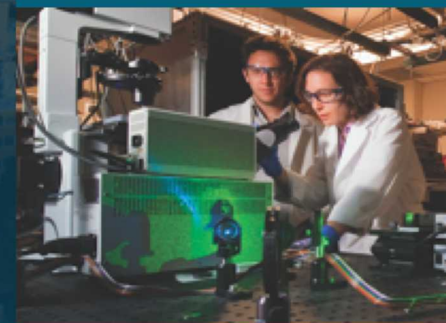
SAND2019-7052C

Sandia National Laboratories

Sandia National Laboratories Fire Science and Engineering Research Directions



The International FORUM of Fire Research Directors Annual Meeting
June 26th - June 28th, 2019 Newtownabbey, BT37 0QB, UK

PRESENTED BY

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Sandia National Laboratories SAND2019-TBD

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Evolution of a Mindset: From Simple to Complex

- Peak radiative heat fluxes to engulfed objects is a function of fuel type, pool size, obstructions/accident geometry, and presence of cross-flow
- As cross-flow and geometric complexity of accident scenarios increase, SNL has found that transitioning from a Reynolds-Averaged Navier-Stokes (RANS) to a more predictive Large-eddy simulation (LES) approach is required → HPC on Next-Gen platforms

RANS-based → LES-based

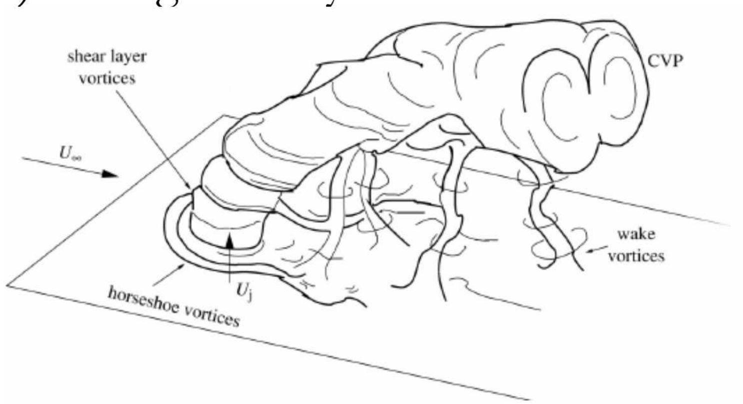
Quiescent; q''_r ~ 100 kw/m^2

Cross-flow; q''_r ~ 200 kw/m^2

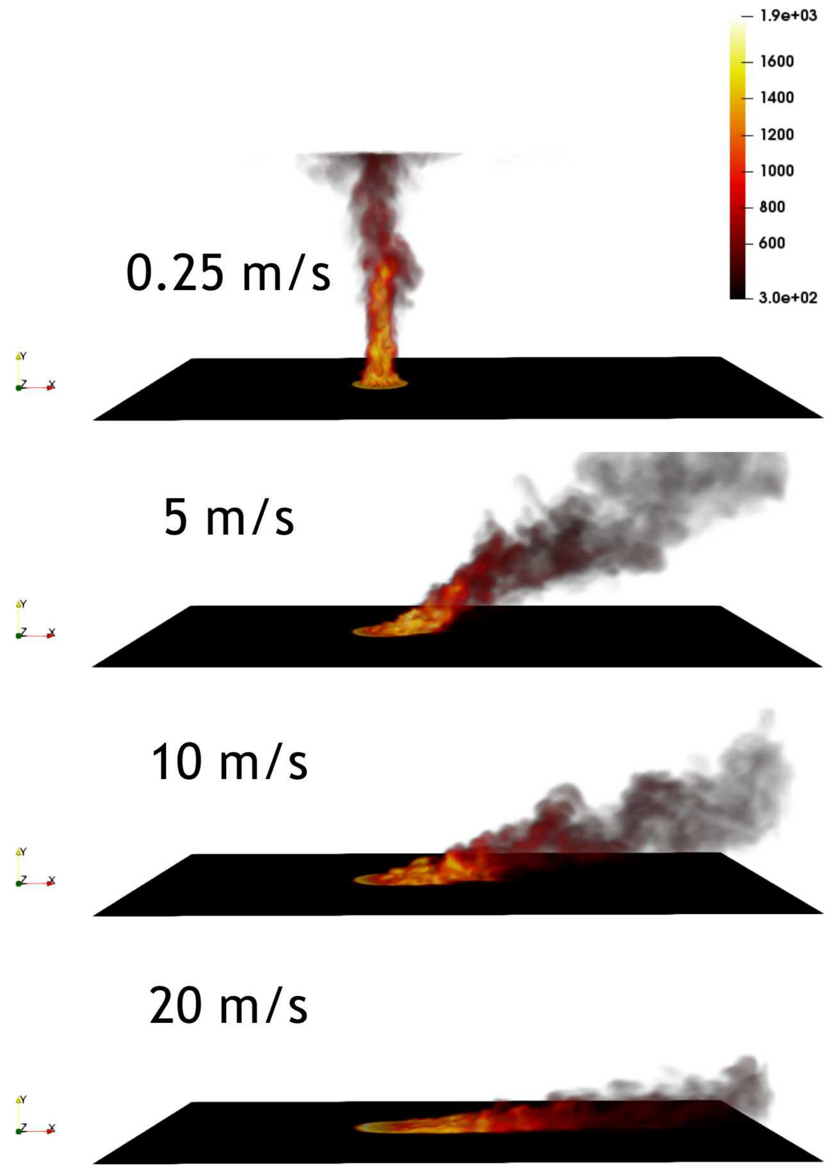
Whirls >> 200 kw/m^2

Core Research Objective: Understand Large-Scale Fire Dynamics

- The coupling of cross-wind with a hydrocarbon fire event drives large-scale column vortex formation – very similar to classic jet-in-cross flow behavior (see below)
- Increased mixing yields increased radiative heat fluxes
- Although lab-scale efforts exist for quantities such as flame drag distance and tilt angles, none exist for scale of interest to SNL, e.g., 10 meters and beyond
- SNL is quantifying large-scale fire physics (Γ, θ, ect.) through theory and simulation



