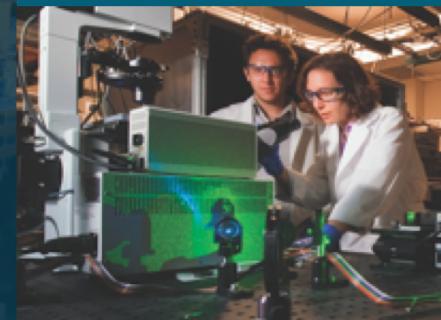


Guest Lecture Stanford ME469: A Validation Methodology: Code and Solution Verification



Sandia
National
Laboratories



*PRES*ENTED 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

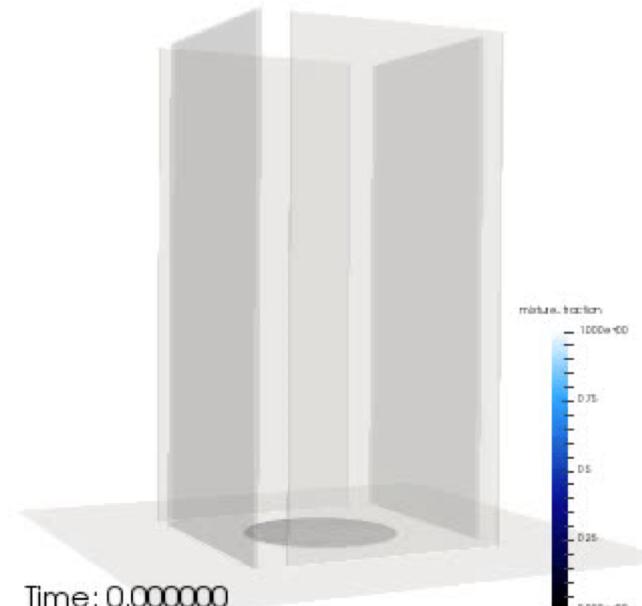
3 Objective: Deploy a High-Fidelity Tool to Predict a Fire



- 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



R1, 20cm

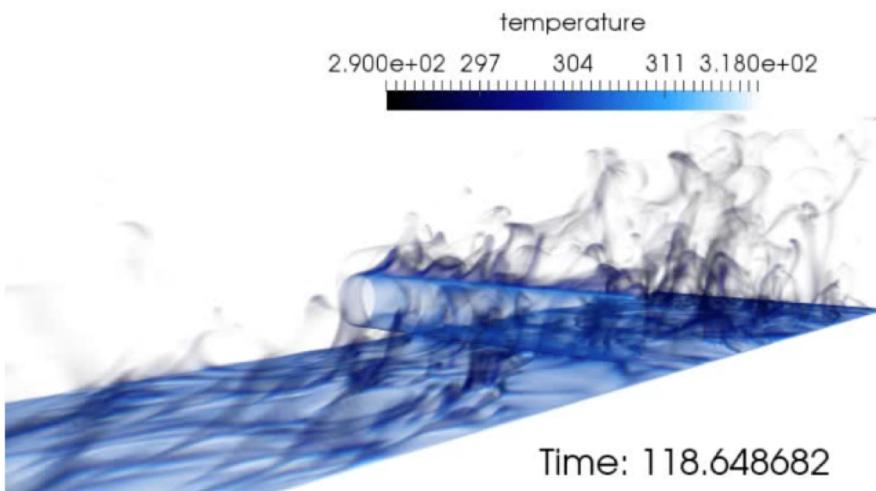


Volume rendered mixture fraction

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

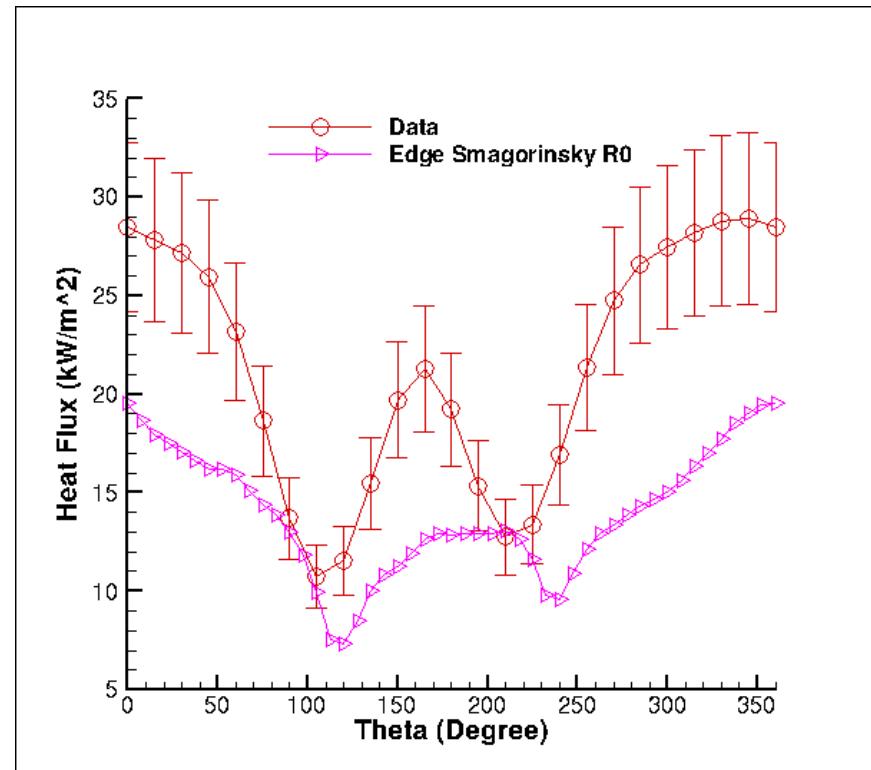


- One mesh, one model, no code pedigree...



