SAND2016-8589PE

Exploring model-form uncertainties in Large Eddy Simulation (LES)

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1541, Comp. Thermal and Fluids Mechanics
September 6th, 2016
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Exceptional service in the national interest

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Outline

- Abnormal/Thermal Environment; Turbulence Basics
- Methodology for Validation (Step 1:n)
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- What about *Physics-form* Error?
- Future Efforts

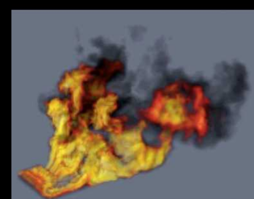
Abnormal/Thermal Stockpile Stewardship

SNL TTC

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

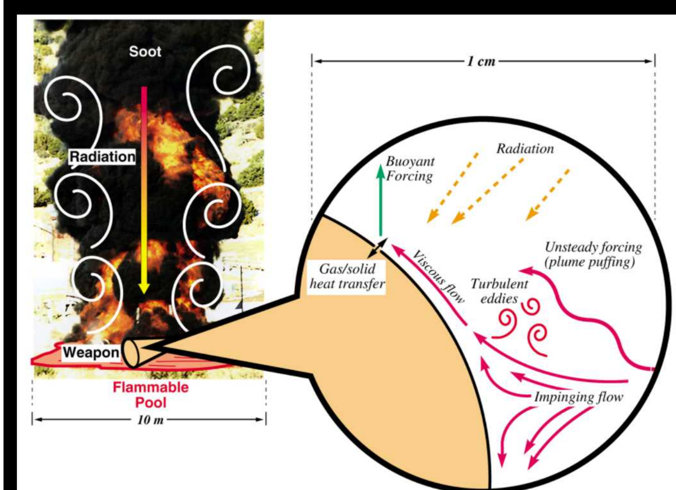
XTF for Cross Wind Fire

FLAME for Quiescent Fire



Previous studies; Hybrid-RANS
(volume-rendered T)

Heat Transfer Modes in a Fire



P henomena
I dentification
R anking
T able (PIRT)…

A process that is used to identify physics that:

- you know
- you think you know
- … and know that you "..know not of"

- For the fire physics, radiation, convection and conduction are dominant

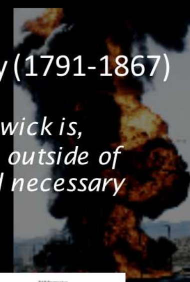
Evolution of a Mindset… *Quiescence*

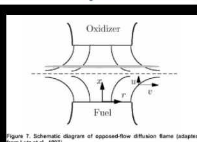
"I PURPOSE, in return for the honor you do us by coming to see what are our proceedings here, to bring before you, in the course of these lectures, the Chemical History of a Candle"

The Chemical History of a Candle, Michael Faraday (1791-1867)

Fig. 62

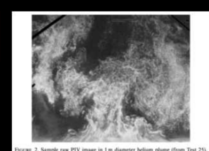
"In the middle of the flame, where the wick is, there is this combustible vapor; on the outside of the flame is the air which we shall find necessary for the burning of the candle"

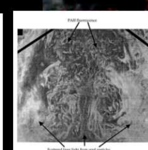




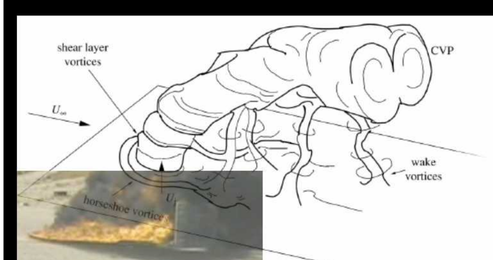
ODF; Martins et al, 2005


FLAME facility


O'Hern et al, JFM, 2005


Tieszen et al, C&F 2002

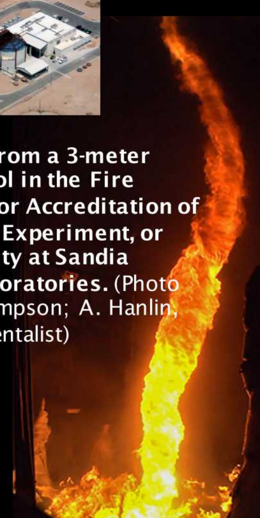
Evolution of a Mindset… *Cross Flow*



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

Conclusion: The inclusion of a cross-flow wind profile couples vorticity of the pool and streamwise momentum which drives the formation of column vortices, increases the importance of mixing and, therefore, convective loads on the object become more important

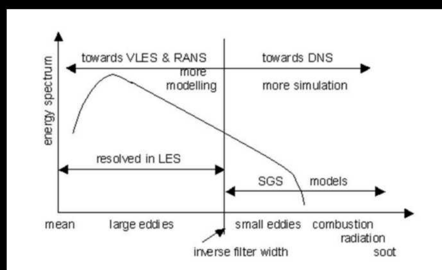
Change in mindset: Invest in Validation cases highlight the importance of convection physics



Fire whirls from a 3-meter diameter pool in the Fire Laboratory for Accreditation of Modeling by Experiment, or FLAME, facility at Sandia National Laboratories. (Photo by Richard Simpson; A. Hanlin, lead experimentalist)

Resolved Scale is *User* Defined

Direct Numerical Simulation (DNS), Large Eddy Simulation (LES) and Reynolds-Averaged Navier-Stokes (RANS) approaches define the computationally required time- and length scales



Direct Numerical Simulation:
- Simulation captures all relevant length- and time-scales
- No turbulence modeling
- Very expensive; total cost ~Re^3

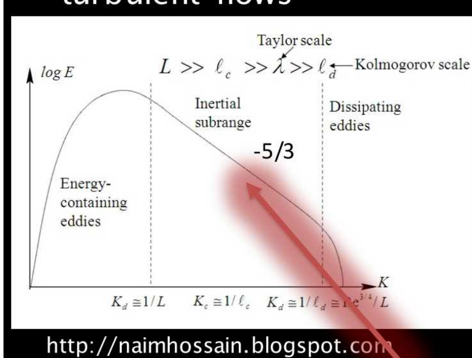
Large Eddy Simulation
- Resolve the large-scale motion that contains most of the flow's energy
- Model small scale based on scale- similarity
- Model = f(D)

Reynolds-Averaged Navier-Stokes
- Model the turbulence spectrum
- Empirical in nature

https://sites.google.com/site/smokeisnojoke/lesrans2.jpg

Towards LES Subgrid Models (PEM[1])

The standard turbulence decay (at least at the affordable LES scale) for momentum driven flows (shown below) does not apply to buoyancy generated turbulent flows



http://naimhossain.blogspot.com

Rayleigh/Taylor and Kelvin/Helmholtz instabilities

Are we ever really this resolved in engineering LES?