LES of pulsed jet in cross flow; Coussement et al, JFM, 2012

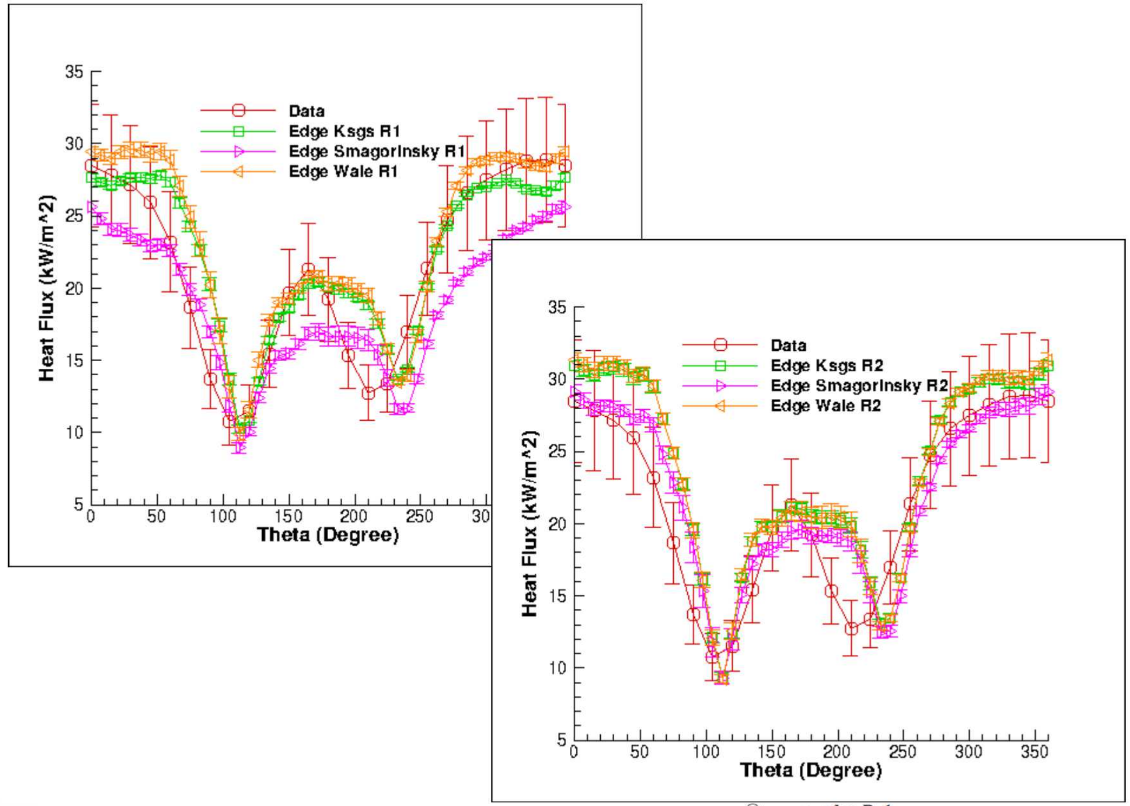


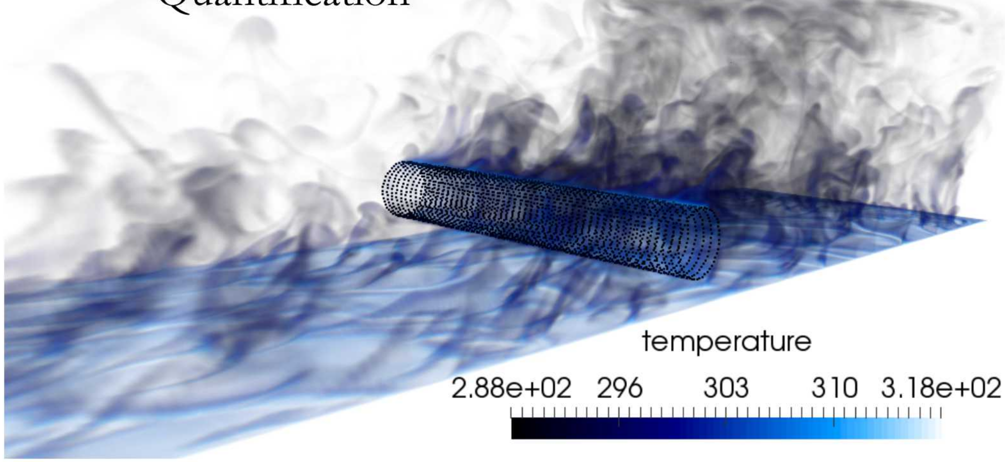
10 m pool fire
LES-based numerical study

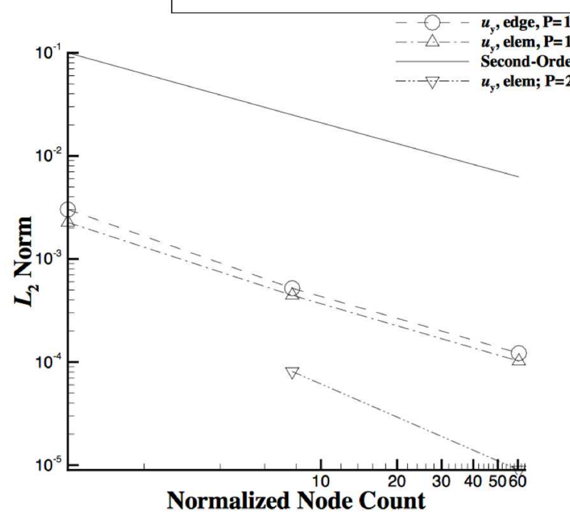
Core Research Objective: Support High-quality VVUQ Process

Goal: Define a sound verification and validation process (with uncertainty quantification) that includes the following attributes:

- Definition of key physics, PIRT
- Code implementation
- Code verification
  - Including higher-order unstructured
- Solution Verification (meshes with converged statistics)
- Structural Uncertainty (model form) Quantification



