SAND2016-4084C

Supporting Efforts in Deploying Large Eddy Simulation for Production Abnormal/Thermal Environment Analysis

Exceptional service in the national interest

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1541, Computational Thermal and Fluids Mechanics
University of Utah PSAAP-2 meeting
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Outline

Description of the Abnormal/Thermal Environment

Verification & Validation and Physics & Engineering Modeling FY16 Project Problems of interest

MMS Description and Order-of-Accuracy

Model Form Error Study

Incorporation of Buoyant Effects in LES Subgrid Models

Unstructured higher order

Path Forward/Conclusions

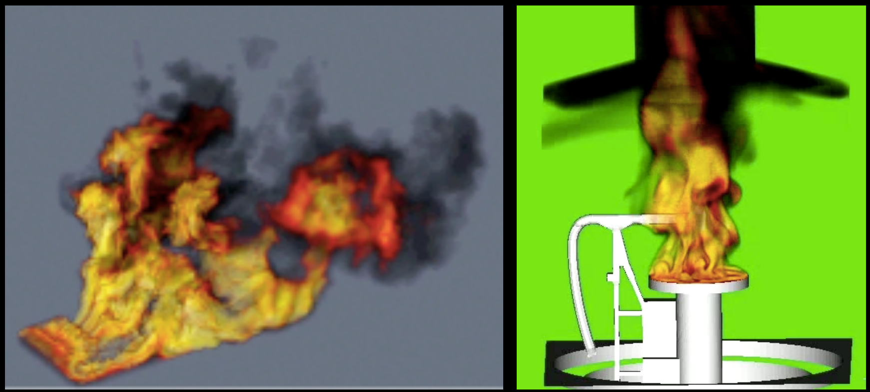
Abnormal/Thermal Environment

SNL TTC

10 meter outdoor JP-8
(Nakos, lead experimentalist)

XTF for Cross Wind Fire

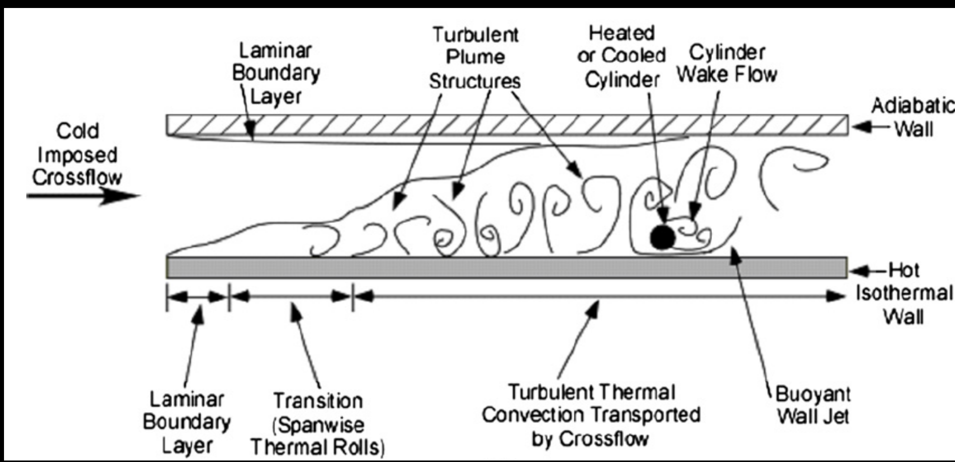
FLAME for Quiescent Fire

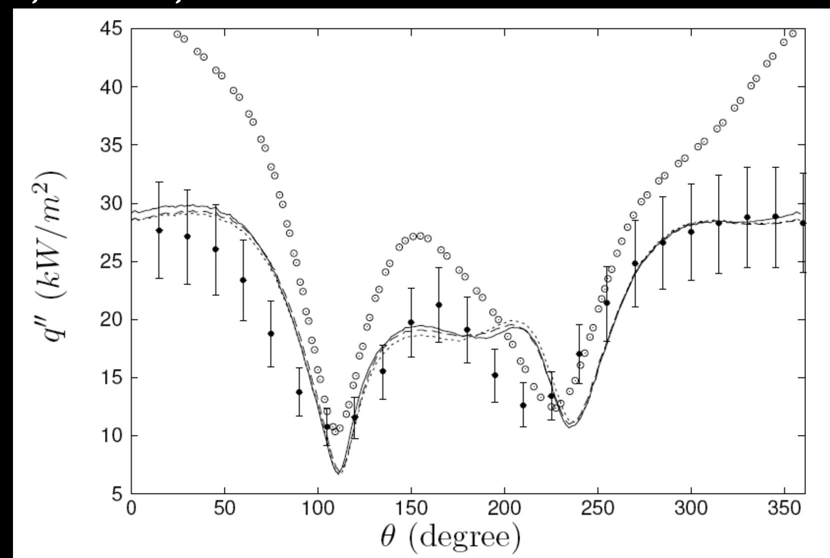


76-1 Qualification study

Towards Model Form Error (V&V[1])

