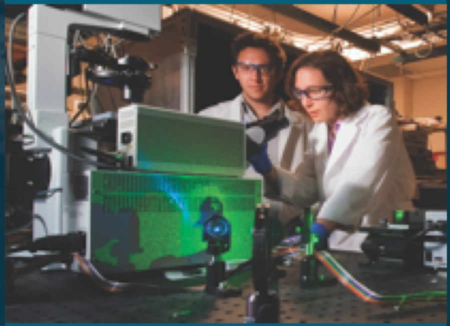
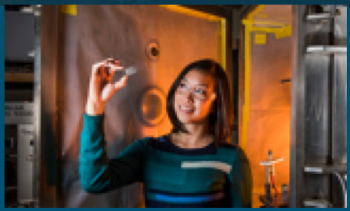
Guest Lecture Stanford ME469: A Validation Methodology: Code and Solution Verification





PRESENTED BY

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Computational Thermal and Fluid Mechanics

Sandia National Laboratories SAND2018-4536 PE

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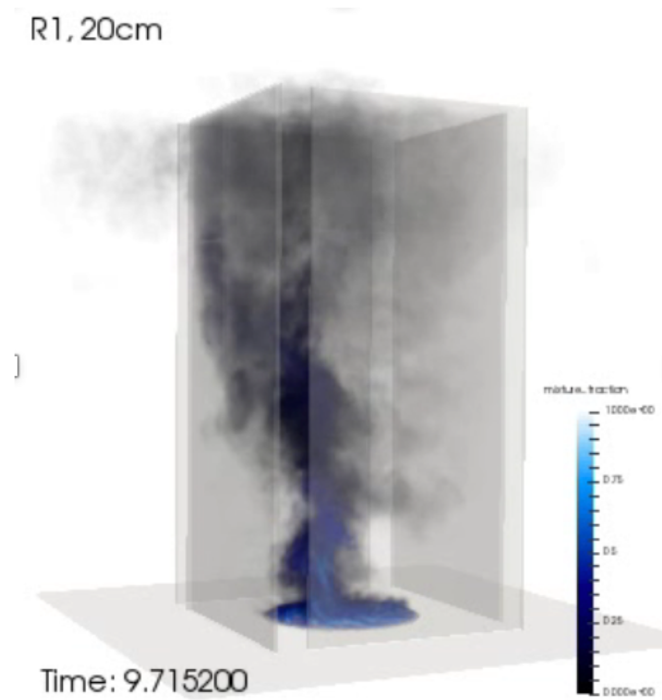
A Validation Methodology: Code and Solution Verification: Outline

- Elements of a Poor-Quality Validation Study
- Overview of a Phenomena Identification Ranking Table (PIRT)
- Overview of Code Verification, including the Method of Manufactured Solutions (MMS)
- Solution Verification
- Structural Uncertainty
- Conclusions

Objective: Deploy a High-Fidelity Tool to Predict a Fire

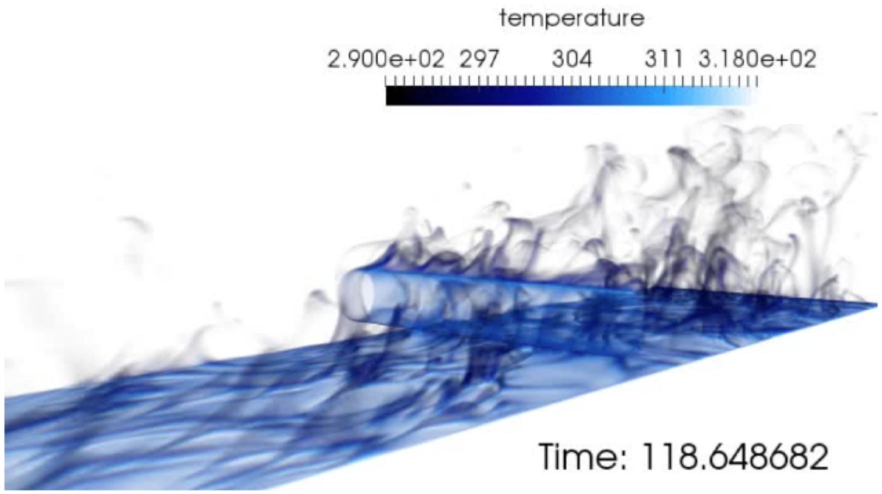
- Consider that we want to develop and deploy a foundational understanding in fire physics and deploy a simulation tool to support production analysis
- Consider the fire-environment with elements of the following physics:
  - Chemical reactions, soot, buoyancy, turbulent fluid mechanics, thermal radiation heat transfer, convective heat transfer, object heat-up/response, and sometimes propellants



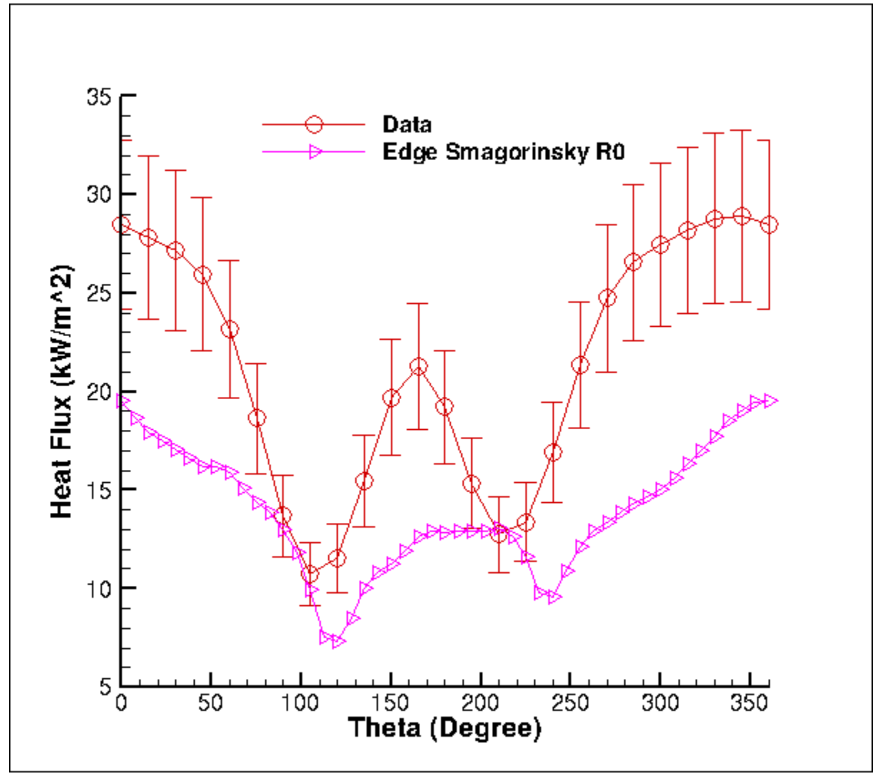
Volume rendered mixture fraction

Conceptual Challenge: Distinguishing Between Model-form Error, Discretization Error, and Code Error