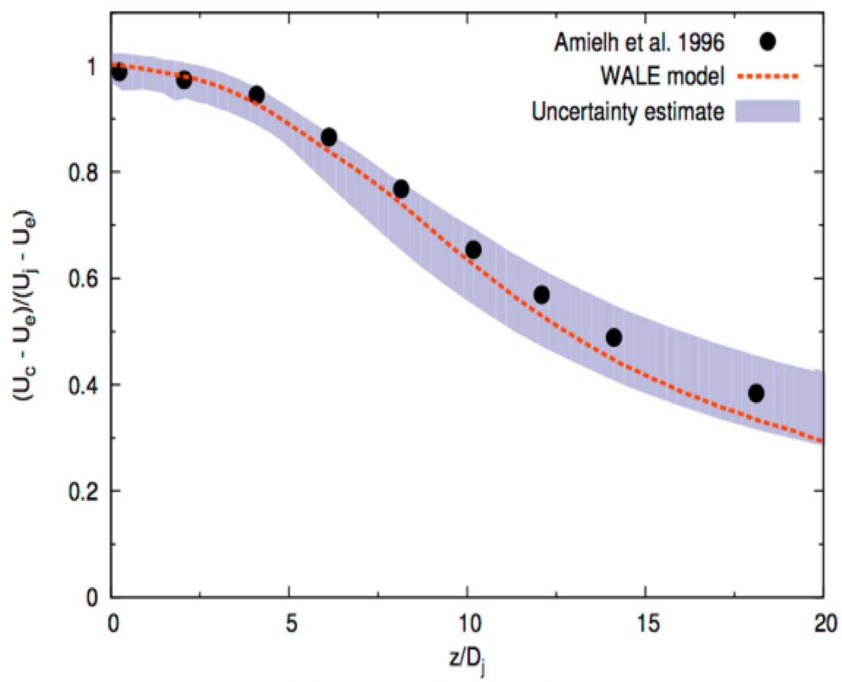




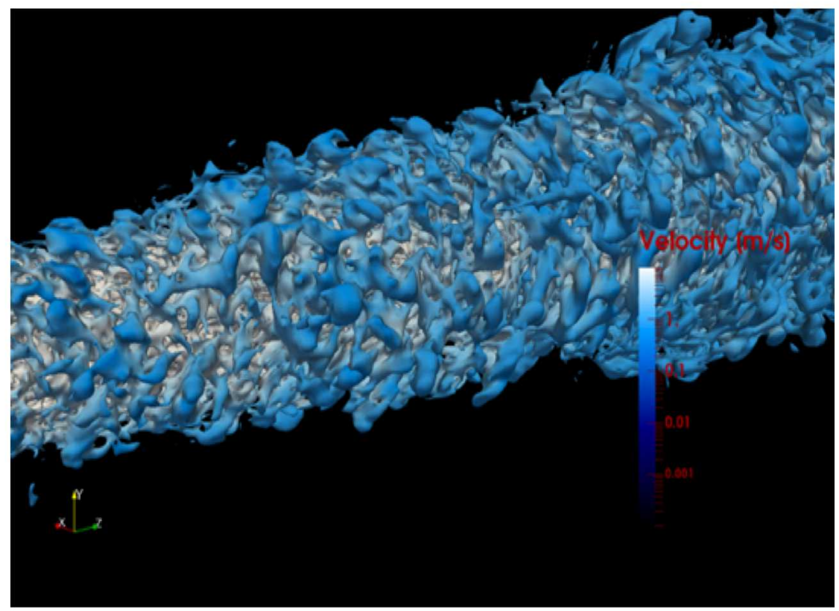
Heated cylinder in cross flow "An assessment of atypical mesh topologies for low-Mach LES", Domino et al, 2019

Core Research Objective: Automatic Structural Uncertainty

- A Direct Numerical Simulation (DNS) data set was developed by the Domino VVUQ/Stanford PSAAP-2 partnership
- Educated eigenvalue perturbations conduced within a suite of LES models to provide an uncertainty bound for a turbulent axisymmetric jet (ramifications for machine learning)
- See, "Eigensensitivity analysis of subgrid-scale stresses in large-eddy simulation of a turbulent axisymmetric jet", Jofre, Domino, and Iaccarino, 2019