Heat flux to the cylinder
Volume-rendered temperature

- What credible scientific hypothesis can be tested in this context?
- Was a Phenomenological 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”



Time-averaged heat flux to cylinder

Step I: 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:

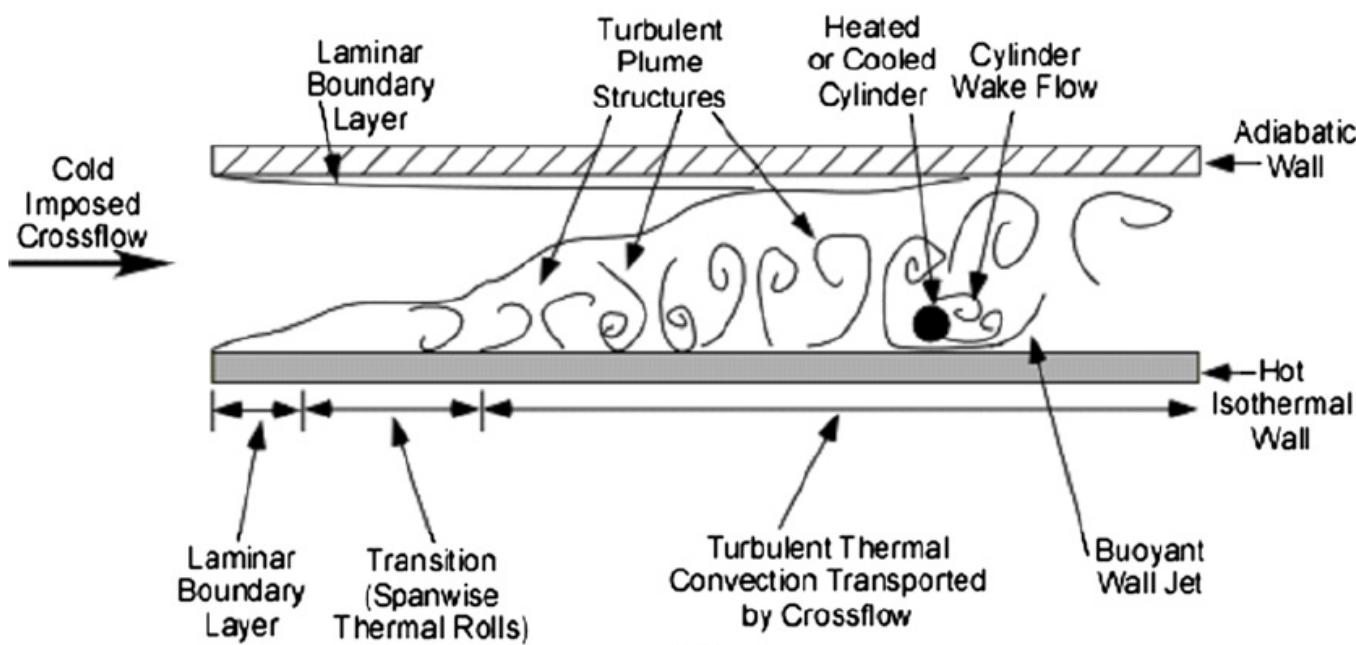
	Import	Adequacy			
		Phen	Mod	Code	Val
Convective Processes					
Convective heat transfer	M	M	L	L	

- 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

6 Cylinder in Cross Flow Validation



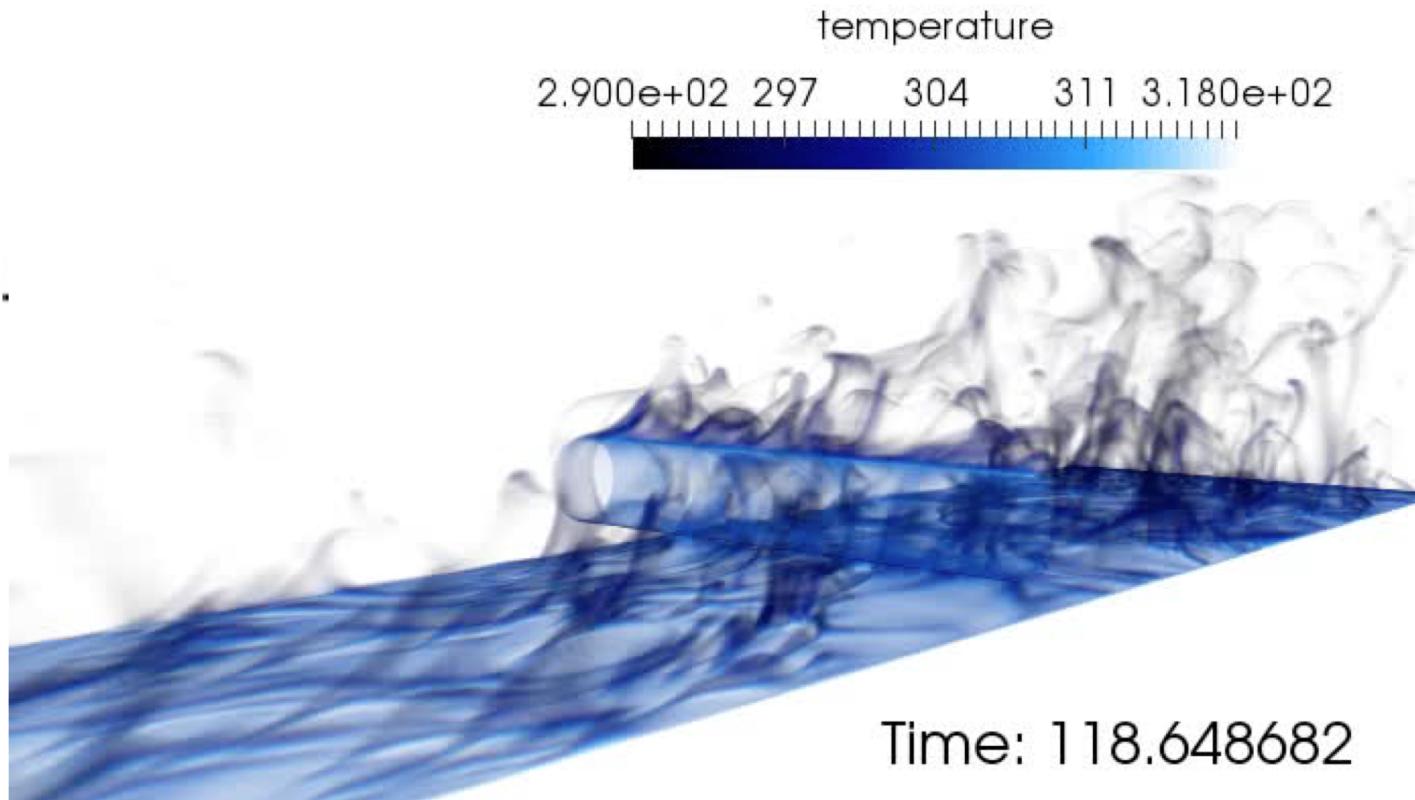
- Kearney et al, “Experimental investigation of a cylinder in turbulent thermal convection with an imposed shear flow”, 2004
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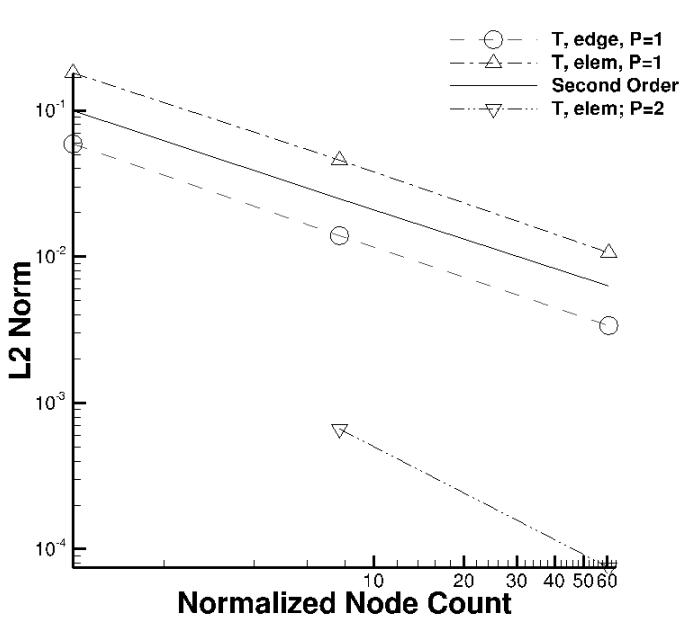
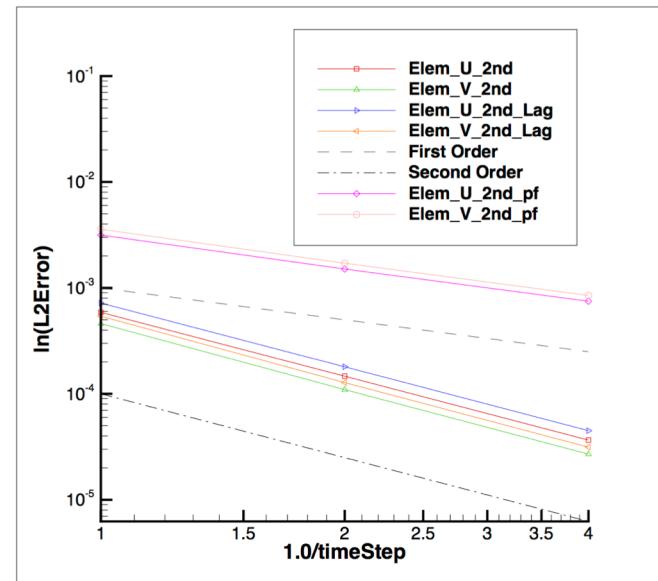
Cylinder in Cross Flow Validation