- One mesh, one model, no code pedigree…



Heat flux to the cylinder
Volume-rendered temperature



Time-averaged heat flux to cylinder

- What credible scientific hypothesis can be tested in this context?
- Was a Phenomalogical Identification and Ranking Table (PIRT) was conducted:
  - Process that defines 1) what you know, 2) what you think you know, and 3) what "you know not of"

Step 1: Phenomena Identification and Ranking Table (PIRT)

- Objective: Define a process that defines 1) what you know, 2) what you think you know, and 3) what "you know not of"
- Once a particular use-case is understood and a PIRT is complete, one can proceed down the path of simply closing the gaps in the modeling, code implementation, and model validation process
- Focus on one such element of convective heat transfer:

	Import	Adequacy			
	Phen	Mod	Code	Val	Mats
Convective Processes					
Convective heat transfer	M	M	L	L	

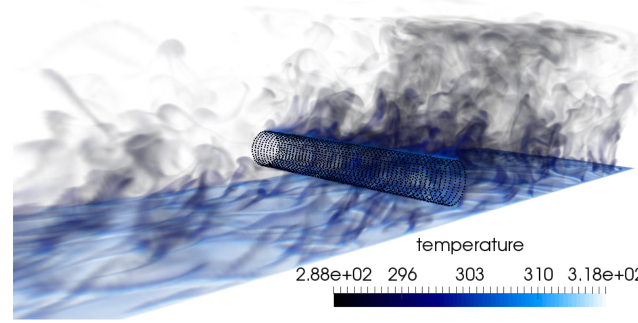
- We think we have a good understanding of the modeling requirements

- and the code seems to have the models that we want – given our current understanding

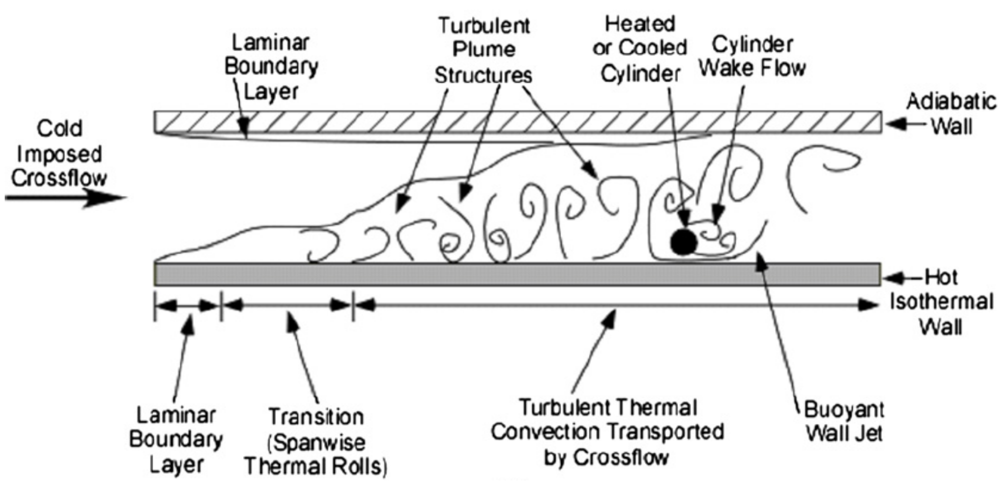
- However, high-quality validation experimental data is missing
- Investment: Experimental campaign for mixed-convective heat transfer

Turbulence Modeling in the Presence of Mixed Convection

- Model Configuration: SNL-based Sean Kearney Experiment, "Experimental investigation of a cylinder in turbulent convection with an imposed shear flow", *AIAA*, 2005
- Present day RANS Conclusion: The presence of the heated bottom wall significantly challenged ability to predict the QoI (normal heat flux to cylinder)



Domino et al., *CTRSP*, 2016



Kearney experimental configuration

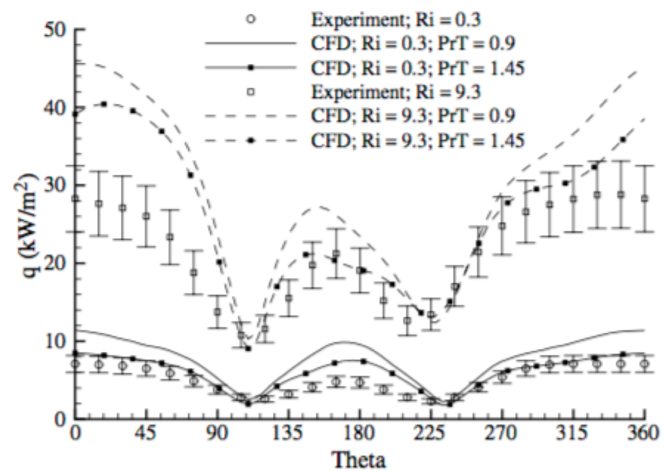


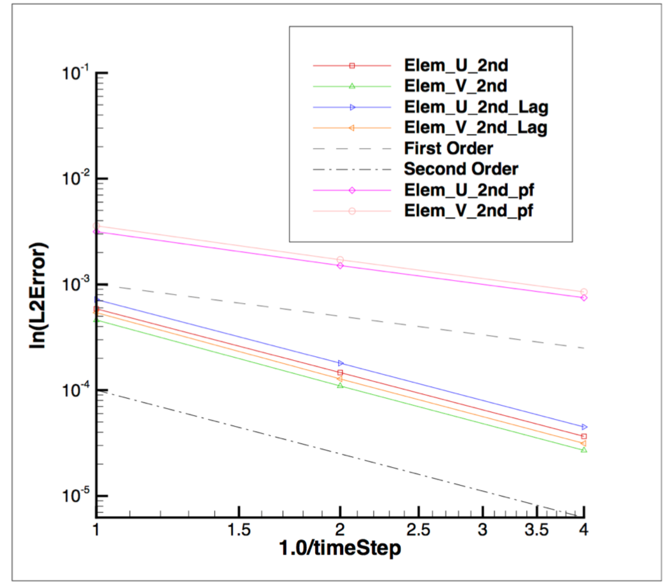
Fig. 13. Effect of turbulent Prandtl number on cylinder heat flux predictions for cases 3 (cooled cylinder) and 4 (heated cylinder).