1. Development of subgrid LES models that include the effect of buoyancy; PL, Domino (P&EM)

Filtered LES low-Mach Equation Set

$$\int \frac{\partial \bar{\rho}}{\partial t} dV + \int \bar{\rho}\tilde{u}_j n_j \, dS = 0$$

Given filter: $\overline{\phi(\boldsymbol{x},t)} \equiv \int_{-\infty}^{+\infty} \phi(\boldsymbol{x}',t) G(\boldsymbol{x}'-\boldsymbol{x}) \, \mathrm{d}\boldsymbol{x}'$

$$\int \frac{\partial \bar{\rho}\tilde{u}_i}{\partial t} \mathrm{d}V + \int \bar{\rho}\tilde{u}_i\tilde{u}_j n_j \mathrm{d}S = \int \tilde{\sigma}_{ij} n_j \mathrm{d}S - \int \tau_{ij}^{sgs} n_j \mathrm{d}S + \int (\bar{\rho}-\rho_\circ)\, g_i \mathrm{d}V$$

$$\int \frac{\partial \bar{\rho}\tilde{h}}{\partial t} \mathrm{d}V + \int \bar{\rho}\tilde{h}\tilde{u}_j n_j \mathrm{d}S = -\int \bar{q}_j n_j \mathrm{d}S - \int \tau_{h,j}^{sgs} n_j \mathrm{d}S - \int \frac{\partial \bar{q}_i^r}{\partial x_i} \mathrm{d}V + \int \left(\frac{\partial \bar{P}}{\partial t} + \tilde{u}_j \frac{\partial \bar{P}}{\partial x_j}\right) \mathrm{d}V + \int \overline{\tau_{ij} \frac{\partial u_i}{\partial x_j}} \mathrm{d}V$$

Subgrid Stress (SGS): $\tau_{ij}^{sgs} \equiv \bar{\rho}(\widetilde{u_i u_j} - \tilde{u}_i\tilde{u}_j)$

$\tau_{h,j}^{sgs} \equiv \bar{\rho}\left(\widetilde{h u_j} - \tilde{h}\tilde{u}_j\right)$

Closure: $\tau_{ij}^{sgs} - \frac{1}{3}\delta_{ij}\tau_{kk}^{sgs} = -2\mu^t S_{ij}^*$

$$\int \frac{\partial \bar{\rho}\tilde{u}_i}{\partial t} \mathrm{d}V + \int \bar{\rho}\tilde{u}_i\tilde{u}_j n_j \mathrm{d}S + \int \left(\bar{P} + \frac{2}{3}\bar{\rho}k\right) n_i \mathrm{d}S = \int 2(\mu+\mu_t)\left(\tilde{S}_{ij} - \frac{1}{3}\tilde{S}_{kk}\delta_{ij}\right) n_j \mathrm{d}S + \int (\bar{\rho}-\rho_\circ)\, g_i \mathrm{d}V$$

$$\mu_t = \rho\,(C_s\Delta)^2\,|\tilde{S}|$$

Smagorinsky: $\mu_t = \rho\,(C_s\Delta)^2\,|\tilde{S}|$

Ksgs: $\mu_t = C_{\mu_\epsilon}\Delta k^{\mathrm{sgs}\,\frac{1}{2}}$

WALE: $\mu_t = \rho\,(C_w\Delta)^2 \dfrac{\left(S_{ij}^d S_{ij}^d\right)^{3/2}}{\left(S_{ij}S_{ij}\right)^{5/2} + \left(S_{ij}^d S_{ij}^d\right)^{5/4}}$

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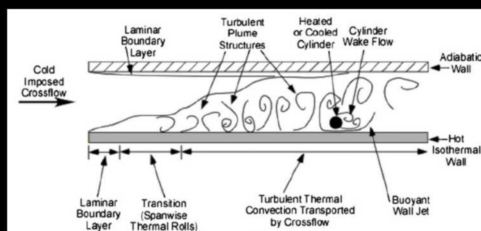
Definition of Validation Case

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, 2005

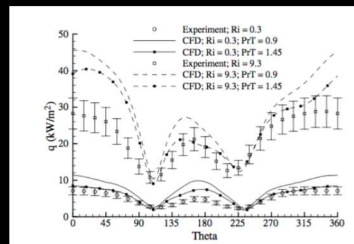


Fig. 13. Effect of turbulent Prandtl number on cylinder heat flux predictions for cases 3 (cooled cylinder) and 4 (heated cylinder).

Laskowski et al., 2007

RANS Conclusion: The presence of the heated bottom wall significantly challenged ability to predict the QoI; q"

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

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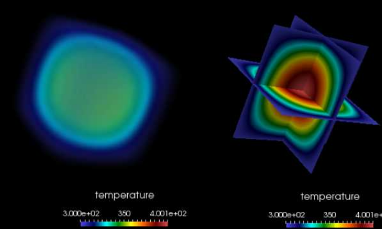
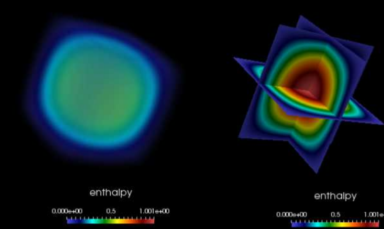
Variable Density MMS, non-Isothermal

Density is a function of static enthalpy transport via standard ideal gas $\rho = f(P, M, R, T)$

Temperature range ~maps to Kearney (400-500 K); g_i is arbitrary and misaligned



Temperature

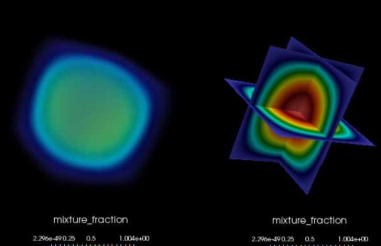


Enthalpy

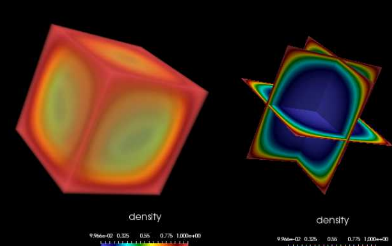
Variable Density MMS, non-Uniform

Density is a function of species transport via standard mixture fraction weighting $\rho = f(Z)$

