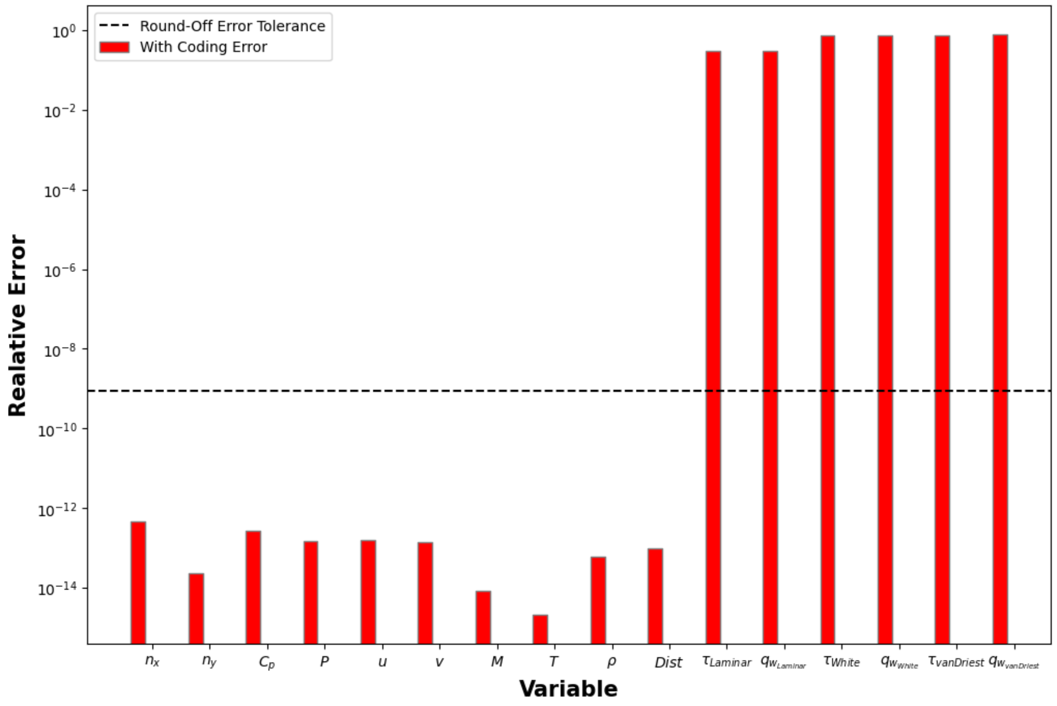


Initial code verification results

- Code verification of inviscid variables have been previously completed
- Compute ε_∞ for each QoI
  - Coding error exists if $\varepsilon_\infty > 10^{-10}$
  - Coding error does not exists if $\varepsilon_\infty < 10^{-10}$
- The shear stress and heat flux for all three viscous models have coding errors
- Debugging of these models can now start



Flat Plate Problem



Inclined Plate Problem

Code bugs found

Code Bug in Laminar Equations

- A code bug was identified in the laminar coefficient of skin friction calculation
  - Impact shear stress and heat flux
  - All other inputs into this equation were verified

$$C_f = \frac{0.664\sqrt{C^*}}{\sqrt{Re_{xe}}}$$

$$C^* = \frac{\rho^* \mu^*}{\rho_e \mu_e}$$

$$\mu^*_{bug} = C_{visc} \boldsymbol{T_w} \frac{\sqrt{\boldsymbol{T_w}}}{\boldsymbol{T_w} + S_{visc}} \qquad \mu^*_{correct} = C_{visc} \boldsymbol{T^*} \frac{\sqrt{\boldsymbol{T^*}}}{\boldsymbol{T^*} + S_{visc}}$$

Code Bug in Turbulence Equations

- A code bug was identified in the turbulent coefficient of skin friction calculation
  - Impact shear stress and heat flux
  - All other inputs into this equation were verified

$$C_f \approx \frac{0.455}{S^2 \ln^2\left(\frac{0.06}{S} Re_{xe} \frac{\mu_e}{\mu_w} \sqrt{\frac{T_e}{T_w}}\right)}$$