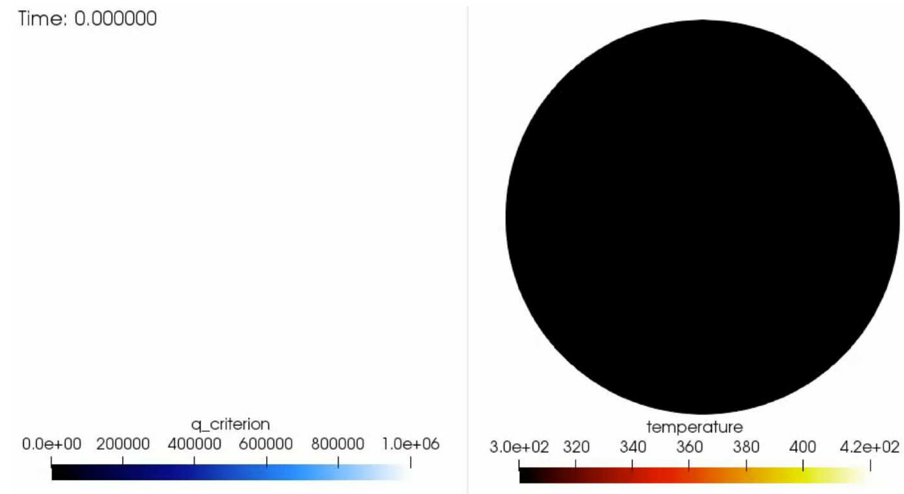
Axial centerline velocity



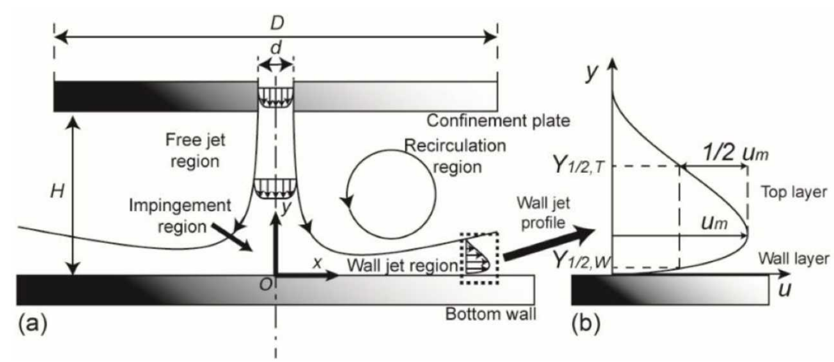
Q-crit isosurface colored by velocity magnitude

Core Research Objective: Capturing Complex *Internal* Physics for Fully Engulfed Objects

- Systems within the Abnormal Thermal Environment experience pressurization due to internal thermal decomposition of common materials
- At critical component pressures, venting of hot combustible gas occurs either by system design or structural failure
- Venting events are characterized by an impinging turbulent non-isothermal jet blowdown
- This year, a Direct Numerical Simulation (DNS) effort is being conducted to understand low-Mach non-isothermal jet impingement (hot jet, cool surface)
- Simulations are being run up to 15 billion mesh nodes on up to 384,000 processors (6000 KNL nodes at 64 MPI-rand/node)
- This DNS is supporting Machine-learning objectives for, e.g., ML-based wall-modeled LES,