Density ratio maps to a helium plume, e.g., ~10x; g_i is arbitrary and misaligned



Mixture Fraction



Density

CVFEM Discretization

The core discretization used in the NW low-Mach code base has been the Control Volume Finite Element Method, CVFEM

An elemental basis is defined from which interpolation and gradients within the element are determined

The test function is defined to be piece-wise constant

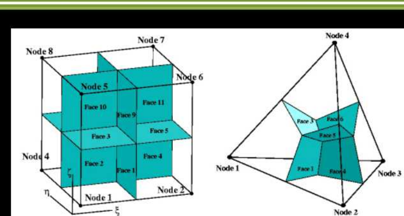
This method can best be described as a Petrov-Galerkin method

The canonical 27-point stencil is recovered

$$\int w \frac{\partial \bar{\rho} \tilde{u}_j \tilde{\phi}}{\partial x_j} d\Omega = -\int \bar{\rho} \tilde{u}_j \tilde{\phi} \frac{\partial w}{\partial x_j} d\Omega + \int w \bar{\rho} \tilde{u}_j \phi n_j \, d\Gamma$$

$$w = w_I; \frac{\partial w_I}{\partial x_j} = -\delta(x - x_{scs})$$

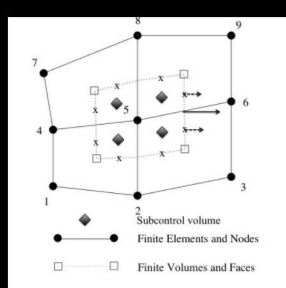
$$\int w \frac{\partial \bar{\rho} \tilde{u}_j \tilde{\phi}}{\partial x_j} d\Omega = \sum_{ip} \left(\bar{\rho} \tilde{u}_j\right)_{ip} \tilde{\phi}_{ip} n_j dS = \sum_{ip} \dot{m}_{ip} \tilde{\phi}_{ip}$$



Hexahedral Dual Mesh (L)
Tetrahedral Dual Mesh (R)

Edge-based Vertex Centered Discretization

In this method, the dual mesh is defined to establish geometric values at the edge midpoint (area vector) and node (volume)

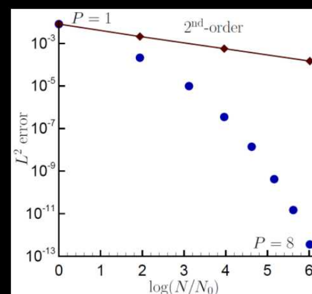


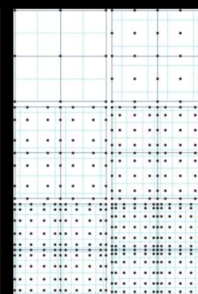
Quadrature points for edge-based scheme

Ramifications for the edge-based finite volume (EBFV) structure are as follows:

- Reduced stencil (27-point to 7-point for structured hex)
- Simple L/R data structure allows for simple interpolation and orthogonal gradient contributions
- Lack of elemental basis requires a diffusion operator in terms of orthogonal to the edge and non-orthogonal correction that requires projected nodal gradients
- 2-4x faster than CVFEM or GFEM
- Limited to second order in-space

CVFEM: Extension to Spectral Convergence



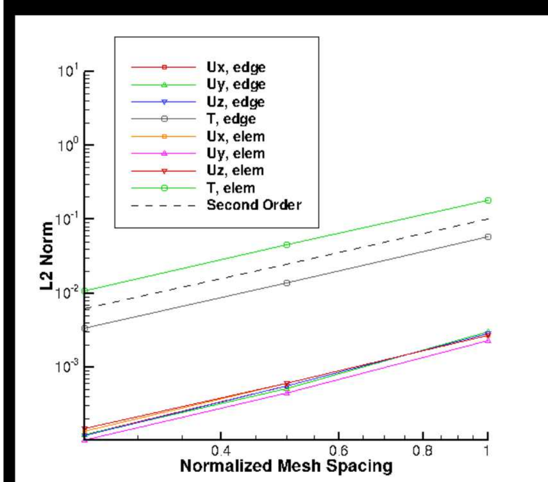


1-meter helium plume simulation comparing P=1 (left) and P=4 (right) on the same number of node mesh (shown: volume-rendered density)

Spectral CVFEM convergence (left) and polynomial promotion (right) from P=1 to P=6 outlining the dual mesh configurations (four-element patch)

Simulations conducted by R. Knaus (1532) in support of ASC IC Research (Hu, PI)

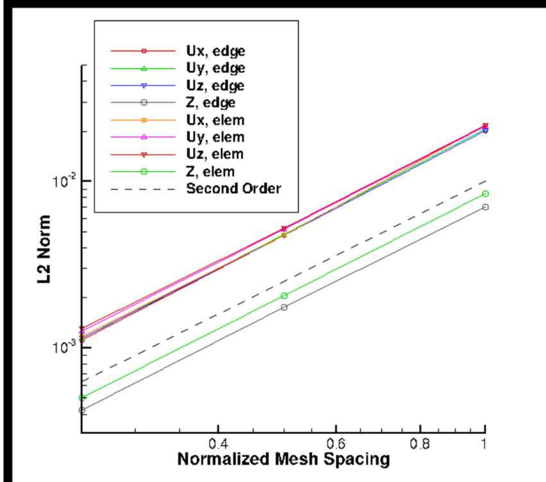
Variable Density MMS, non-Isothermal



Findings:

- MMS study revealed no surprises
- P=1 is O(2) for both edge- and element-based schemes
- Mixture fraction-based analysis/validation efforts can proceed now
- Unit testing of turbulence models due to algebraic nature
- ✓ Core kernels shared between all scalar transported variables, e.g., Z, h, Ksgs, etc

Variable Density MMS, non-Uniform



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What about *Physics-form* Error?