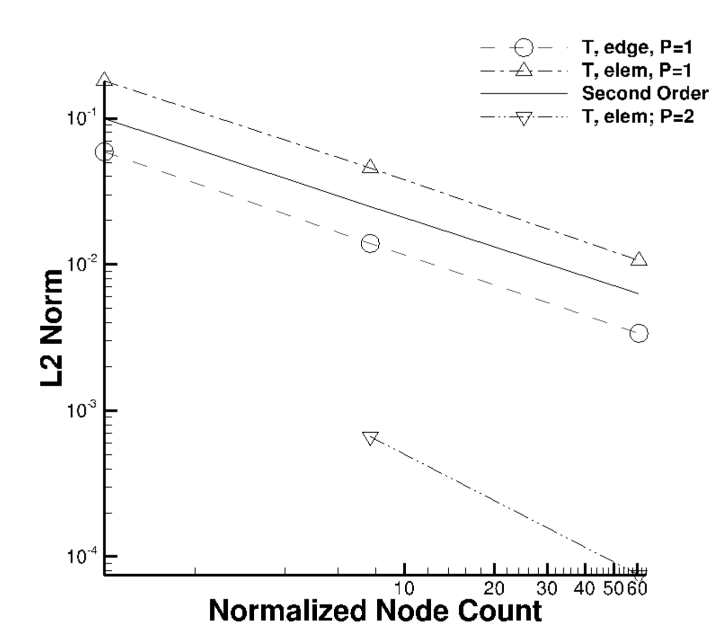
Laskowski et al., *AIAA*, 2007

RANS-based simulation (v2-f, k-e) study conducted by Laskowski et al., *AIAA*, 2007

Essentials of Code Verification

- Taxonomy: One *verifies* code and *validates* models
- Code verification establishes the numerical accuracy of the underlying discretization for the given partial differential equation set
- Code verification seeks to provide the temporal and spatial accuracy of the underlying discretization approach
- For temporal discretization error,
  - a two-state Backward Euler time integrator should be first-order in time, specifically the error should scale with Δt
  - a three-state BDF2 time integrator should scale with Δt^2
  - a multi-stake Runga-Kutta schemes can achieve higher-order accuracy
- For spatial discretization error, a method is design-order if the observed order of accuracy is Δx^{P+1}, where P is the underlying polynomial order for interpolation





Introduction to the Method of Manufactured Solutions (MMS)

Providing confidence that the code implementation converges to the proper solution

- For complex low-Mach fluid flow applications, there are very few analytical solutions
- Consider an approach whereby the solution is manufactured (Roache, et al, 1990)
- Simple thermal heat conduction PDE:

$$\rho C_p \frac{\partial T}{\partial t} - \frac{\partial}{\partial x_j} \lambda \frac{\partial T}{\partial x_j} = 0$$

- with manufactured analytical form for T:

$$T^{MMS} = \frac{1}{4}[\cos(2\alpha\pi x) + cos(2\alpha\pi y) + \cos(2\alpha\pi z)]$$

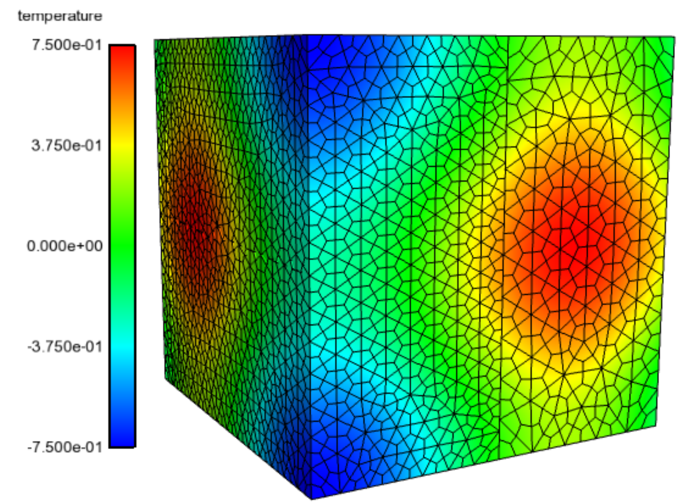
- Placing this MMS back into model PDE:

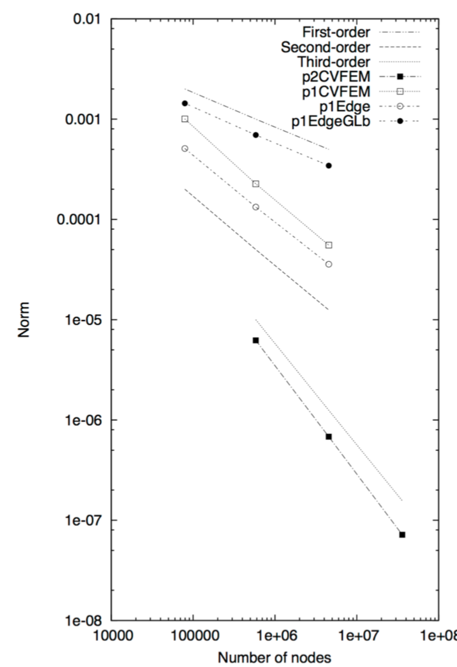
$$\rho C_p \frac{\partial T^{MMS}}{\partial t} - \frac{\partial}{\partial x_j} \lambda \frac{\partial T^{MMS}}{\partial x_j} = S^{MMS}$$

provides the source term:

$$S^{MMS} = \frac{\lambda}{4}(2\alpha\pi)^2[cos(2\alpha\pi x)+cos(2\alpha\pi y)+cos(2\alpha\pi z)]$$