Model Configuration: SNL-based Sean Kearney Experiment, "Experimental investigation of a cylinder in turbulent convection with an imposed shear flow", AIAA, 2005





Kearney experimental configuration

Laskowski et al. RANS / Kang et al. DNS study (taken with permission from G. Iaccarino)

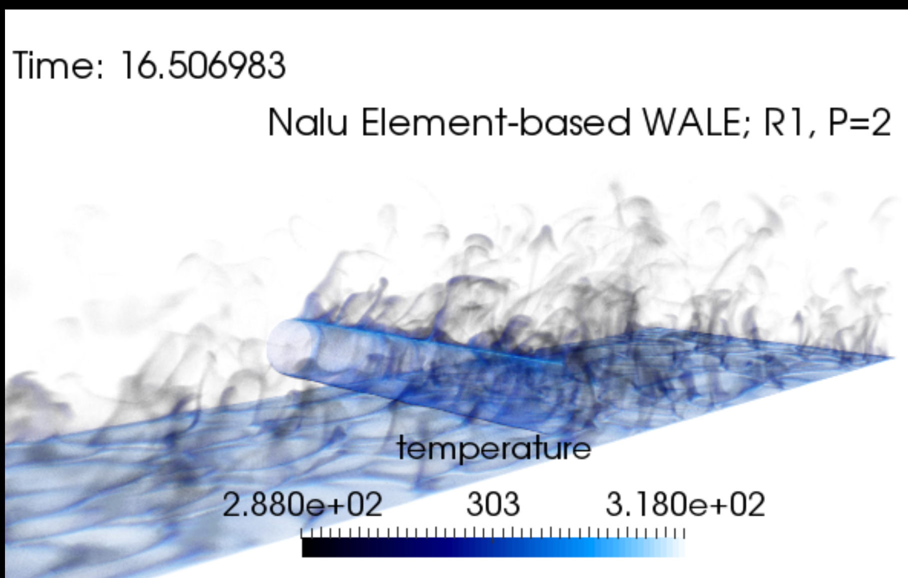
RANS-based simulation (v2-f, k-e) study conducted by Laskowski et al., AIAA 2007
DNS-based simulation study conducted by Kang et al., JCP, 2009

1. V&V Approaches to support the Abnormal/Thermal Environment; PI, Domino (V&V)

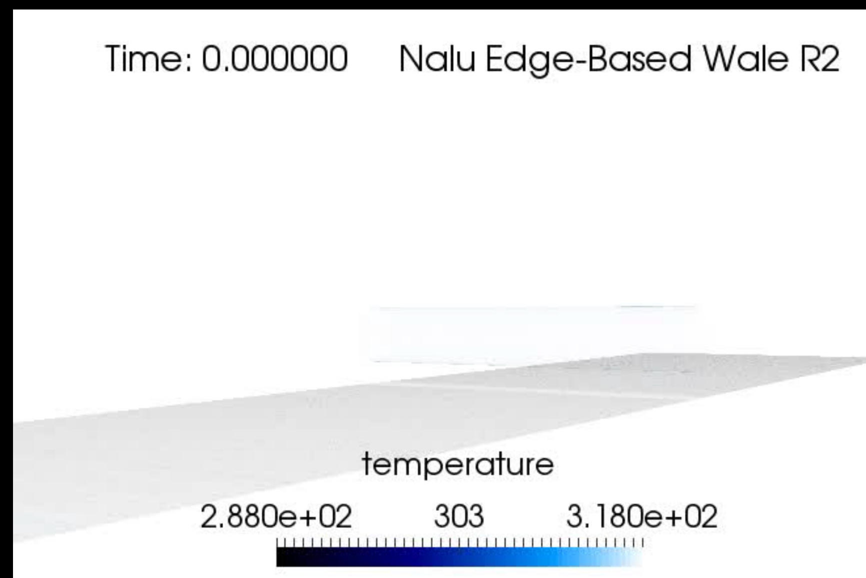
Towards Model Form Error (1/2)