Future Efforts

Testing Matrix

Three numerical methods:

Low order edge- element-based (P=1); element-based (P=2); with code verification

Three core LES models

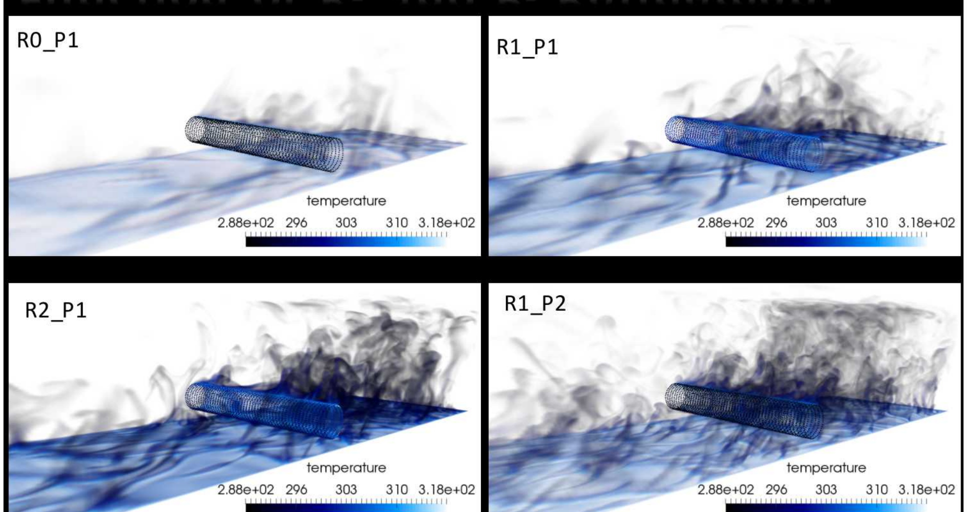
Three mesh resolutions (R0, R1 and R2)

O(10) simulations run to establish model-form error

O(10) simulations run to establish physics-form error

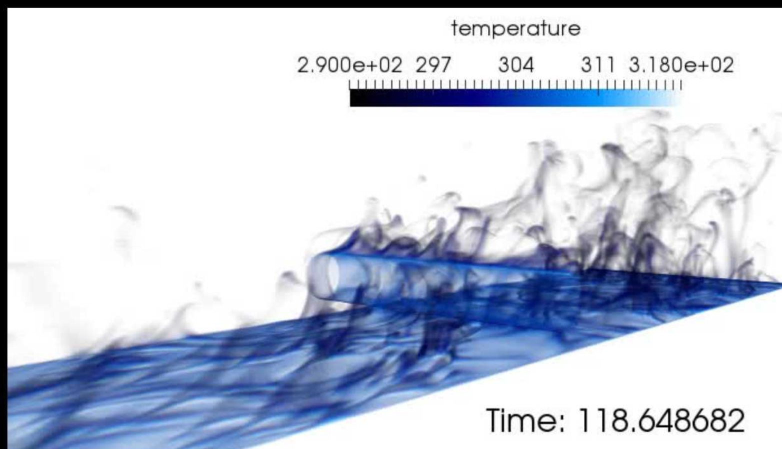
In the end, ~2.5 million CPU hours, however, not capability-based computing (2048 max core)

Thermal Plume Structure as a Function of R- and P- Refinement

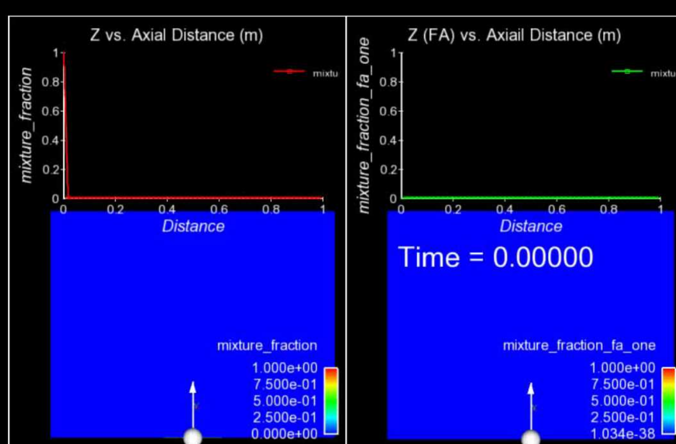


Note: Increased resolution yields finer plume structure; higher order ++

R2_P1 Volume-rendered Temperature Field

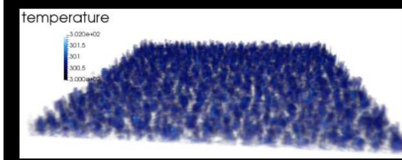


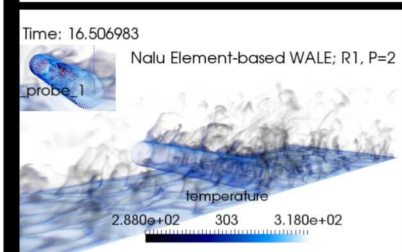
The Bane of Transient Turbulent Simulations: Many flow-through-times required for convergence

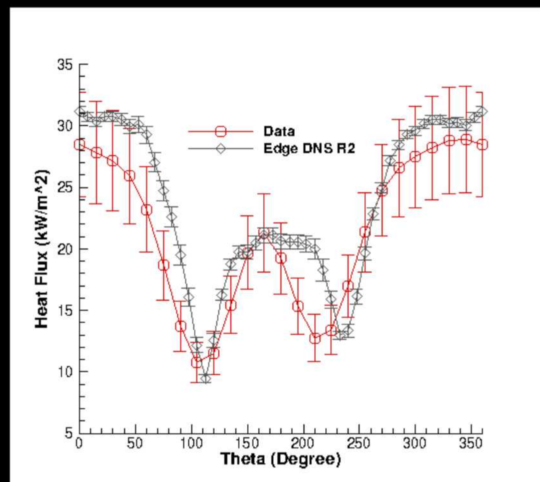


Typical LES/DNS simulation must proceed until converged statistics, above shown for a 1-meter helium LES

For the X-flow Simulation, Statistical Convergence is Expensive



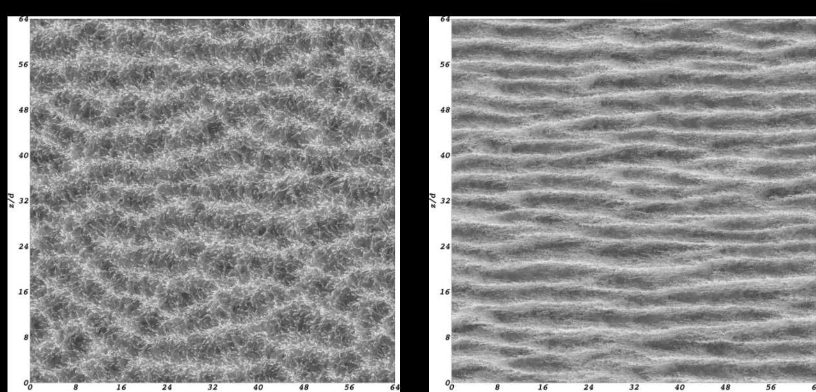




Rayleigh Bernard simulation (Top) X-flow (Bottom; inset L-O-S); both volume-rendered temperature