with error now provided by: $T^E = T - T^{MMS}$

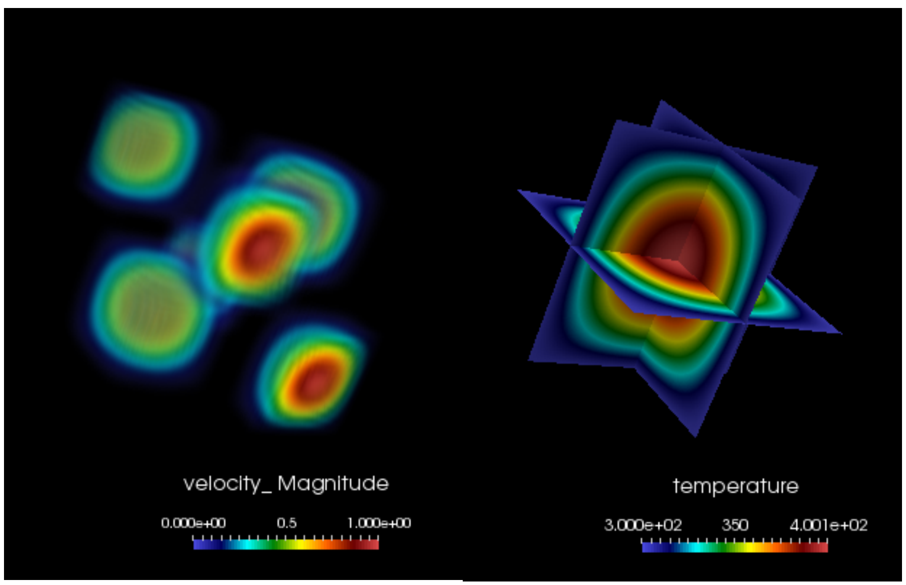




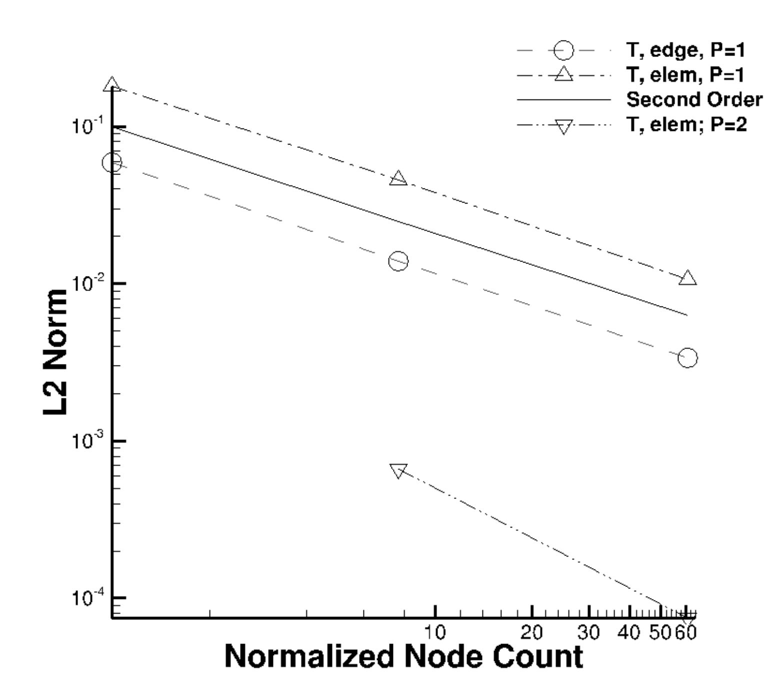
Spatial Code Verification for a low-Mach, Variable-Density Flow

	Import	Adequacy			
	Phen	Mod	Code	Val	Mats
Convective Processes					
Convective heat transfer	M	M	L	L	

- Density is a function of static enthalpy transport via the standard ideal gas, $\rho = f(P,M,R,T)$
- Temperature range maps to experiment
- Arbitrary buoyancy source term via rotated gravity vector
- Collective study now provides confidence in the interplay between numerical and modeling accuracy



Velocity Mag Temperature



See, "Exploring model-form uncertainties in large-eddy simulations", Domino et al, 2016

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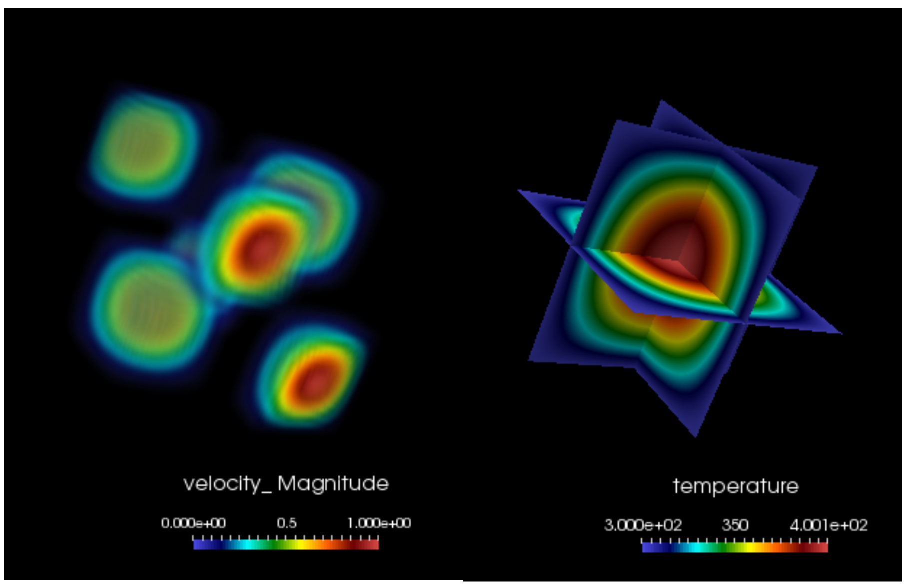

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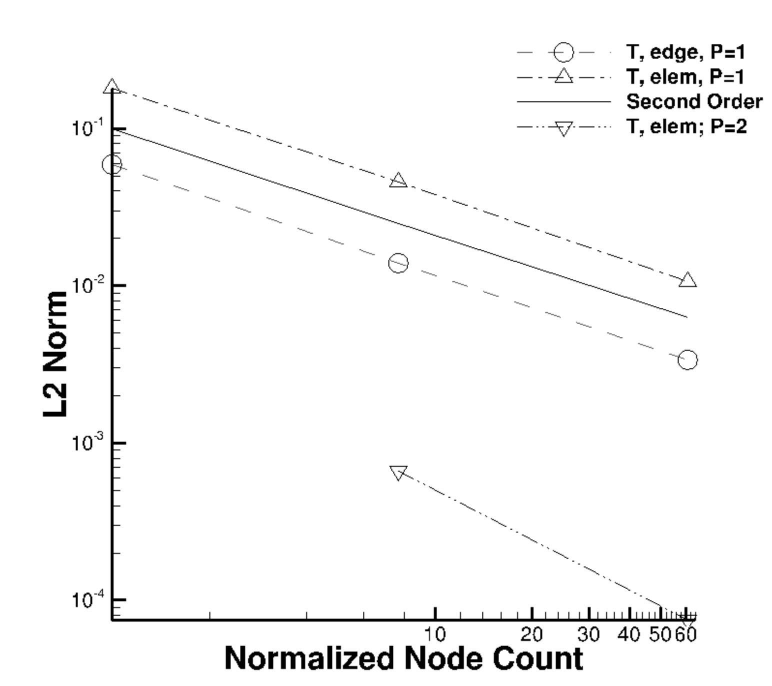