Goal 1: Deploy standard V&V study (h- and P-refinement) with current set of LES models

WALE, Ksgs, and Smagorinsky model
- P=1 R0, R1 and R2; R2 ~O(100) million nodes
- P=2 R1



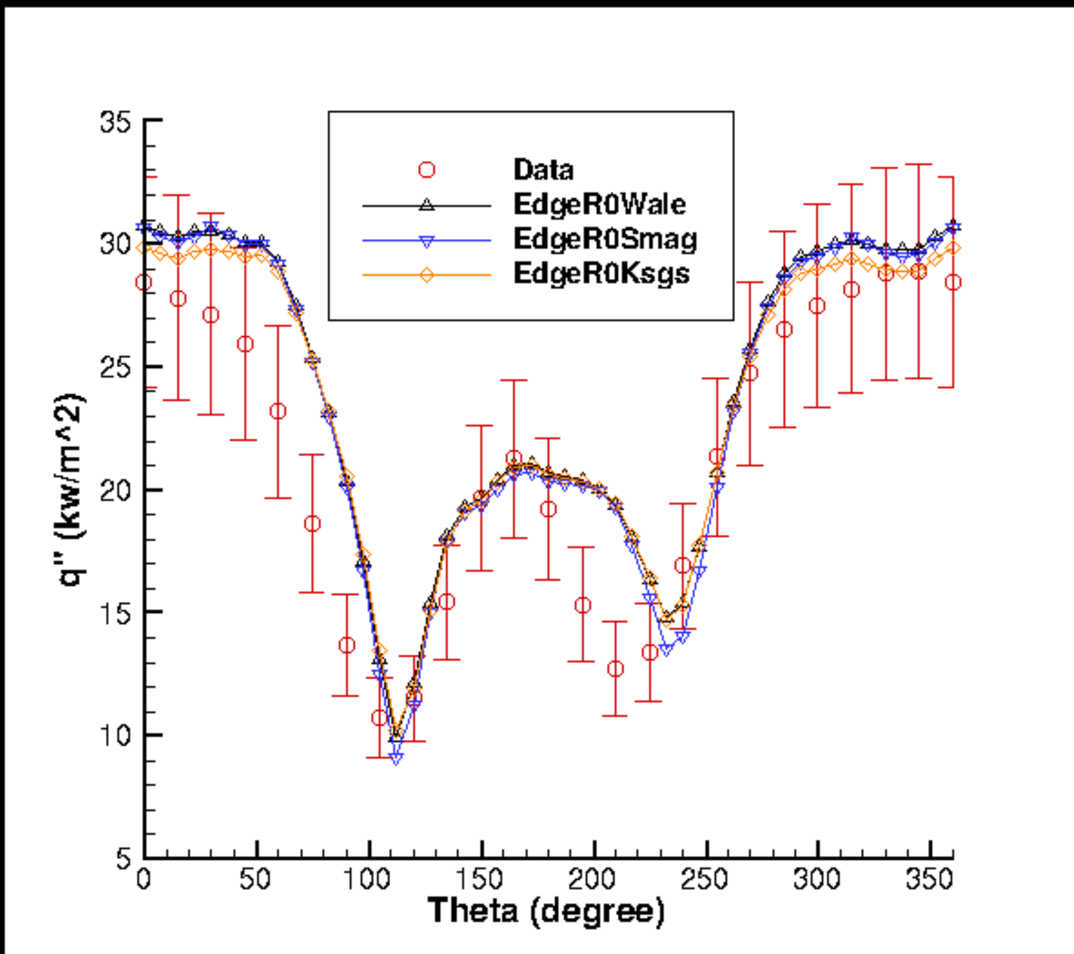
Typical Volume-rendered Temperature Field



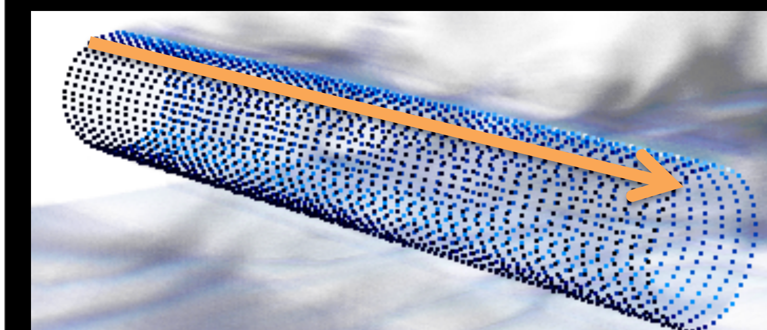
….. and P=1, EBVC movie

Towards Model Form Error (2/2)