Simulation deemed converged when mean QoI ~ 1%; σ ~3%; ~250 seconds of M-N-T

Leveraging DNS work of Curtis Hamann



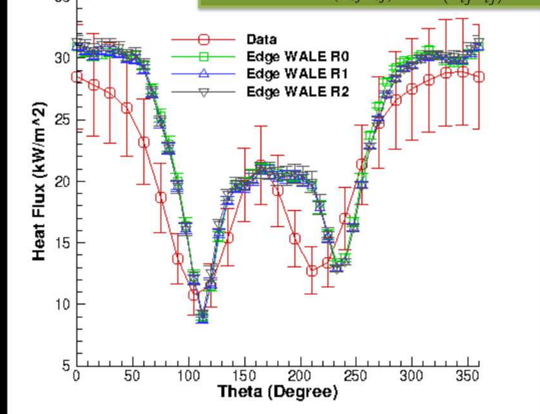
Temperature (white: hot; dark:cool) for a Rayleigh/Bernard configuration; Left (low cross flow); Right (high cross flow)

- Streaks observed in low-Ra DNS similar in structure and spanwise size

Personal communication of currently unpublished results

LES Solution Verification (WALE)

$$\mu_t = \rho (C_w \Delta)^2 \frac{(S^d_{ij} S^d_{ij})^{3/2}}{(S_{ij} S_{ij})^{5/2} + (S^d_{ij} S^d_{ij})^{5/4}}$$

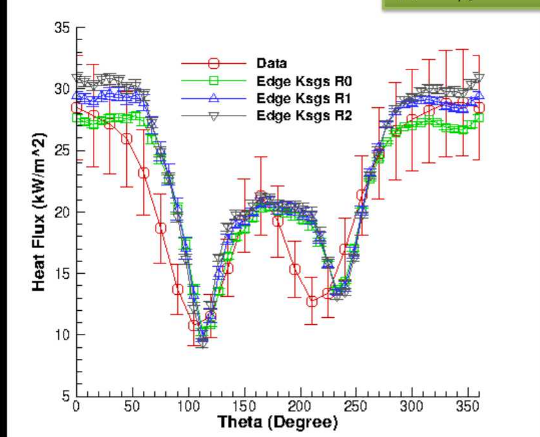


Attributes of Wall-adapting local-eddy viscosity (WALE):
Nicoud and Ducros, 1999

- Algebraic LES model
- Isotropic eddy viscosity assumption in which turbulent viscosity = f(Δ,S_{ij} invariants)
- proper scaling near the wall ($\mu^t \sim y^3$)
- Dynamic procedure possible as per Germano's identity (Germano, 1991); $T_{ij} = \tau_{ij} + L_{ij}$

LES Solution Verification (Ksgs)

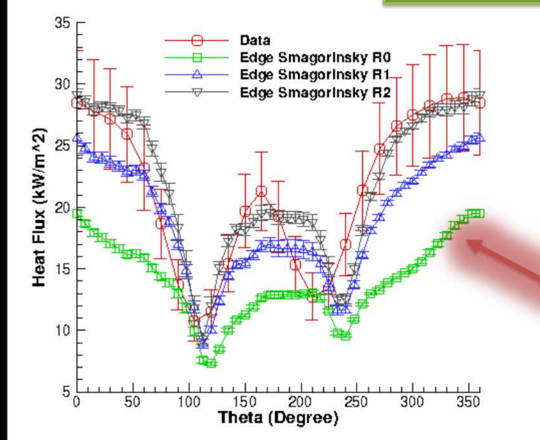
$$\mu_t = C_{\mu_\epsilon} \Delta k^{\mathrm{sgs}\,\frac{1}{2}}$$



Attributes of Ksgs:

- PDE-based LES model derived from the mechanical energy equation (filtered, subtracted, etc)
- Isotropic eddy viscosity assumption in which turbulent viscosity = f(Δ,Ksgs)
- Allows for increased model fidelity for, e.g., buoyant flows
- Dynamic procedure possible as per Germano's identity (Germano, 1991); $T_{ij} = \tau_{ij} + L_{ij}$

LES Solution Verification (Smagorinsky)

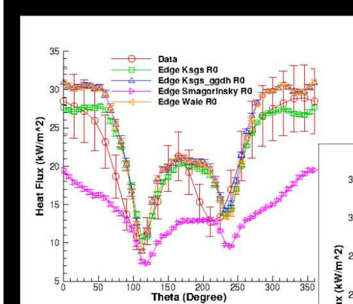


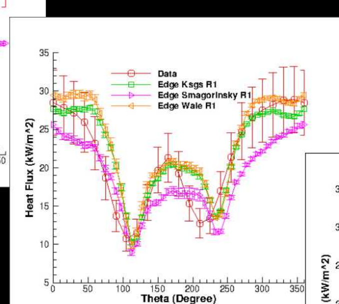
$\mu_t = \rho (C_s \Delta)^2 |\tilde{S}|$

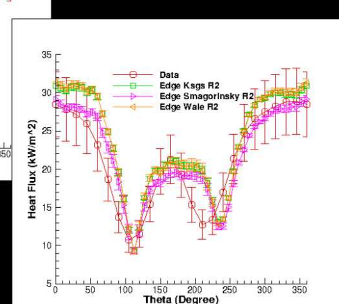
Attributes of Smagorinsky:
Smagorinsky (1963)

- Simplest of any LES model (period)
- Isotropic eddy viscosity assumption in which turbulent viscosity = f(Δ,|S|)
- In general, poor for most flows
- Lack of proper scaling near the wall ($\mu^t \sim y^3$) requires either damping functions (Van Driest, exponential dampening, 1956) or a dynamic procedure
- Dynamic procedure possible as per Germano's identity (Germano, 1991); $T_{ij} = \tau_{ij} + L_{ij}$