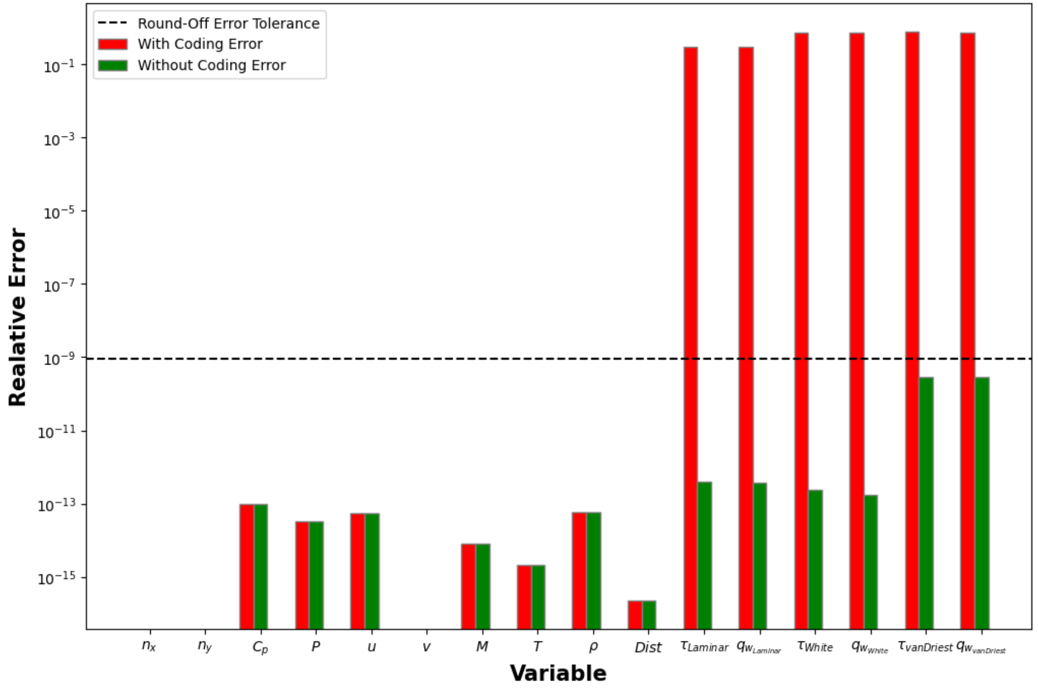
$$S_{bug} = \frac{\sqrt{\frac{T_{aw}}{\boldsymbol{T_w}}}}{\sin^{-1} A + \sin^{-1} B} \qquad S_{correct} = \frac{\sqrt{\frac{T_{aw}}{\boldsymbol{T_e}}}}{\sin^{-1} A + \sin^{-1} B}$$