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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-stage Runge-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:

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

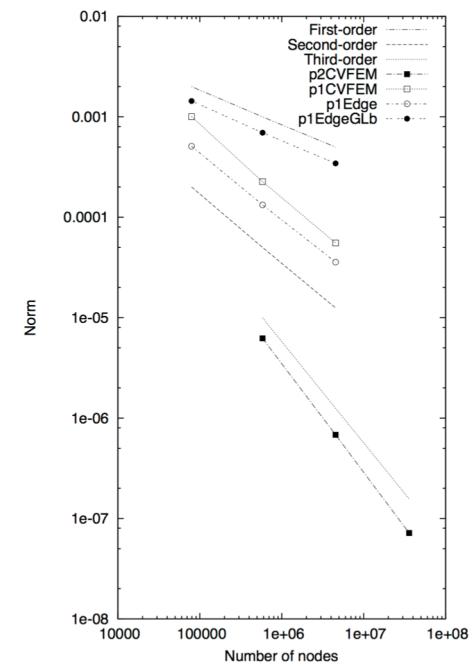
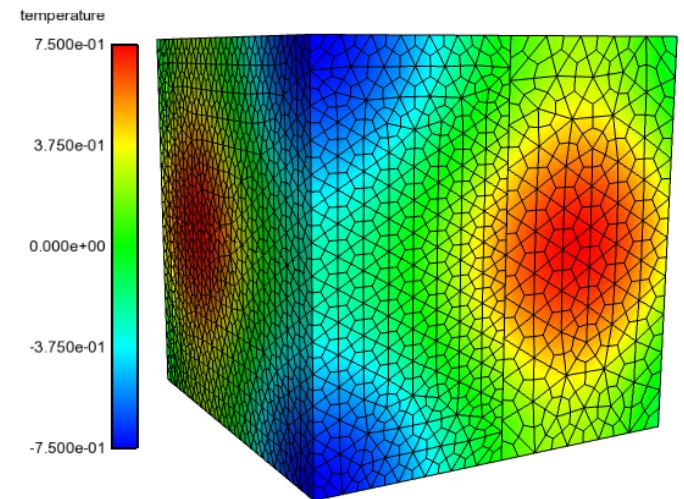
- with manufactured analytical form for T:
- $$T^{MMS} = \frac{1}{4} [\cos(2\alpha\pi x) + \cos(2\alpha\pi y) + \cos(2\alpha\pi z)]$$
- Placing this MMS back into model PDE:

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

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: $T^E = T - T^{MMS}$

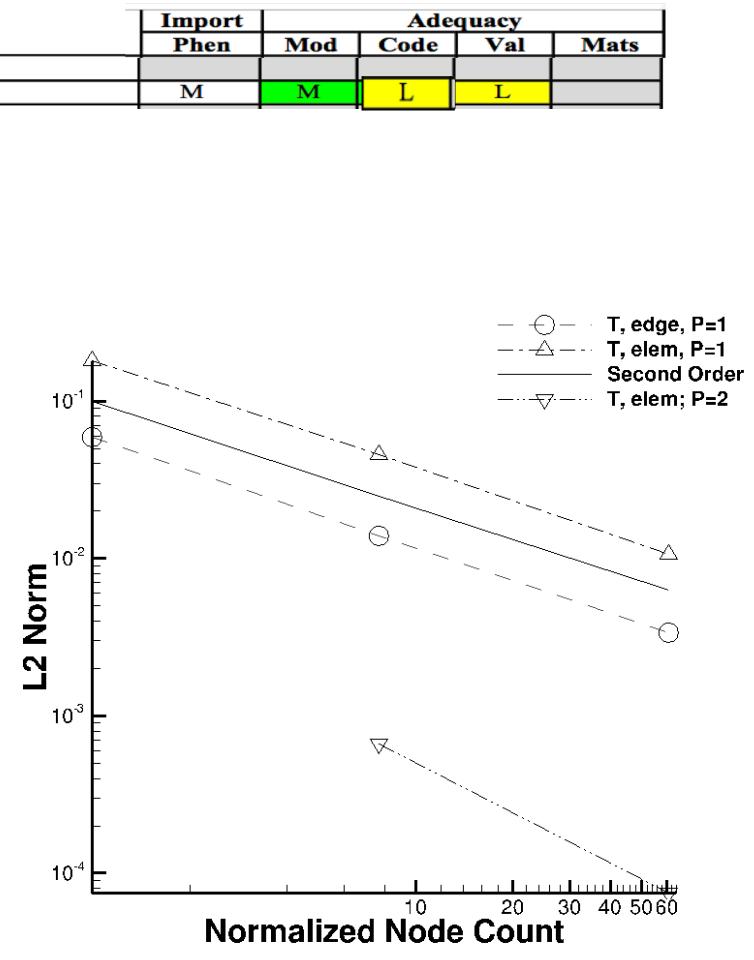
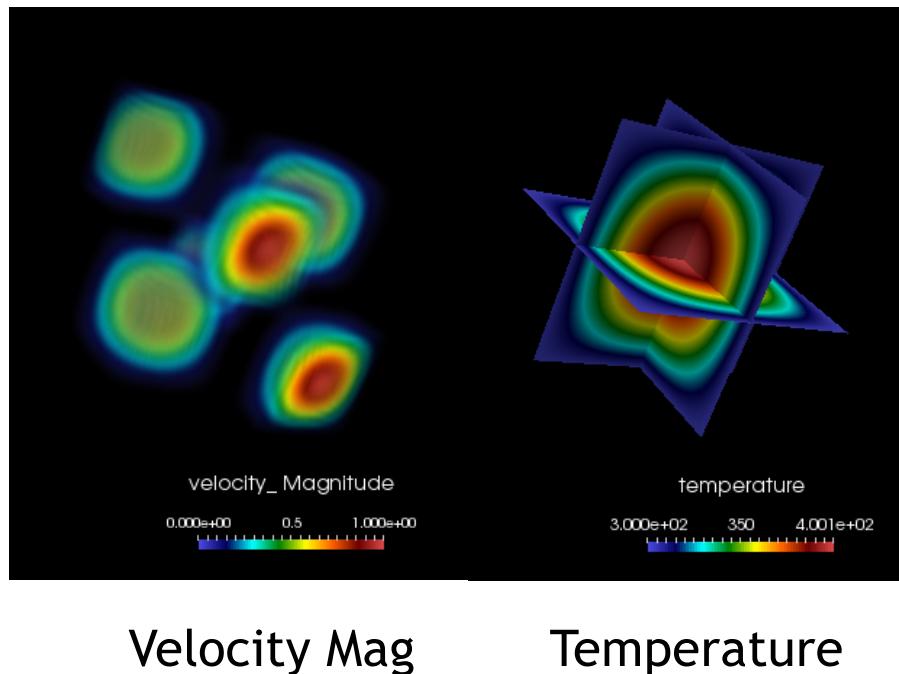


Spatial Code Verification for a low-Mach, Variable-Density Flow



	Import	Adequacy			
		Phen	Mod	Code	Val
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



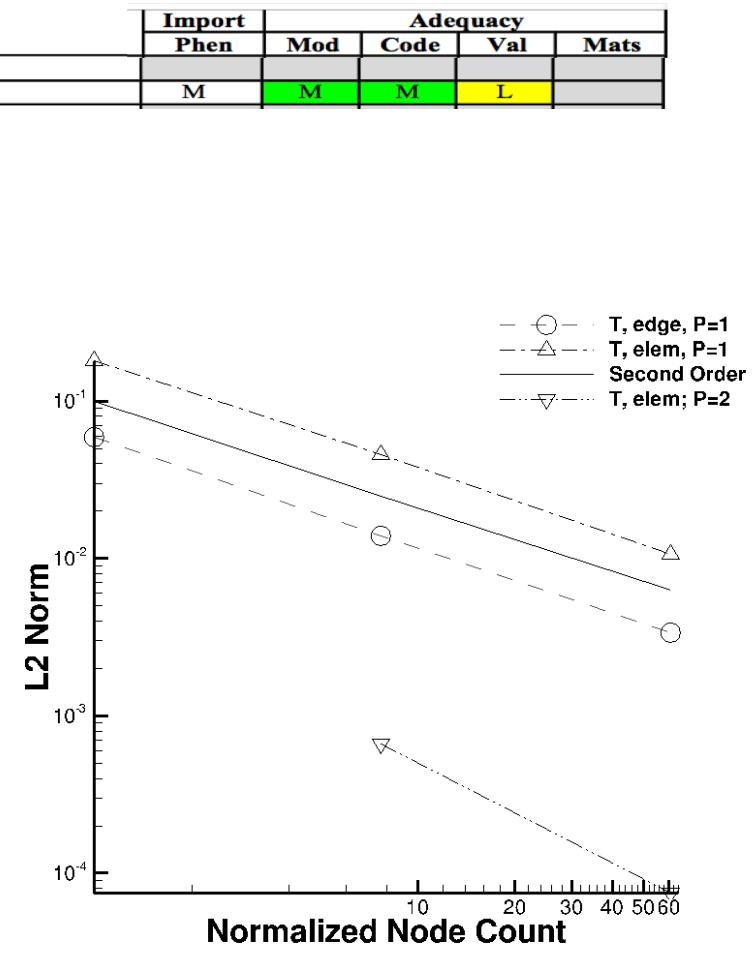
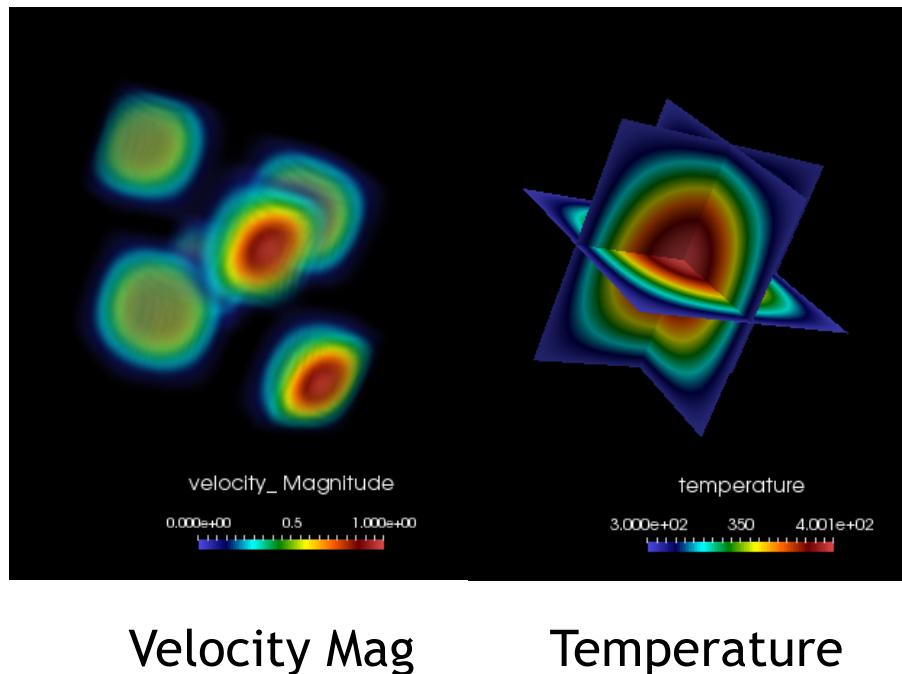
See, “Exploring model-form uncertainties in large-eddy simulations”, Domino et al, 2016