Edge-based R0/R1/R2 Model-form

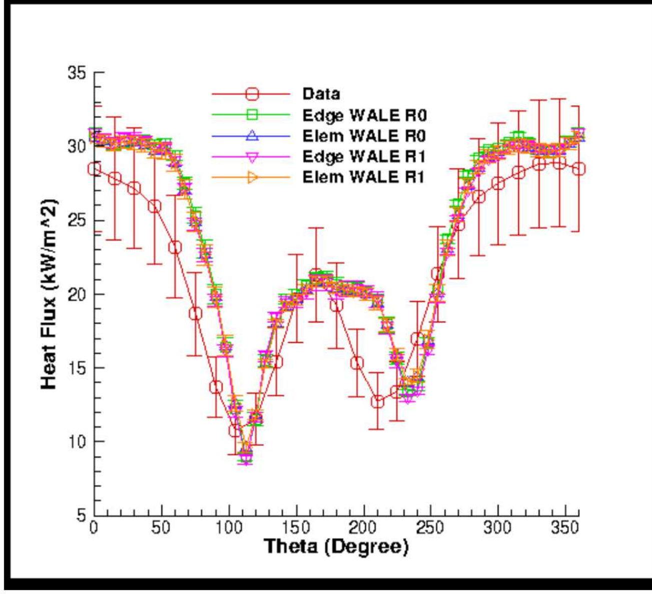






Conclusion: All models other than Smagorisnky are seemingly convergent (at this mesh resolution range) *[however, not to the data…]*

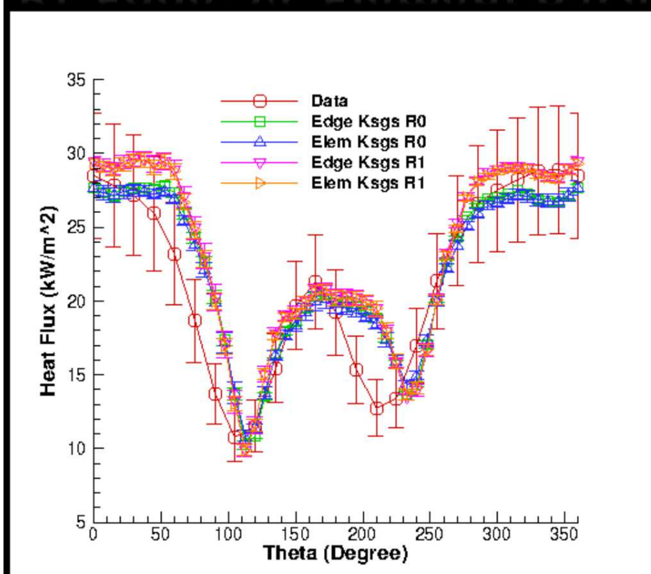
P1 Edge- vs Element-based; (WALE)



Findings

- WALE model seems insensitive to numerical method at both R0 and R1
- Low-order edge- and element-based seem to provide the same simulation results wrt QoI

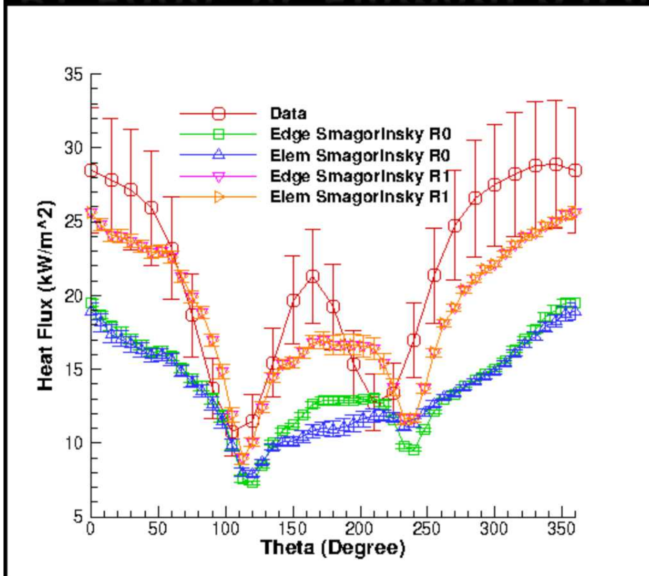
P1 Edge- vs Element-based; (Ksgs)



Findings

- Ksgs model also seems insensitive to numerical method within the mesh resolution range
- Low-order edge- and element-based seem to provide the same simulation results wrt QoI

P1 Edge- vs Element-based; (Smagorinsky)

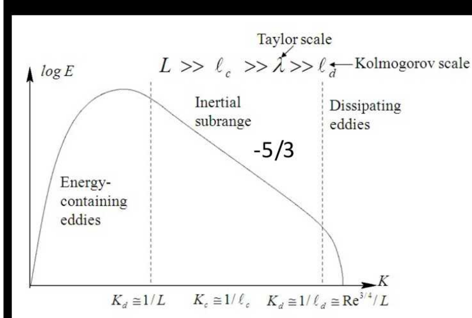


Findings

- Smagorinsky model shows sensitivity to mesh over discretization ranges only at R0 mesh
- Low-order edge- and element-based seem to provide the same simulation results wrt QoI at finest mesh

LES Model-form Scaling

Why is the sensitivity to numerical method so low?



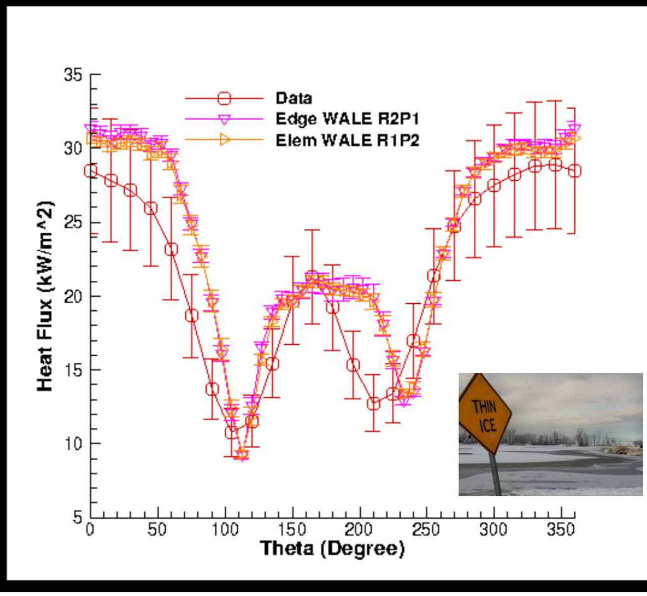
http://naimhossain.blogspot.com

Kolmogorov's second similarity hypothesis:

For every turbulent flow at sufficiently high Re, statistics of the motions of scale *lc* within the inertial subrange *have a universal form*

- Within the inertial subrange, motions are determined by inertial effects with viscous effects negligible
- Within the dissipation range, motions are driven by viscous effects
- This drives velocity scale as ~$u^{1/3}$
- Turbulent kinetic energy ~$k^{-2/3}$

Edge(P1R2)- vs Element(P2R1)-based; (WALE)



Possible explanation for insensitivity of LES results on underlying numerical discretization/order?