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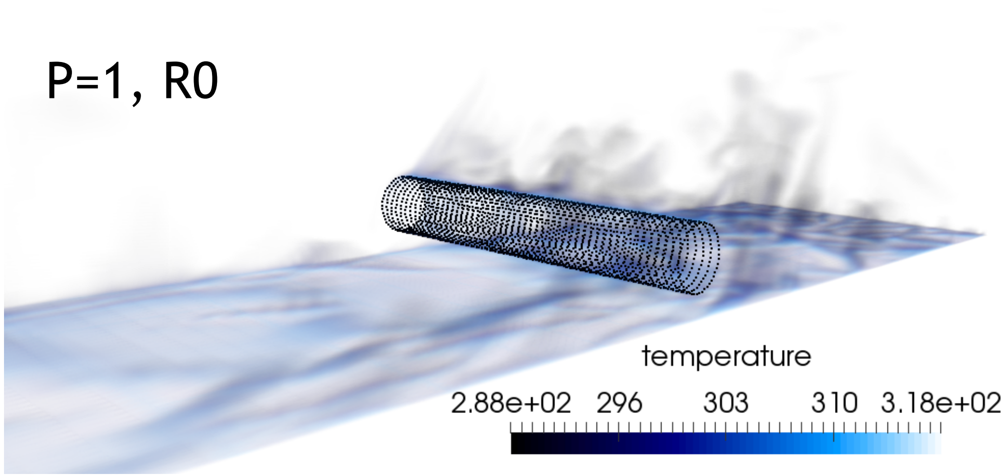
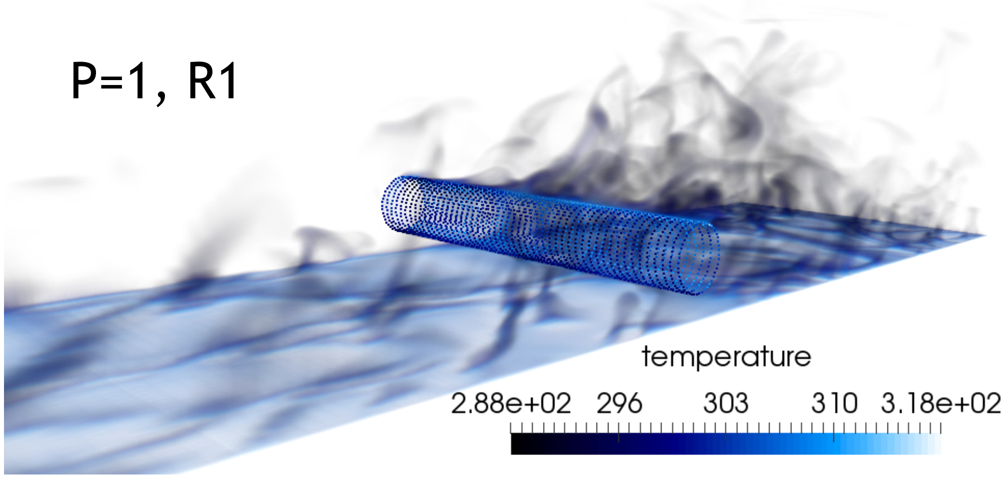
The Effect of Polynomial (P) and Mesh Spacing (H) Refinement

- For the heated cylinder-in-cross flow, either mesh resolution or polynomial promotion provides a more accurate result with more turbulence structure