$A = f(b)$ and $B = f(b)$

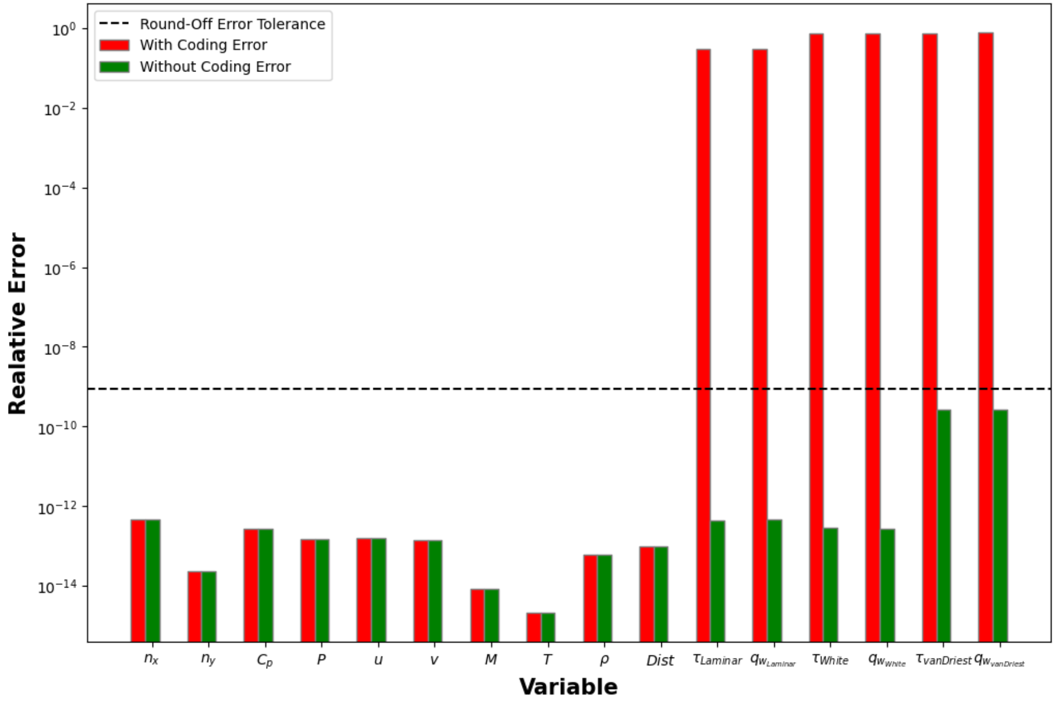
$$b_{bug} = \frac{T_{aw}}{T_w} \qquad b_{correct} = \frac{T_{aw}}{T_w} \boldsymbol{- 1}$$

Initial code verification results

- Once the coding errors were fixed, the simulations were reran
- Computed ε_∞ for each QoI
  - Coding error exists if $\varepsilon_\infty > 10^{-10}$
  - Coding error does not exists if $\varepsilon_\infty < 10^{-10}$
- Since all variables have $\varepsilon_\infty < 10^{-10}$, no coding errors exist
- Code verification activities can continue for more complex scenarios



Flat Plate Problem



Inclined Plate Problem

Measuring the impact

- Now that the model is bug free, let's measure the impact on a validation study
- Using the HIFiRE-1 wind tunnel test data, we are able to see the impact of these coding errors on assessing model form error
- This process also highlights the importance of completing code verification before a validation study
- Both a laminar case and a turbulent case results are shown