Model form comparison using common LES sgs closure



Line-of-side post-processing



- Unstructured formulation Requires a line-of-site post processing technique
- 1% standard deviation in q”

LES using P=1 edge-based scheme with low-dissipation operators, BDF2

Goal 2: Advanced Model-Form Uncertainty Techniques

"A framework for epistemic UQ for turbulent scalar flux models for RANS", C. Gorle, 2013; Q3 activity

$$\rho < u_i' h > = -\frac{\mu_t}{Pt}\frac{\partial h}{\partial x_j}$$

Gradient diffusion hypothesis (fails for a simple shear flow)

$$\rho < u_i' h > = -C < u_i' u_j' > \frac{\partial h}{\partial x_j}$$

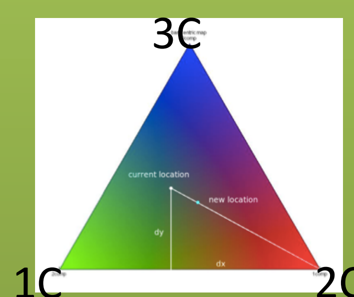
Generalized gradient diffusion hypothesis; Daly and Harlow, 1970

$$< u_i' u_j' > = 2k(\frac{1}{3} + v_{in}\Gamma_{nl}v_{jl})$$

* = perturb

QL-decomposition and GGDH implemented and about to be tested

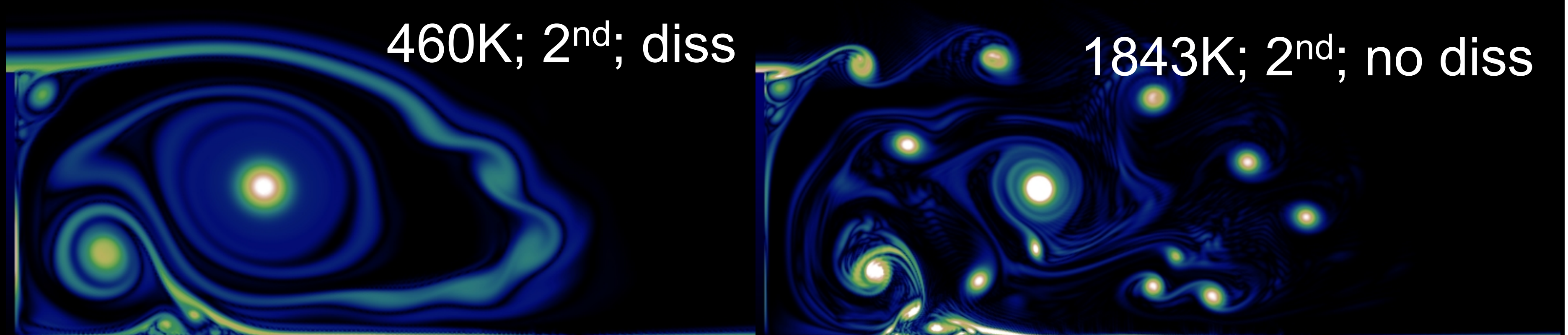
$$= 2k^*(\frac{1}{3} + v_{in}^*\Gamma_{nl}^*v_{jl}^*)$$



Barycentric map (Emory)

The low-Mach application space has extensive experience with low-order, low-dissipation schemes

Production low Mach algorithm for Abnormal/Thermal LES-based simulations is characterized as a low order (P=1), low dissipation (k.e. conserving) generalized unstructured CVFEM formulation



Re ~45K turbulent back step; vorticity magnitude

Question: What is the Viability of high-order schemes in low-Mach?

ASC Research project on continuous higher order methods with efforts on linear solver strategies and low Mach discretization (J. Hu, PI); Advantageous for NGP?

Goal 1: Implement and verify low Mach higher order method building from base CVFEM (P-based promotion; Domino, 2014) [Sweet spot of P=3? PC: M. Ihme; K. Jansen]

Goal 2: Are common pressure stabilization approaches used in low Mach equal-order interpolation design order?