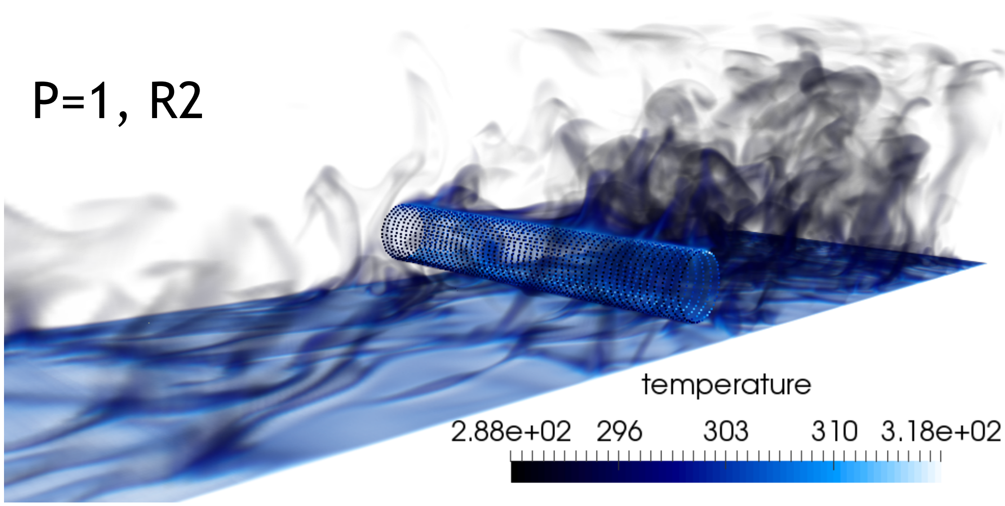
P=1, R0



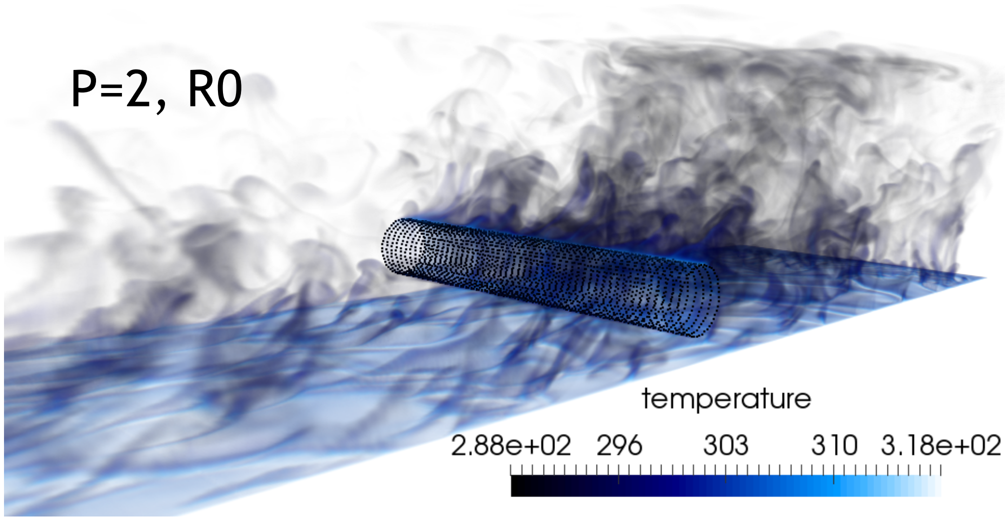
P=1, R1



P=1, R2



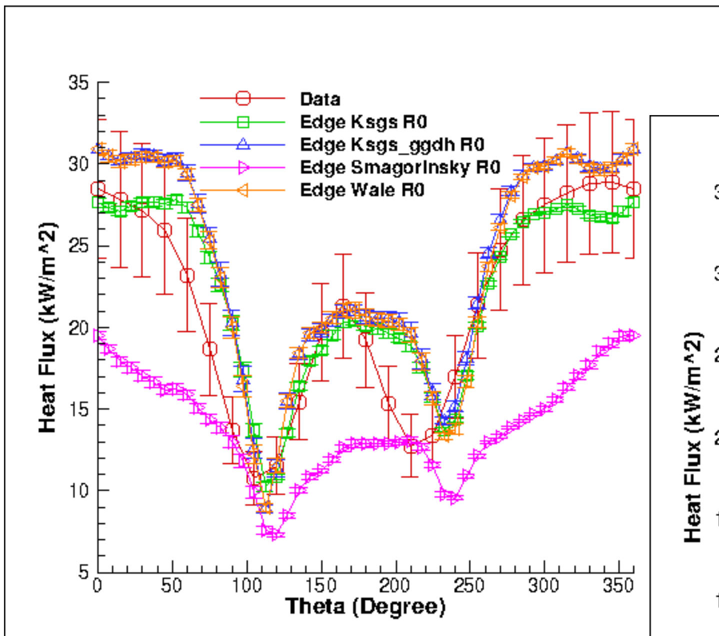
P=2, R0

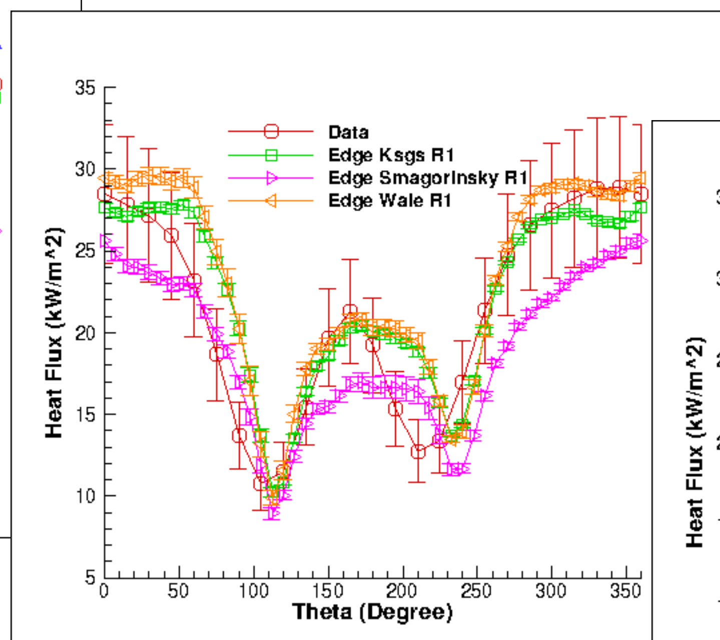


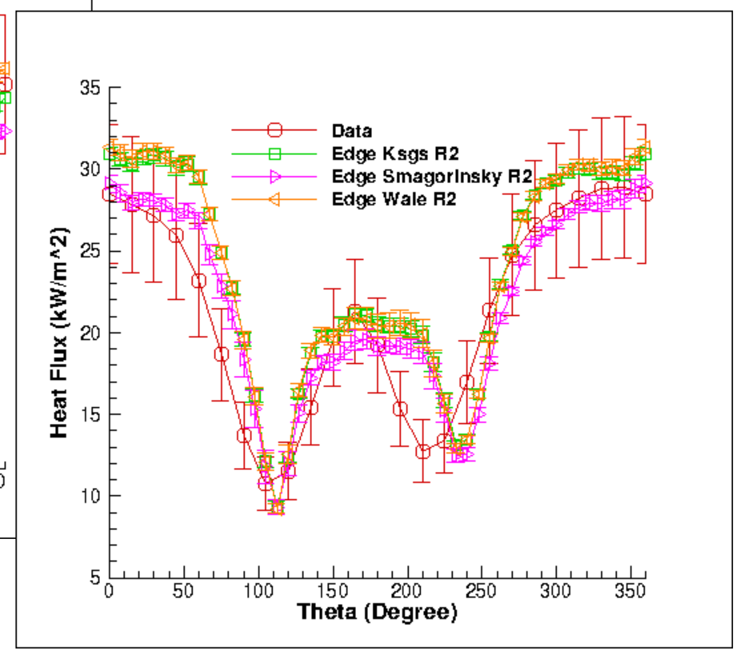
Solution Verification and Due Diligence for Model-form (Structural) Uncertainty

	Import	Adequacy			
	Phen	Mod	Code	Val	Mats
Convective Processes					
Convective heat transfer	M	M	M	L	

- Three meshes, three models
- The heat flux results also show error bars due to time and spatial averaging over a line-of-site







- Can we yet feel confidence in any scientific statement?

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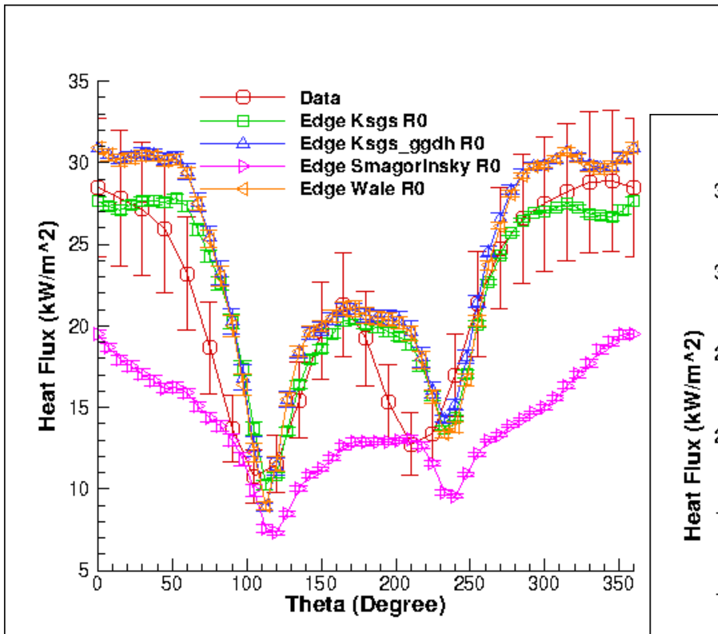