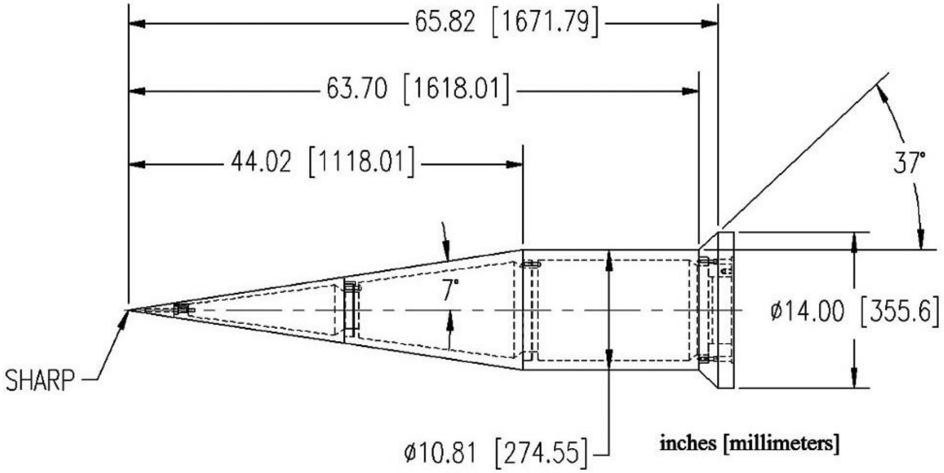
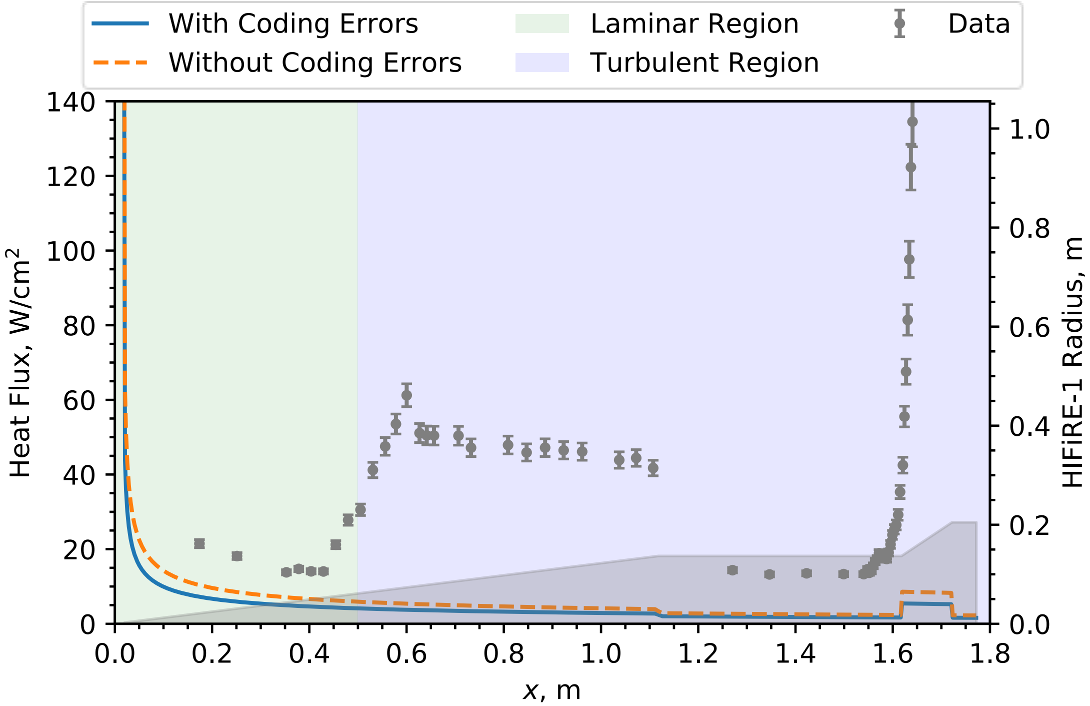


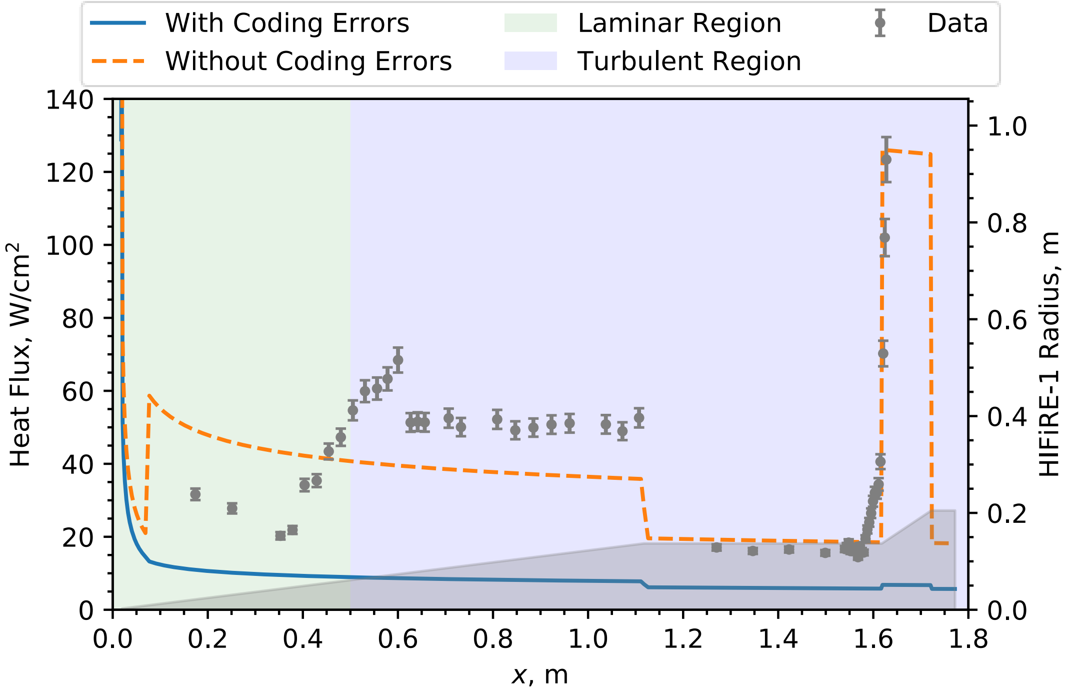
Figure 3: The HIFiRE-1 wind tunnel test geometry that shows the fore-cone on the left, the cylindrical section in the center, and the flare on the right; from Wadhams 2008. The text states that the final nosetip was changed from sharp to a radius of 2.5 mm and the flare angle was changed from 37˚ to 33 ˚.