- Scaling for typical LES SGS models are as follows:
  - Smagorinsky $\sim\Delta^{4/3}$
  - WALE $\sim\Delta^{4/3}$
  - Ksgs $\sim\Delta^{5/3}$
- For a given mesh resolution, final result is generally a function of model + numerics
- At a given mesh resolution, is there a way to choose the optimal P?

Take-away Points for Discretizations

Edge-based scheme provided similar LES quality results for all turbulence models at ~¼ the cost

In general, the community is in a somewhat divided state over low- and higher-order methods for LES
Recall, model form convergence $\sim\Delta^{4/3}$ or $\Delta^{5/3}$

Most agree that low-dissipation low-Mach discretization choices is a critically important attribute

Advance models for LES and higher-order methods are required given the universal scaling of model form error is lower than discretization error (for P > 2)

Outline

Abnormal/Thermal Environment; Turbulence Basics

Methodology for Validation (Step 1:n)

- Step 1: Definition of the Validation Study
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- Step 3: Solution Verification
- Step 4: Advanced LES Model-form Sensitivity

What about *Physics-form* Error?

Future Efforts

Model-form Error in LES?

Algorithmic and modeling constraints for the

^ application of LES to design

Sanjeeb Bose (Cascade, ICME-Stanford) & Frank Ham (Cascade, CTR)

L Shunn, G Bres, D Philips, M Emory, A Saghafian, D Kim, B Hejazi, P Quang [Cascade Tech.]

CASCADE TECHNOLOGIES

Relatively little is known about modeling errors
in the absence of validation data

In the limit when grid convergence to an asymptotic (dissipative) range is infeasible and no DNS/expt. data is available, what can we say about the simulation error?

Current lack a rigorous approach for estimating *modeling* errors in LES
... novel attempts have been made for RANS modeling (Emory et al 2013)

Should make efforts to use the same standard that's used in experiments

In what way can we drive model form *estimation* for LES?

- Topic recently highlighted by Dr Sanjeeb Bose; July 20th, 2016 CTR summer program
- Developing state-of-the-art:
  - parametric studies of model constants, thermal/diffusion parameters, etc.
  - PCE (see Safta et al., IJNMF, 2016)
  - High-/low- fidelity (Eldred and Geraci, 2016)
- Is there a way to incorporate previous RANS-based sensitivity studies to the LES application space?

Eigen-value Decomposition of b_{ij}

"Estimating model-form uncertainty in Reynolds-Averaged Navier-Stokes Closures", M. Emory, 2014

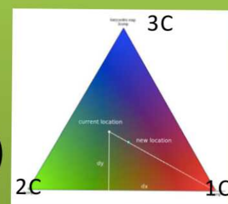
$$a_{ij} = \overline{u_i' u_j'} - \frac{2}{3} k \delta_{ij} \quad b_{ij} = \frac{a_{ij}}{2k}$$

$$< u_i' u_j' >= 2k(\frac{1}{3} + b_{ij})$$

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

Six-dof perturbation + k

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



Barycentric map (Emory)

Γ = matrix of perturbed eigenvalues, v eigenvectors

Extension to Scalar SGS Closure

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

$$\tau_{h,j}^{sgs} = -\frac{\mu_t}{\mathrm{Pr}_t} \frac{\partial \tilde{h}}{\partial x_j}$$

Gradient diffusion hypothesis (fails for a simple shear flow)

$$\tau_{h,j}^{sgs} = -\alpha_c \tau_c \tau_{jk}^{sgs} \frac{\partial h}{\partial x_k}$$

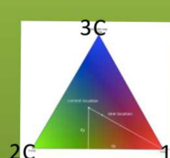
Generalized gradient diffusion hypothesis; Daly and Harlow, 1970

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

QL-decomposition using fast-3x3 algorithm

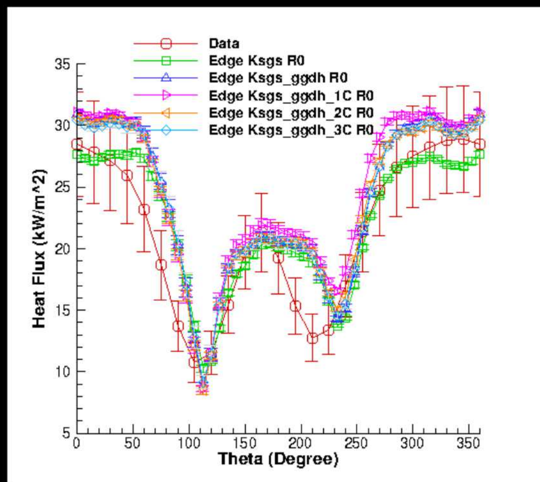
$$= 2k^*(\frac{1}{3} + v_{in}^* \Gamma_{nl}^* v_{jl}^*)$$

* = perturb



Barycentric map (Emory)

Perturbation to 1C, 2C & 3C Poles
(instantaneous τ_{ij} within scalar SGS only)



Findings:

- Minimal sensitivity in Scalar SGS closure; possibly due to plain-shear channel flow

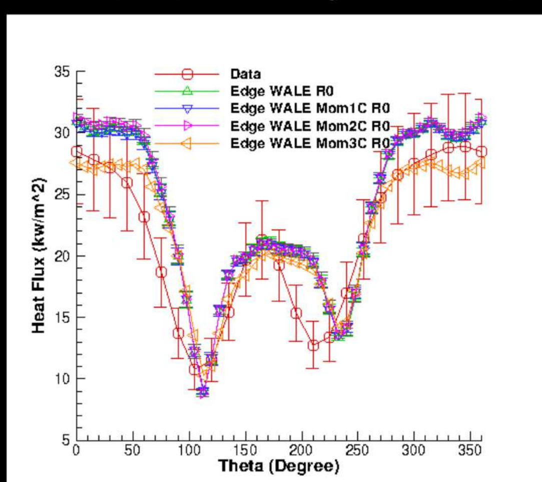
GDH: $\overline{v'c} = -\frac{\nu_t}{\sigma_t}\frac{\partial C}{\partial y}$

GGDH: $\overline{v'c} = -\alpha_c \tau_c \overline{v'v'}\frac{\partial C}{\partial y}$

Q: $\overline{v'c} = -\alpha_c \tau_c \frac{1}{k}[(\overline{u'v'})^2 + (\overline{v'v'})^2]\frac{\partial C}{\partial y}$

- Model form modification pushed closer to DNS, however, further from experimental data (later)
- Is this legal?