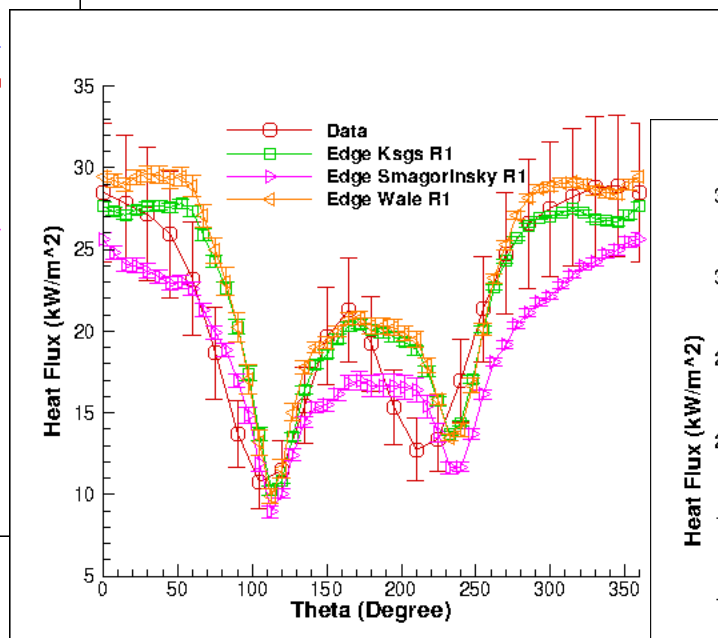

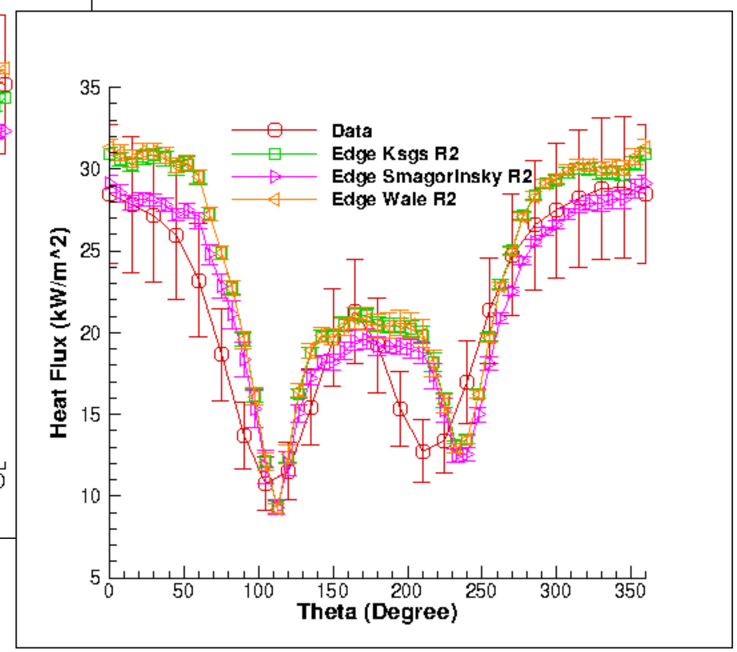

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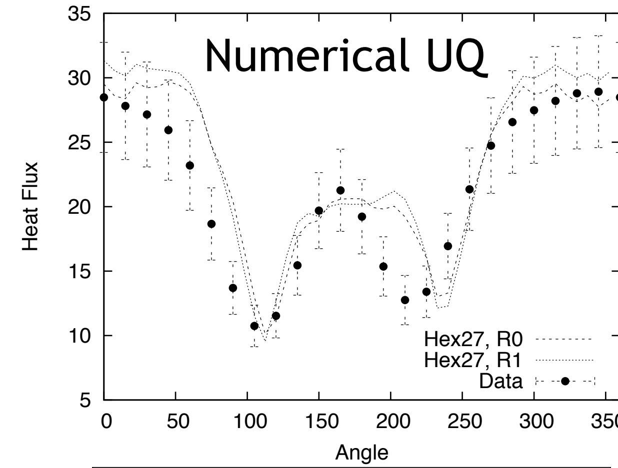
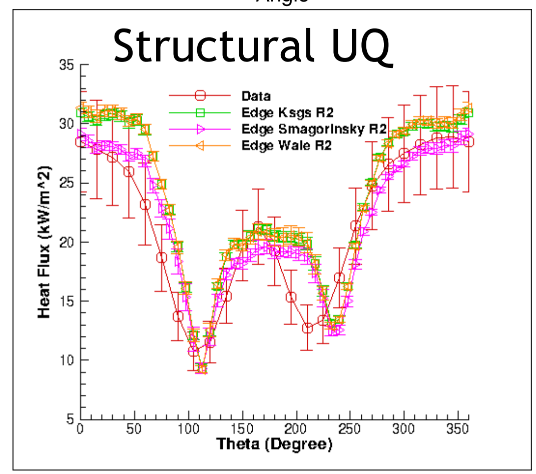
Review of a Strong V&V Process LES-based

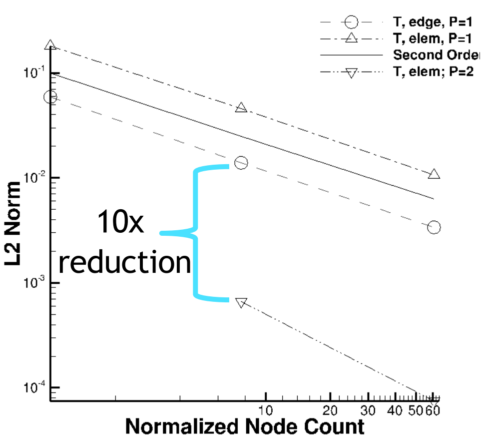
Established a sound LES-based verification and validation process (with uncertainty quantification) that includes the following attributes:

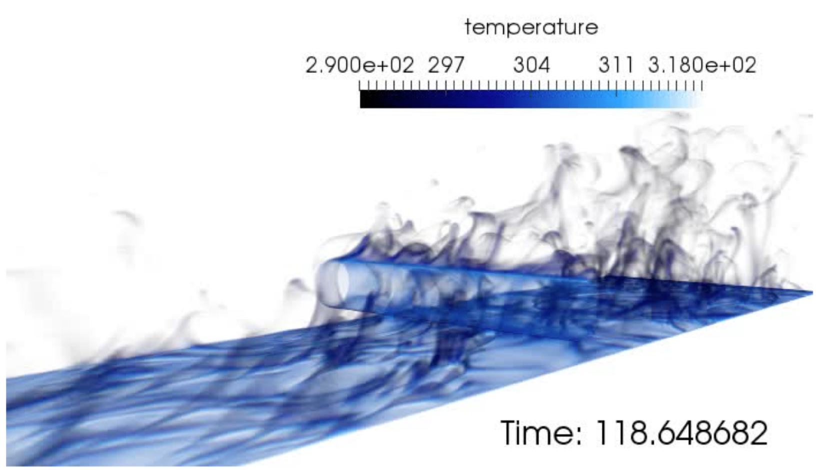
- Definition of key physics, Phenomena Identification Ranking Table (PIRT)
- Code implementation and verification
- Validation including solution verification (meshes with converged statistics)
- Structural uncertainty, i.e., model form, quantification
- Physics assumptions