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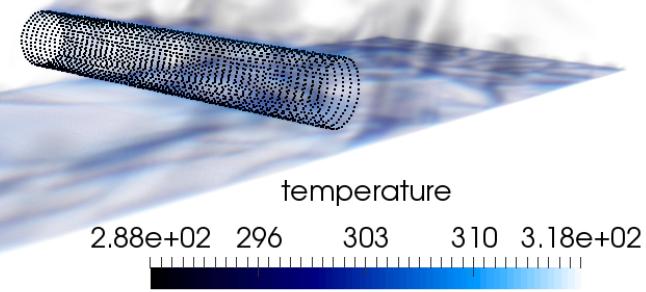
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The Effect of Polynomial (P) and Mesh Spacing (H) Refinement

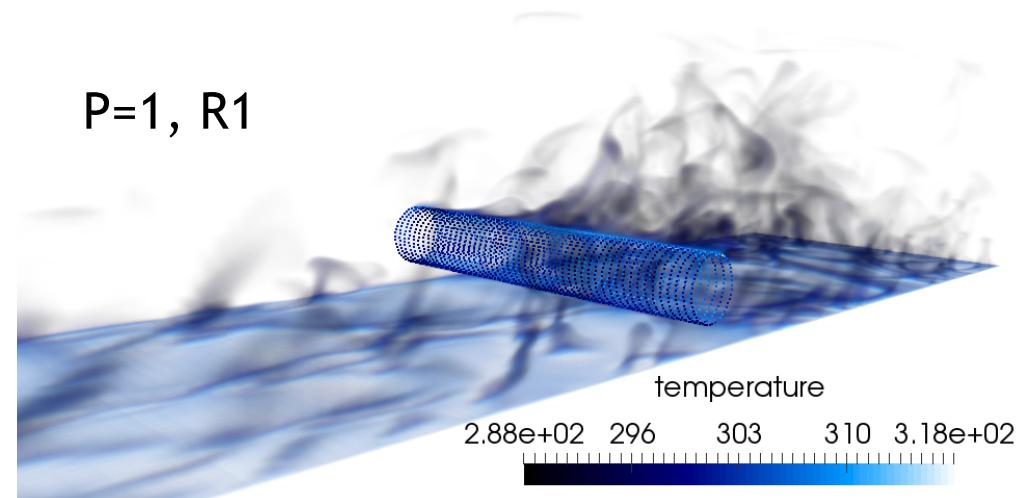


- For the heated cylinder-in-cross flow, either mesh resolution or polynomial promotion provides a more accurate result with more turbulence structure