Goal 3: Efficient linear solver interface/performance

Goal 4: Develop advanced stabilization approaches

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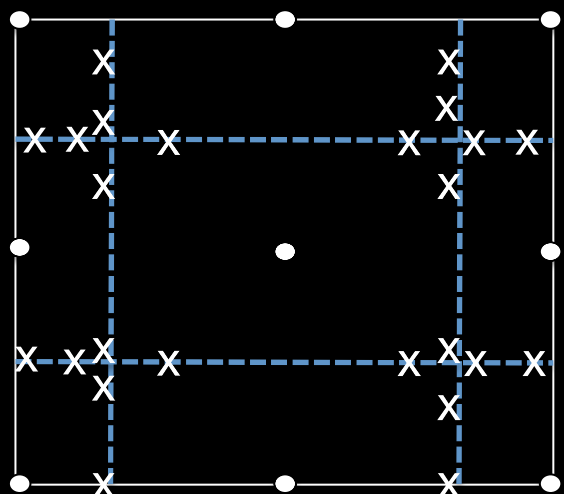
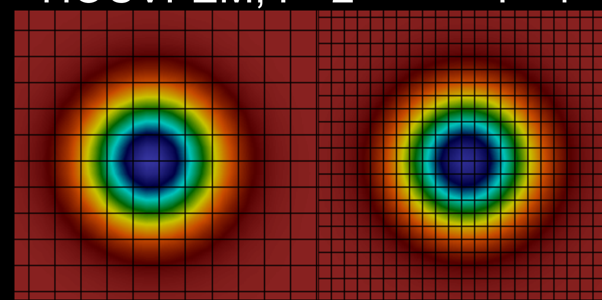
Location, location, location!

Quadrature locations are of the utmost importance!

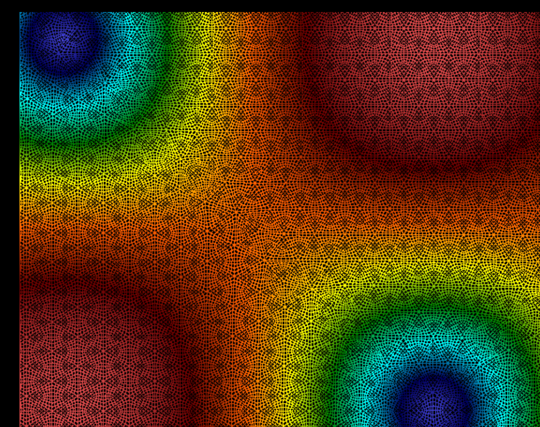


Dual volume definition; P=2
2x2 integration at scs/scv

HOCVFEM, P=2   P=1



Inviscid Taylor Vortex



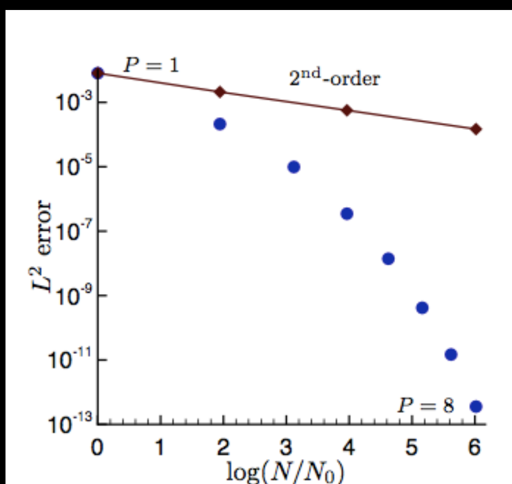
Steady Taylor Vortex

<u>Challenge</u>: pStab ~ $\tau(G_j\phi - d\phi/dx_j)n_j dS$

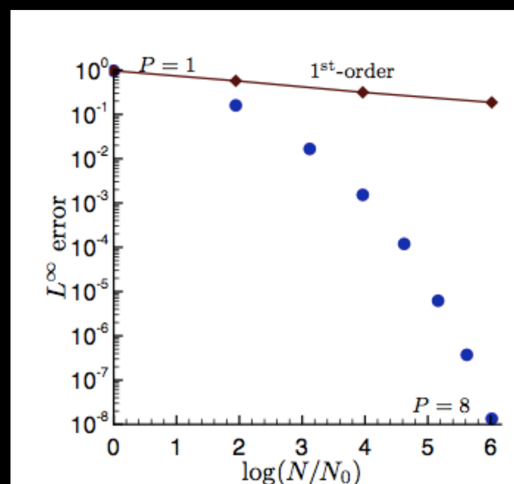
Finding: Current dual volume definition requires consistent integration for time, source, and L2 $G_j\phi$

Most unstructured CV-based methods are difficult to extend to H.O.