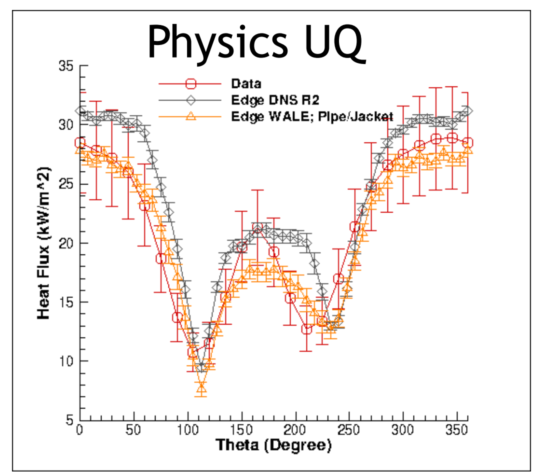




Non-isothermal MMS







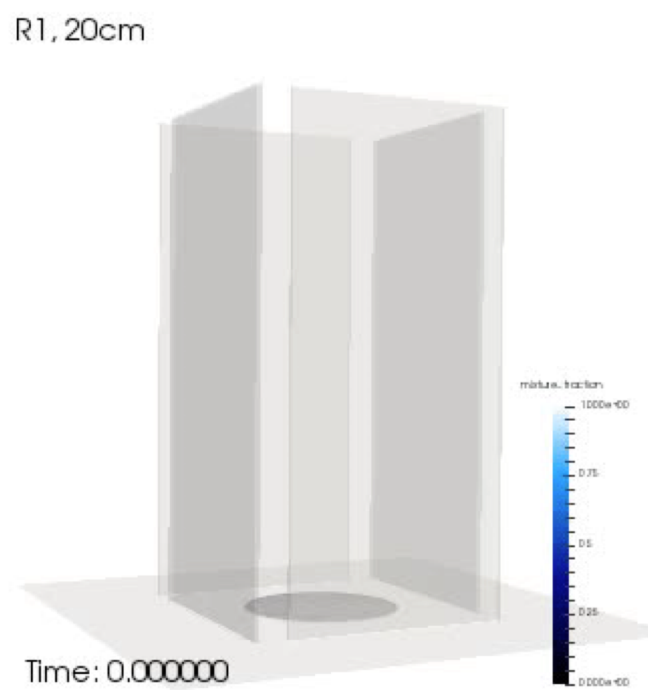
"An assessment of atypical mesh topologies for low-Mach LES", Domino et al., *Comp & Fluids*, 2019

A Validation Methodology: Code and Solution Verification: Conclusions

- A validation pedigree includes understanding what models are to be implemented, what code verification is required, and a detailed solution verification
- A PIRT is a simple process that identifies gaps in models, code, and/or, validation
- Typical validation studies often include one mesh, one model and lack of any code verification
- As a general rule, it takes 10x longer to verify correctness than to implement the code capability
  - Code verification is hard work, however, is critical to numerical methods development
  - Violations of this rule are abundant– especially when the code implementation is really really hard, e.g., NGP on GPU
- For structural uncertainty, i.e., model-form sensitivity, eigenvalue perturbation procedures can be a good approach

Objective: Deploy a High-Fidelity Tool to Predict a Fire

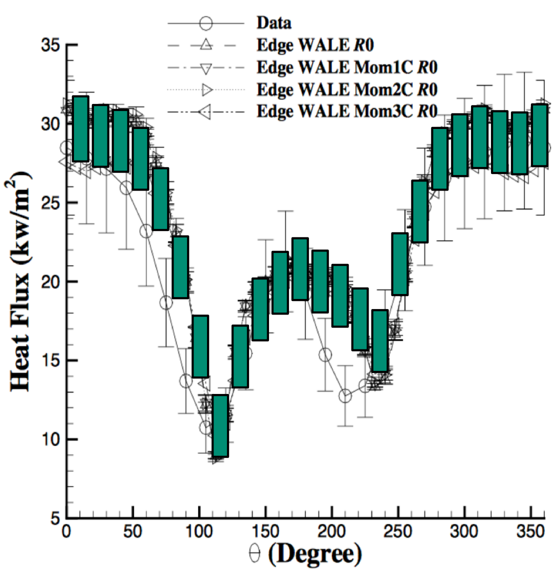
- Consider that we want to develop and deploy a foundational understanding in fire physics and deploy a simulation tool to support production analysis
- Consider the fire-environment with elements of the following physics:
  - Chemical reactions, soot, buoyancy, turbulent fluid mechanics, thermal radiation heat transfer, convective heat transfer, object heat-up/response, and sometimes propellants

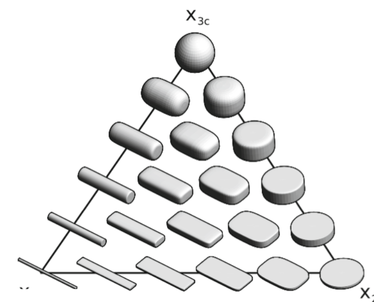


Volume rendered mixture fraction

More Effective/Efficient Structural Uncertainty

- In the previous high-quality LES validation (cylinder in x-flow), three models were implemented and tested
- Is there a more efficient approach? Yes! Eigenvalue perturbation of the SGS stress





$$\tau_{ij}^{sgs} - \frac{\tau_{kk}^{sgs}}{3}\delta_{ij} = -2\nu_{sgs}\bar{S}_{ij},$$

$$a_{ij}^{res} = \frac{1}{\overline{u_k u_k}}\left(\bar{u}_i\bar{u}_j - \frac{\bar{u}_k\bar{u}_k}{3}\delta_{ij}\right) = v_{in}^{res}\Lambda_{nl}^{res}v_{jl}^{res}$$

$$a_{ij}^{sgs} = \frac{1}{\overline{u_k u_k}}\left(\tau_{ij}^{sgs} - \frac{\tau_{kk}^{sgs}}{3}\delta_{ij}\right) = v_{in}^{sgs}\Lambda_{nl}^{sgs}v_{jl}^{sgs},$$

$$\overline{u_i u_j}^* = \bar{u}_i\bar{u}_j + \tau_{ij}^{sgs*} = \bar{u}_i\bar{u}_j + \overline{u_k u_k}^* a_{ij}^{sgs*} + \frac{\tau_{kk}^{sgs*}}{3}\delta_{ij},$$

$$\text{with} \quad \overline{u_k u_k}^* = \bar{u}_k\bar{u}_k + \tau_{kk}^{sgs*} \quad \text{and} \quad a_{ij}^{sgs*} = v_{in}^{sgs*}\Lambda_{nl}^{sgs*}v_{jl}^{sgs*}.$$

- See “Framework for characterizing structural uncertainty in LES”, Jofre et al, 2017

For Transient, Turbulent Flows, Averaging is Required

- The **bane** of turbulent validation: converged statistics require many flow-through times