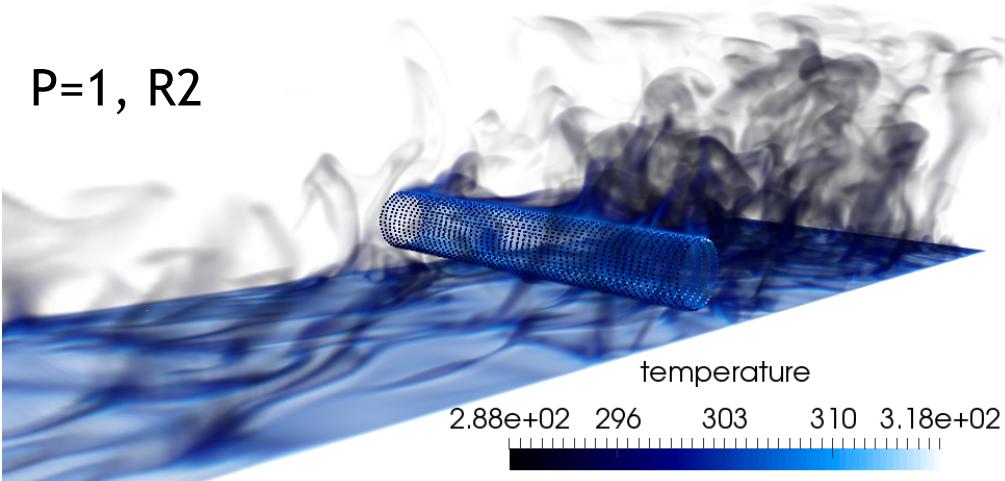
P=1, R0



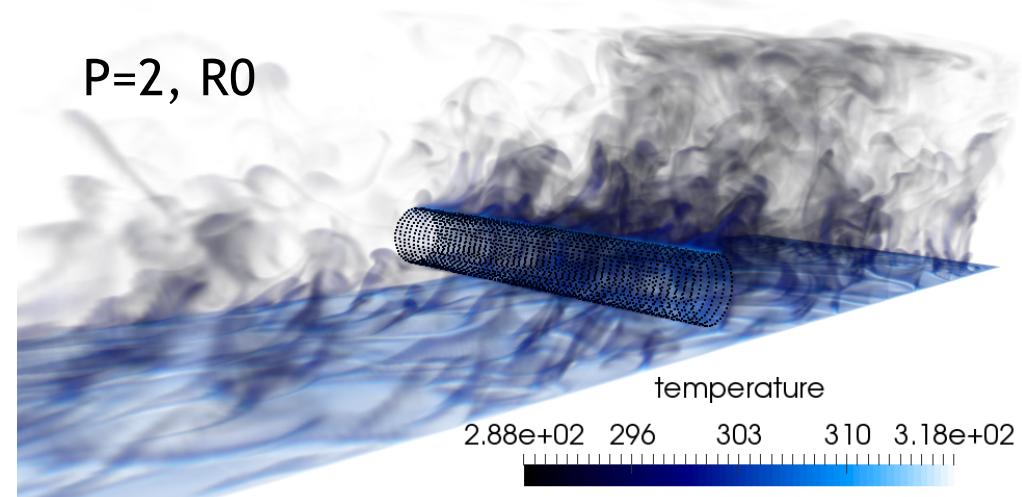
P=1, R1



P=1, R2



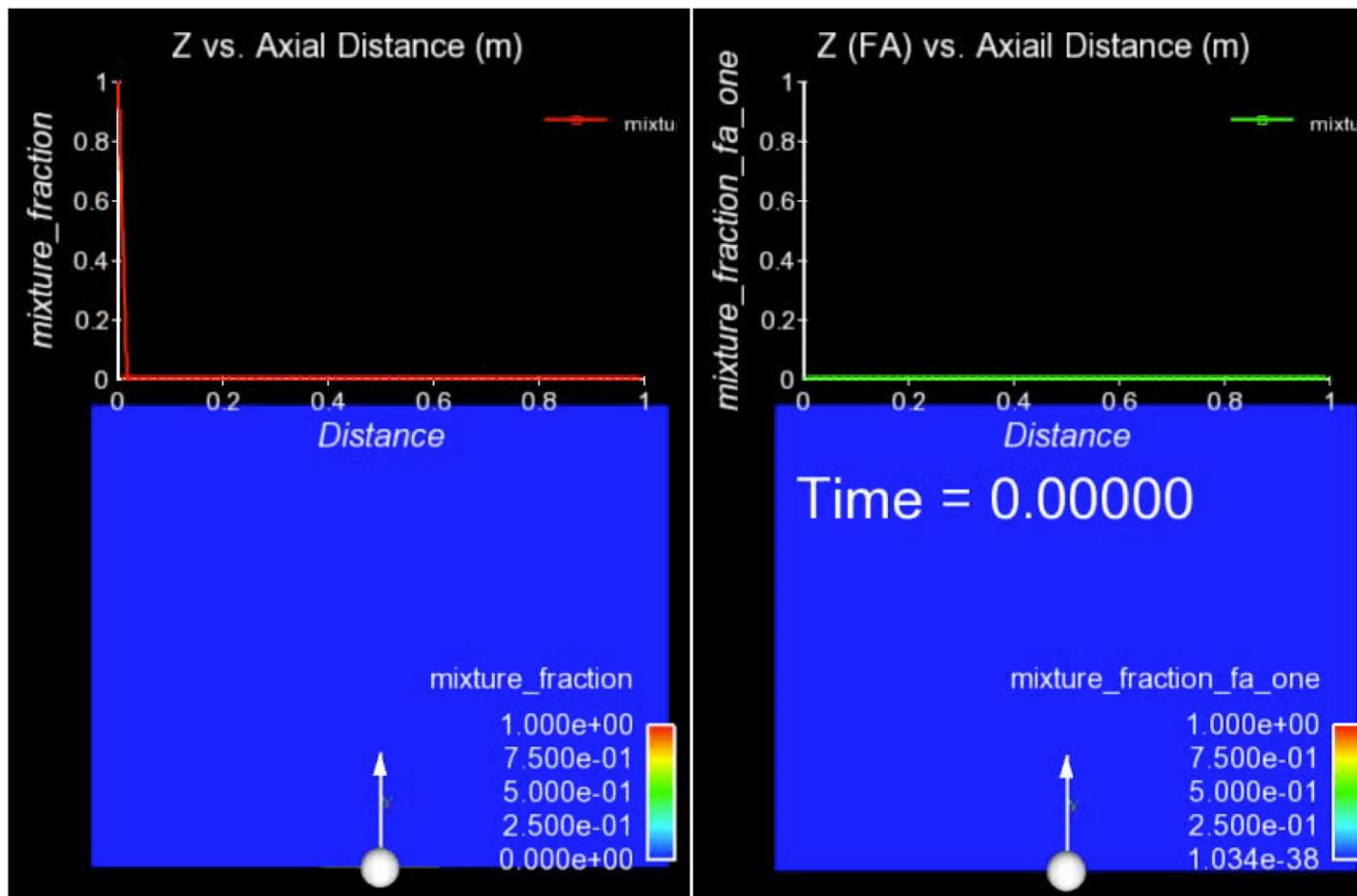
P=2, R0



For Transient, Turbulent Flows, Averaging is Required