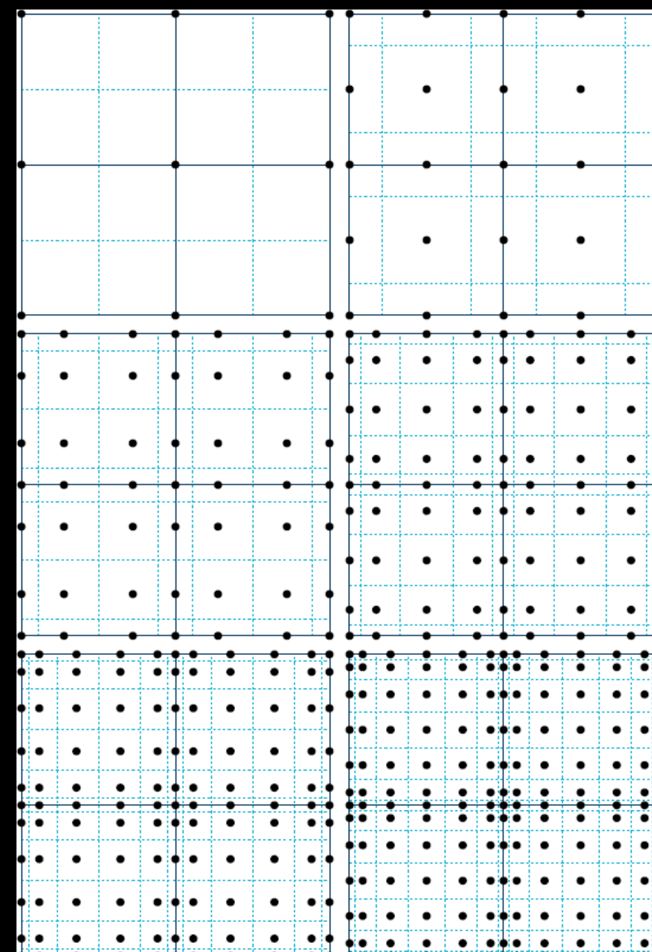
Spectral CVFEM demonstrated



d-o-f; $O(P^{+1})$

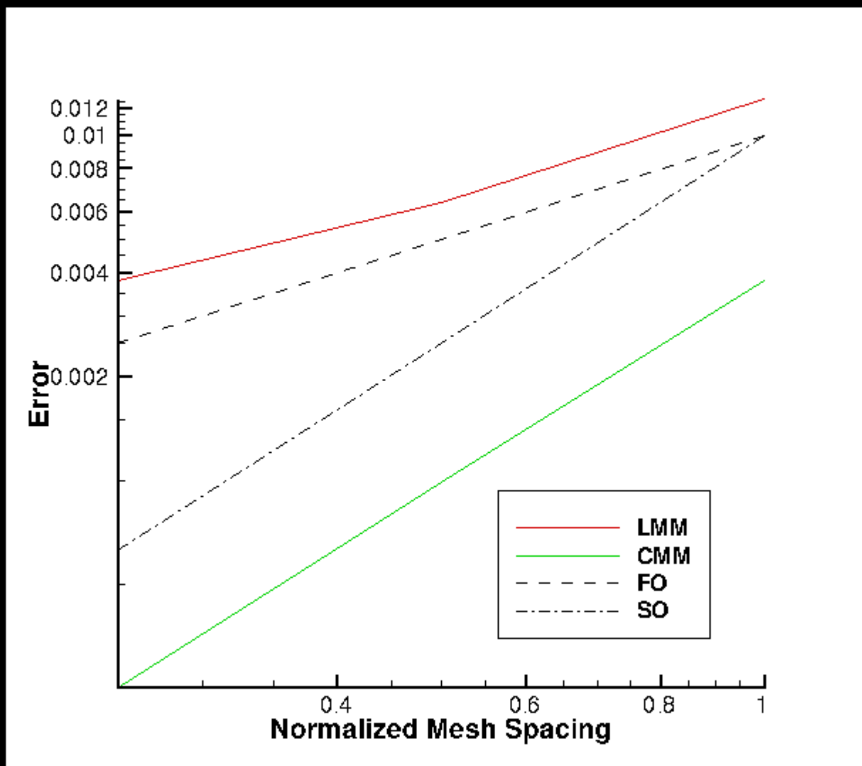


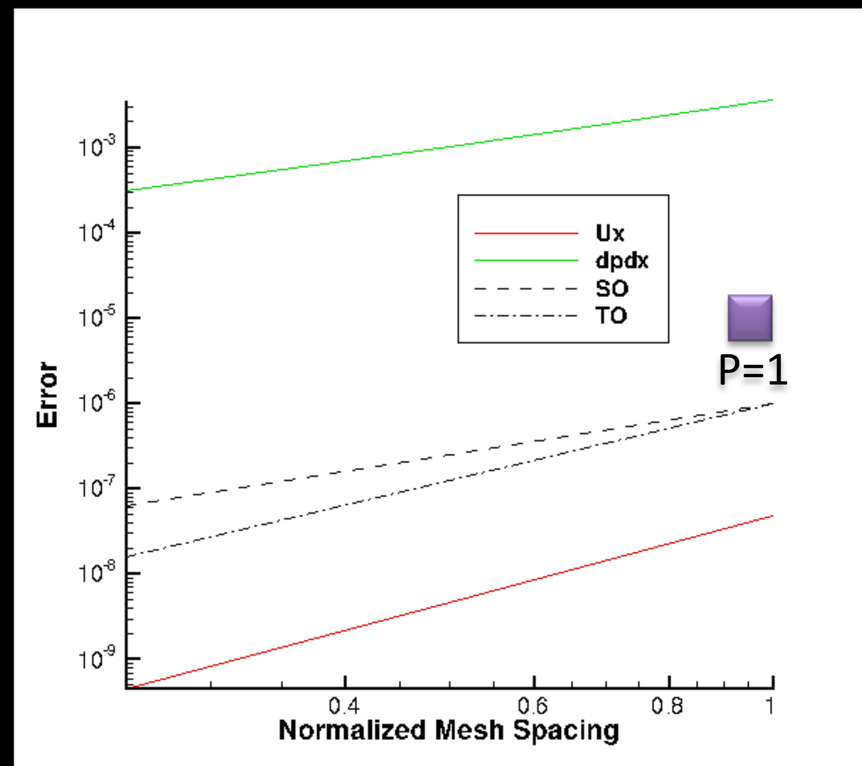
$G_j\phi$; $O(P)$



P=1:6 element integration rules (GLL/GL)

Code Verification (P1 vs P2)





L2 projected nodal gradients must be O(P)
CMM L2 Projection Equation must be solved!

Velocity verified to be O(3)
Pressure gradient O(2)

Lesson leaned: If one is verifying an unstructured scheme then use unstructured meshes !

Advanced Stabilization Approaches

Goal: Advanced the state-of-the-art nonlinear stabilization operators (NSO) (ASC Algorithms)

$$\sum_e \int_\Omega \nu(\mathbf{R}) \frac{\partial w}{\partial x_i} g^{ij} \frac{\partial \phi}{\partial x_j} d\Omega, \quad g^{ij} = \frac{\partial x_i}{\partial \xi_k} \frac{\partial x_j}{\partial \xi_k}, \quad g_{ij} = \frac{\partial \xi_k}{\partial x_i} \frac{\partial \xi_k}{\partial x_j}$$

FEM-based DCO (Shakib, 91)

Co-variant and contra-variant metric tensors

$$\nu(\mathbf{R}) = \sqrt{\frac{\mathbf{R_k R_k}}{\frac{\partial \phi}{\partial x_i} g^{ij} \frac{\partial \phi}{\partial x_j}}}$$