Impact on results

- For the laminar case, small differences are seen along the streamline direction
- This would have a small impact on validation

- For the turbulent case, large differences are seen along the streamline direction, especially at the tail
- This would have a large impact on validation



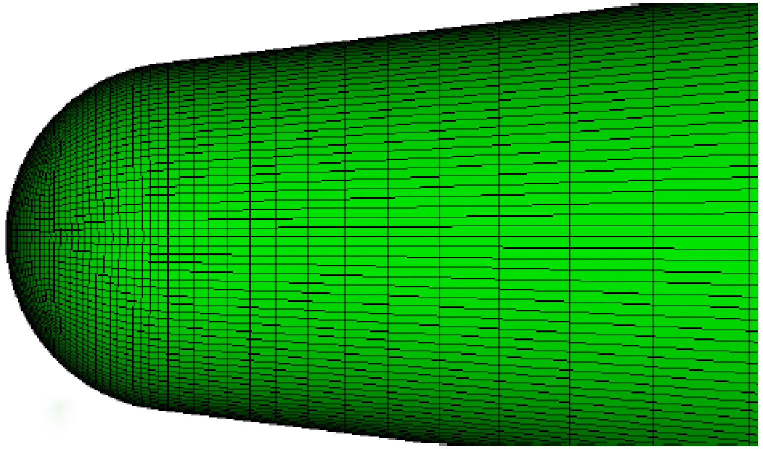


Simulation results generated by
Jared Kirsch of Sandia National Labs

Algebraic models with discretization errors

- For certain problems, numerical errors can be present
  - Geometric discretization
  - Only part of the model is algebraic
  - Iterative errors can still be present
- Break problem up into purely algebraic and discrete if possible
- Initial testing should match analytic solution to round-off for algebraic portion
- Order-of-accuracy testing should cover portions of the code that were not testing in previous testing

- Cone problem introduces geometric discretization
- Additionally, the streamline (Dist) calculation introduces discretization error



Curved Mesh

Conclusions

- We applied code verification methods in a slightly different way
- We apply this methodology to a high-speed compressible flow code
- Three coding errors were identified in the calculation of the coefficient of skin friction
- We showed the impact of the code bug on the HIFiRE-1 wind tunnel test problem
  - This highlights the impact on a validation assessment
- Future work is to continue code verification on the cone problem, which will use order-of-accuracy testing
- When selecting problems, it is valuable to isolate specific errors
  - Start simple and evolve tests to include more possible sources of errors
- Acknowledge that the “verification infrastructure” can be causing issues
  - Add unit testing to cover calculating the analytic solution