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



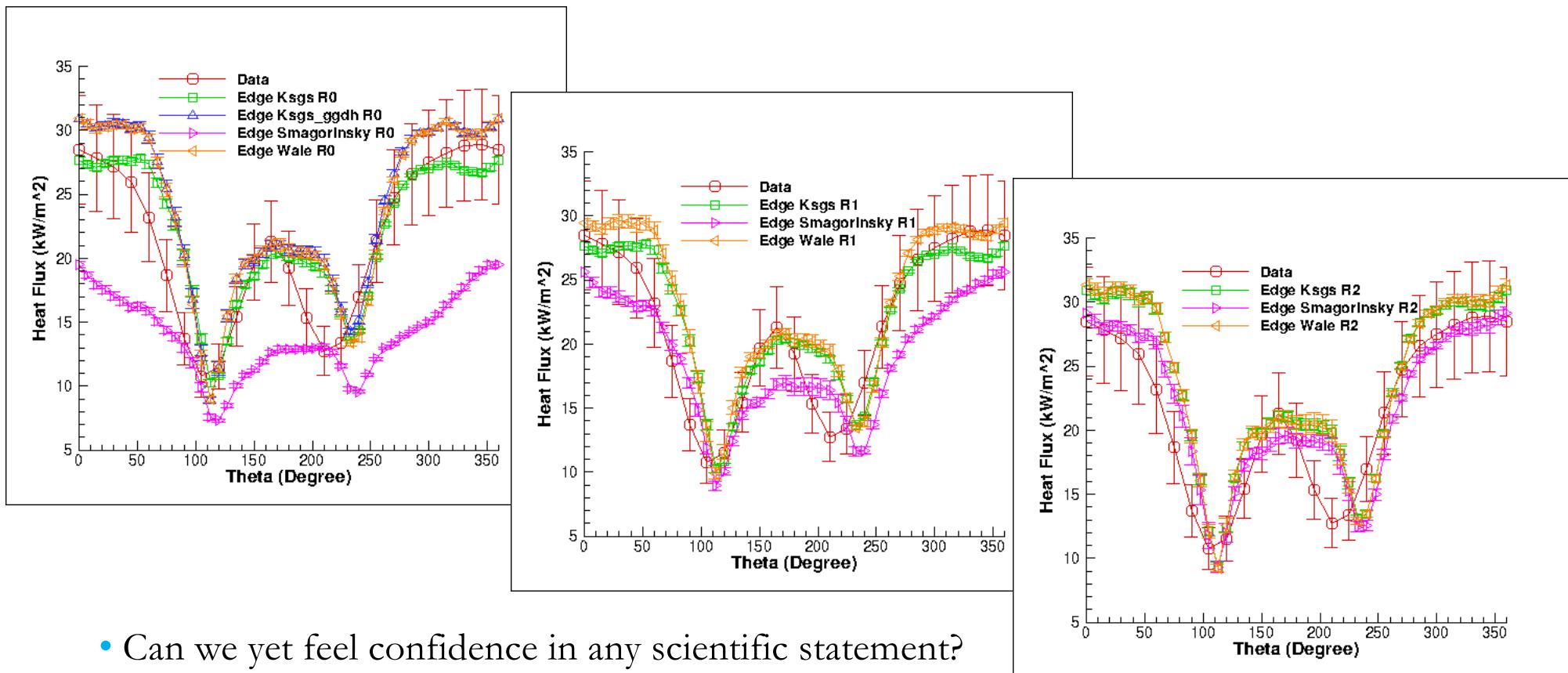
Solution Verification and Due Diligence for Model-form (Structural) Uncertainty