LES Scoping Study
Re = 10,000, T^j = 300C



Guo, 2016

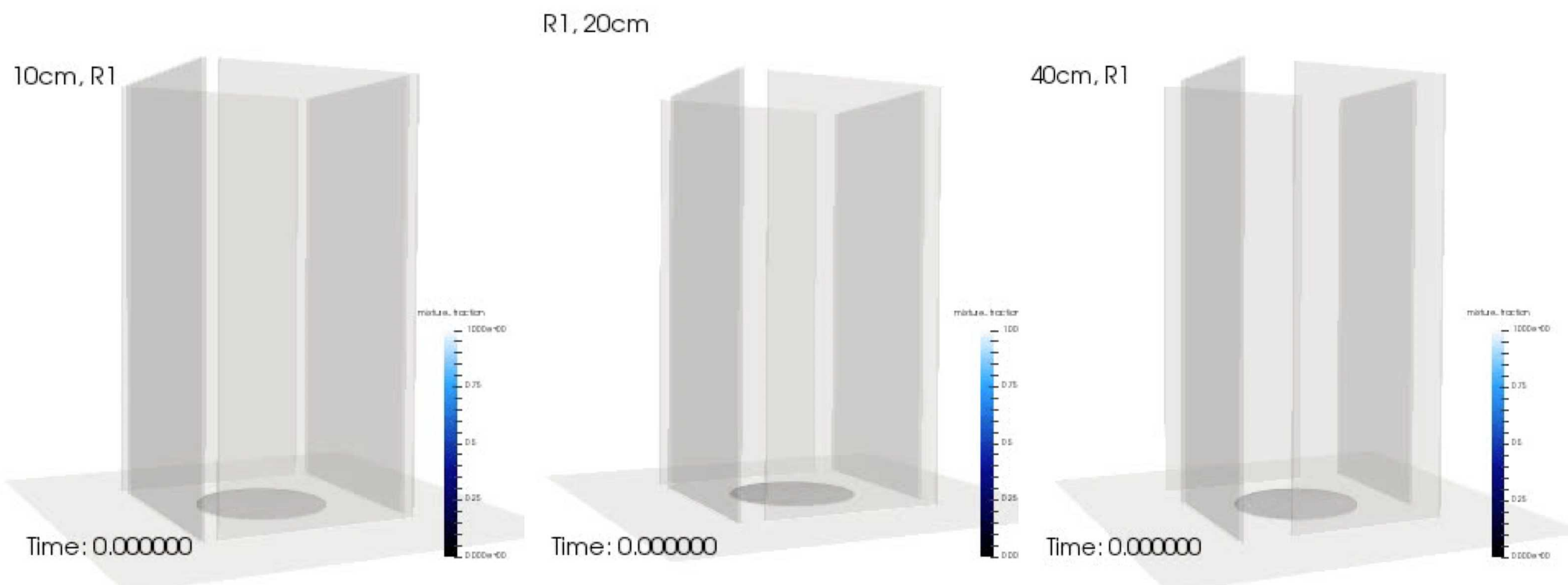
Conclusions

- RANS-based approach to LES-based will increase predictivity of fire-mechanics in complex accident scenarios
- Large-scale fire dynamics understanding is of interest – especially when providing heat fluxes to objects of interest
- High-quality V&V methodology requires quantification of all possible errors including model-form (structural), numerical (solution verification), and parameter uncertainties (epistemic and aleatory)
- Objects within a fire environment often times undergo complex morphology changes that drives new and challenging mod/sim objectives

Extra Slides

Evolution of a Mindset….. Modeling Whirling-like Flow

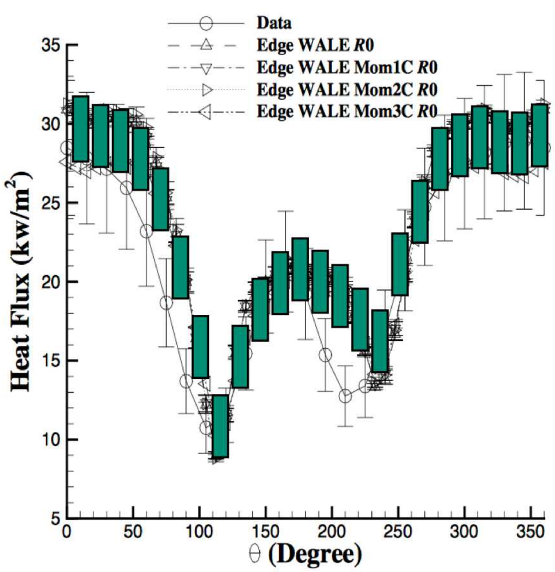
- Idealized chamber in which swirl is provided by selective wall placement in the experimental design
- Gap varied between 10, 20, and 40 cm
- Objective: Can the onset of swirl be predicted? What is the strength?



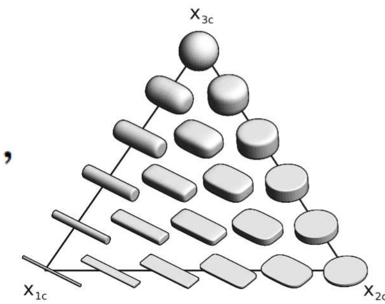
Volume rendered mixture fraction

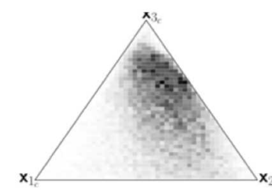
More Effective/Efficient Structural Uncertainty

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



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





Open jet

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

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

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

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

- See “A Framework for Characterizing Structural Uncertainty in Large-Eddy Simulation Closures”, Jofre, Domino, and Iaccarino, 2018