or min…..$\nu^{upw} = C_{upw}(\rho^2 u_i g_{ij} u_j)^{\frac{1}{2}}$

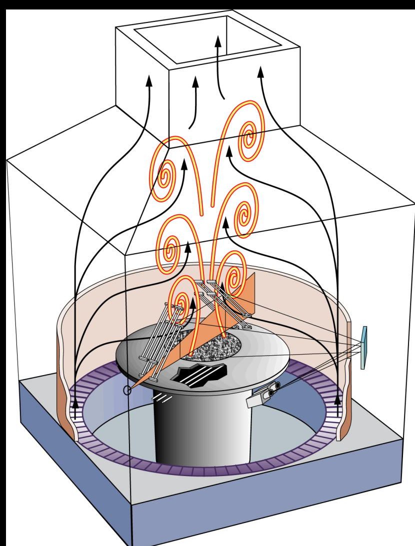
Coefficient based on local residual

Limit the coefficient based on an upwind analogy

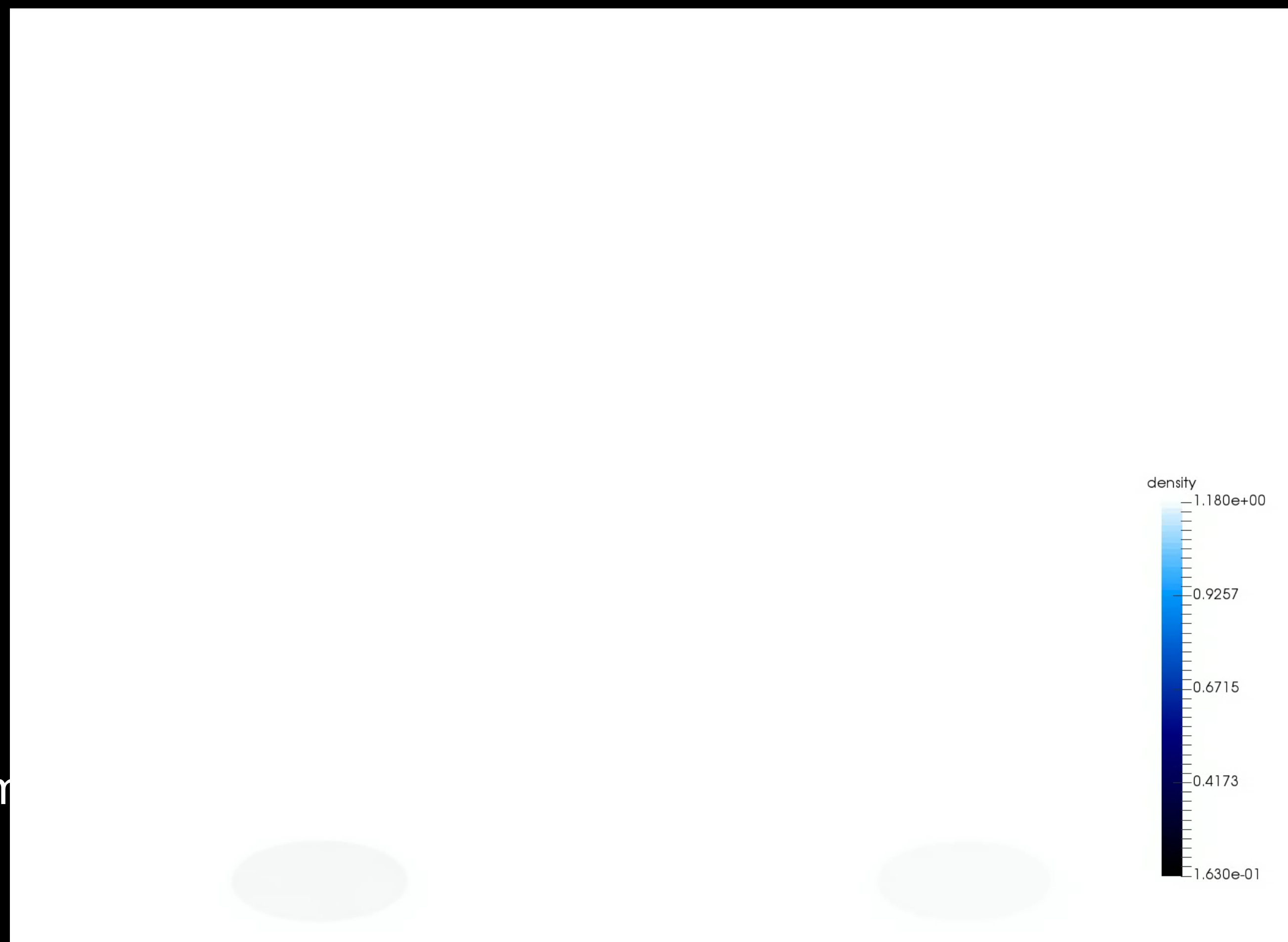
$$-\sum_e \int_\Gamma \nu(\mathbf{R}) g^{ij} (\frac{\partial \phi}{\partial x_j} - G_j \phi) n_i dS$$

Piecewise-constant test function converts to the CVFEM form of interest

Helium Plume DNS



Reduced Geometry from FLAME (above) to simple cylinder



P=1 (left); P=4 (right); same number of nodes

Conclusions

A variety of innovations are required to deploy LES to production ATE simulation studies

Discretization, solver, V&V and PEM activities are in progress to advance the state of the art

MMS First (not shown), model validation second

LES non-isothermal flow V&V study in transit; Model form uncertainties will be explored via λ decomp

Higher order methods look promising; compare to P=1

Models to incorporate buoyancy in LES simulations will be explored; will drive novel DNS study for a 1-m plume