14



	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



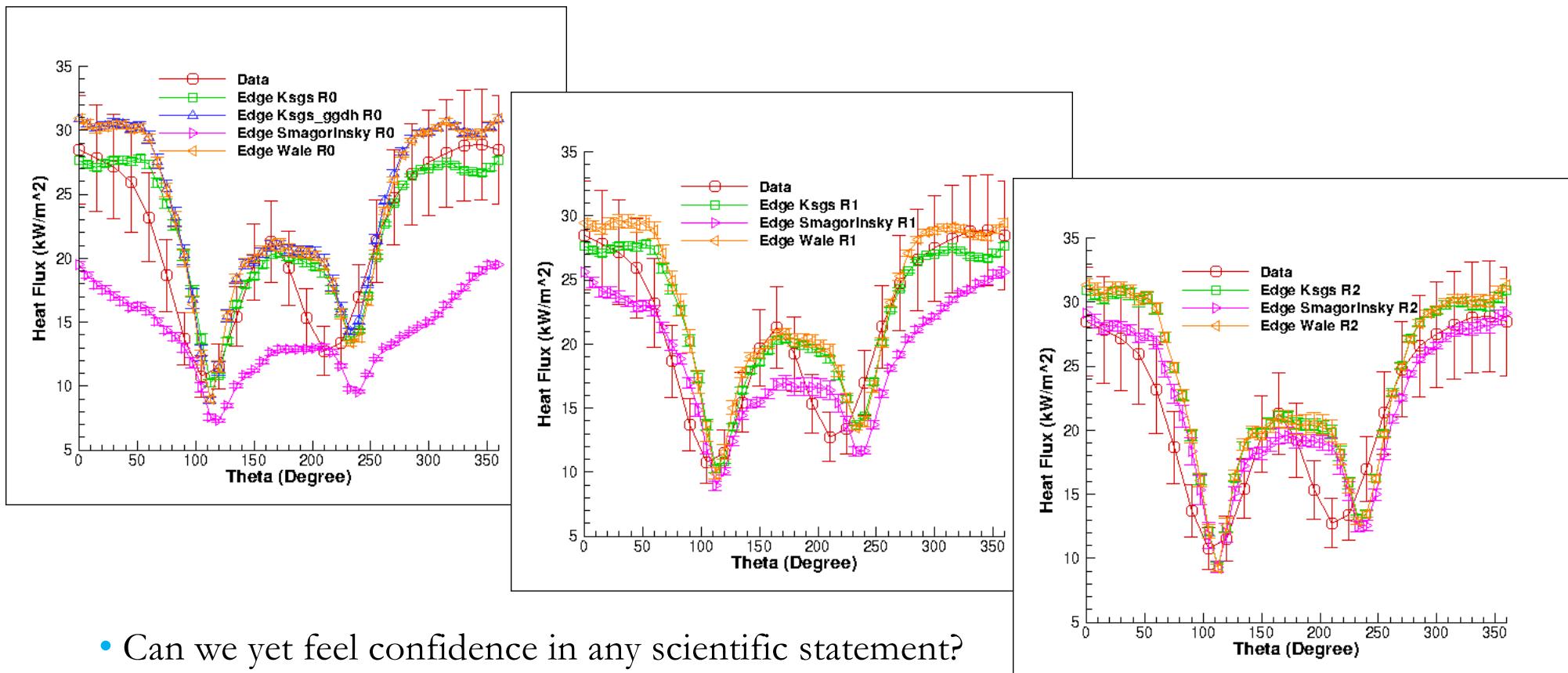
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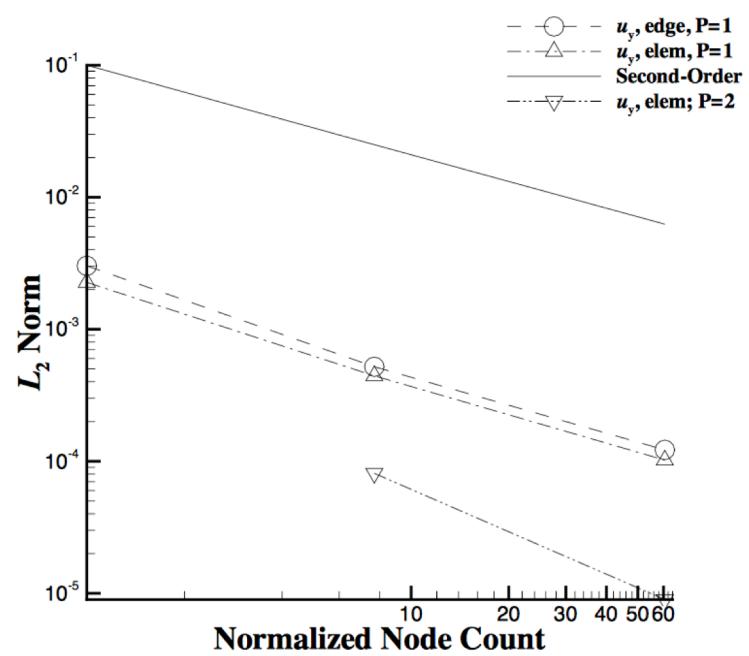
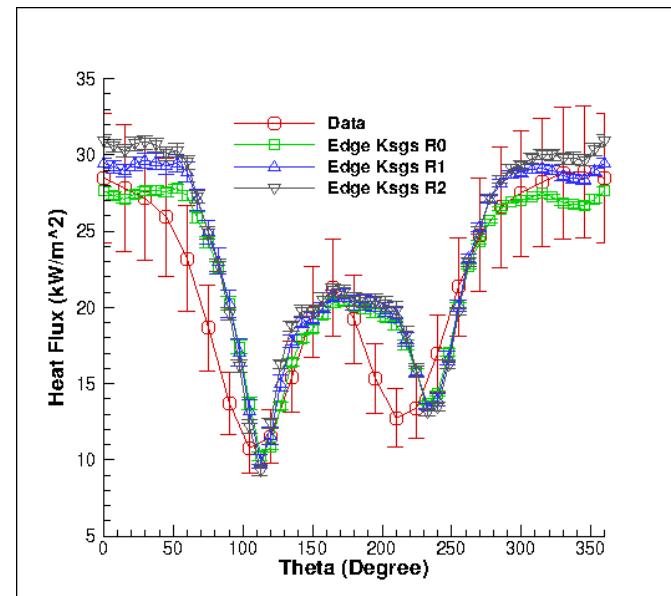
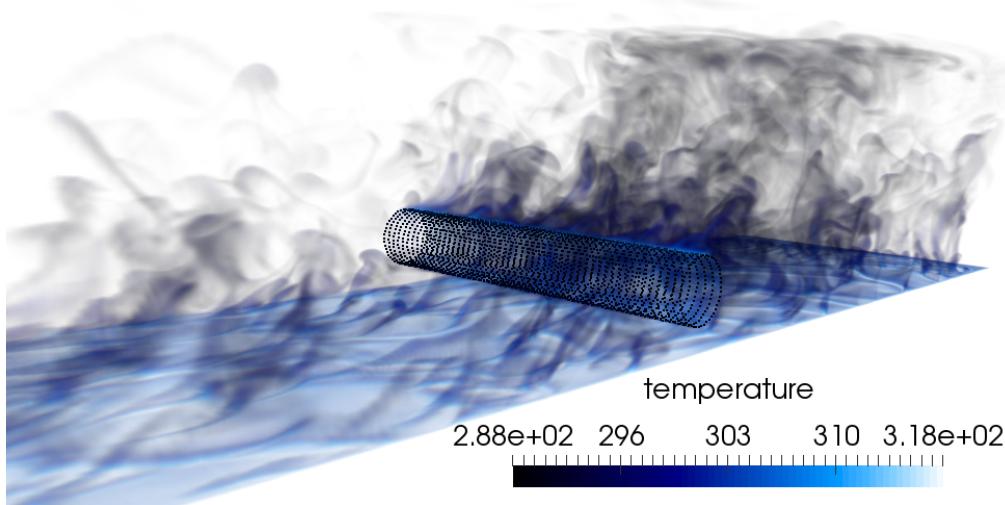
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Review of a Strong V&V Process

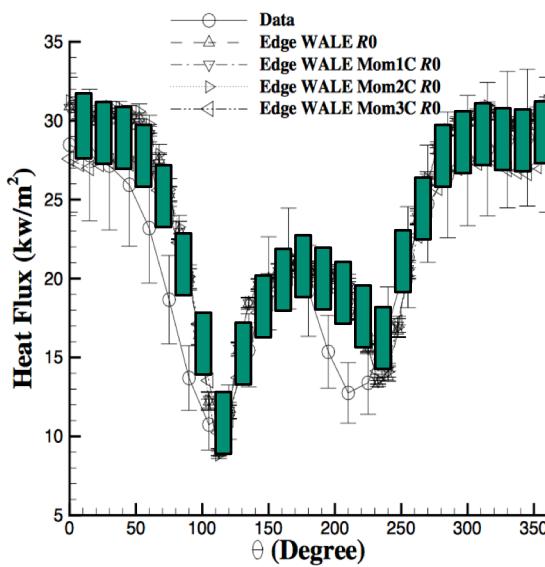
- Objective: Define a sound validation process that includes:
- Definition of key physics, PIRT
- Code implementation
- Code verification
- Solution Verification (meshes with converged statistics)
- Structural Uncertainty Quantification



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



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

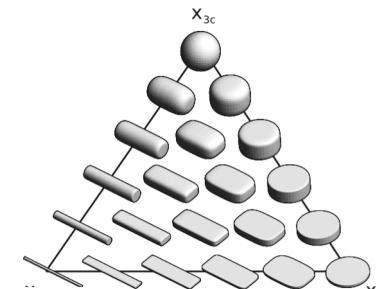
$$a_{ij}^{res} = \frac{1}{\overline{u_k u_k}} \left(\overline{u_i u_j} - \frac{\overline{u_k} \overline{u_k}}{3} \delta_{ij} \right) = v_{in}^{res} \Lambda_{nl}^{res} v_{jl}^{res}$$

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

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

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

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



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 something 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