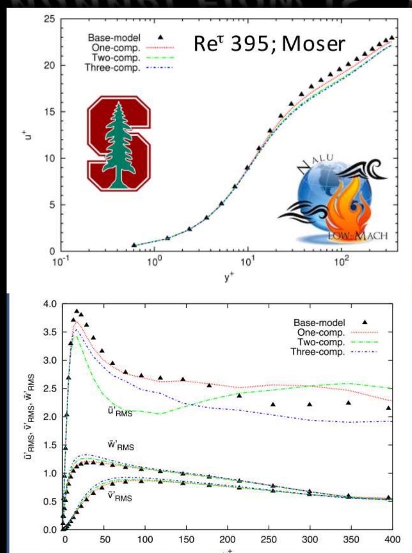
Perturbation to 1C, 2C & 3C Poles
(instantaneous τ_{ij} within momentum SGS only)



Findings:

- Still seems that there is a minimal sensitivity in SGS closure
- However, three-component biasing drastically increased mixing
- Model form modification pushed closer to DNS, however, further from experimental data (later)
- Is this legal?
- Perhaps a more fundamental flow should be explored?

Questions? Reverting to *Plain Channel Flow* is "your best option"



Findings:

- Bounding of data seems to be conceptually different from RANS
- Still on-going questions as to the realizable of the SGS stress tensor (Vreman, JFM, 1994)
- Foundational work is planned both this year (PSAAP-2 interaction) and next FY (subject to V&V project renewal)
- Stanford partnership with G. Iaccarino and L. Jofre during the 2016 CTR summer program
- Interesting WMLES ramifications
- CU@ SIAM CSE2017, "UQ in Turbulent flow Simulations"

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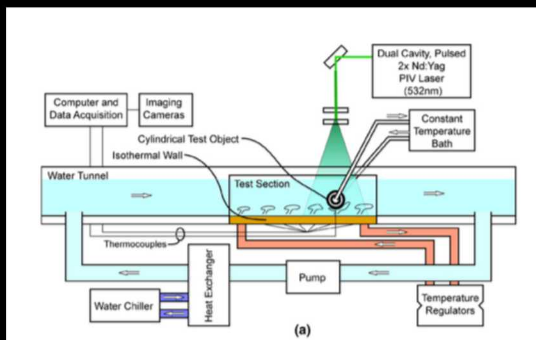
What about *Physics-form* Error?

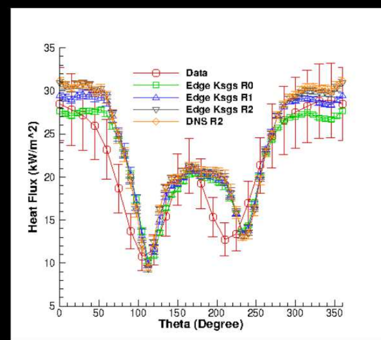
Future Efforts

Physics-Form Error

Finding: The LES is consistent with DNS, however, is different from Kearney's experiment. Why?



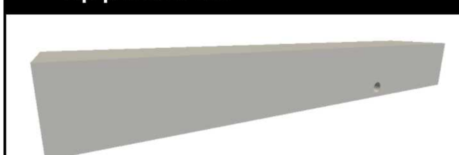
Kearney experimental configuration

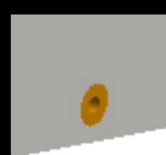


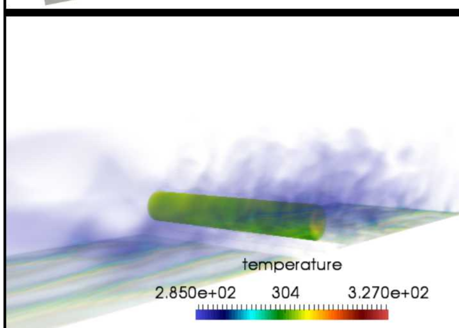
Ksgs convergence with DNS

Physics-Form Error: +inner thermal physics

Classic Fluids/Thermal Conjugate Heat Transfer application





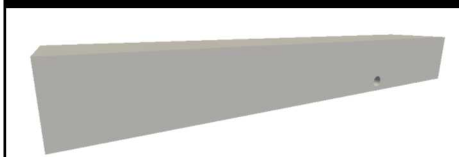


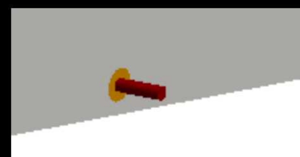
New Specifications

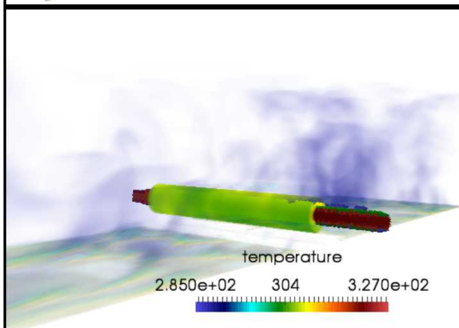
- Internal heat conduction physics added (uniform properties of SS)
- Inner heat flux applied (based on energy balance from experiment)
- Not without precedent; Kang et al, JCP 2009 (DNS with optimization loop)

Physics-Form Error: +inner thermal physics + inner fluids physics

More complex Fluids/Thermal/Fluids Conjugate Heat Transfer application







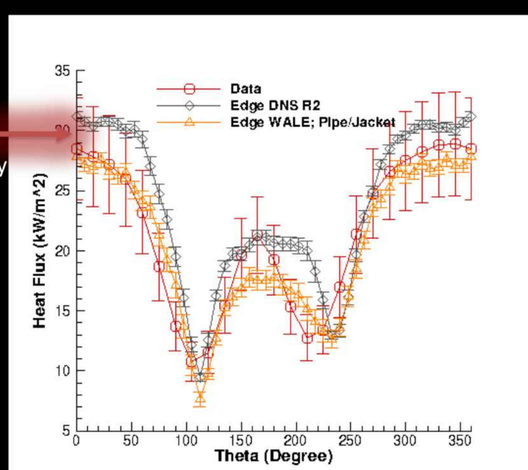
New Specifications

- Inner fluid (water) 1.12 GPM; 327 K; Re ~150K
- As reported in the experiment, inlet and outlet pipe temperature within ~1K
- Disparity in Re-numbers suggest a more sophisticated operator split time advancement; lock step for now (Picard loop)

Physics-Form Error: +inner thermal physics + inner fluids physics

Prediction improved with each added physics!

Inner q”
This aproach slightly drops stagnation point heat flux



Physics-form prevails… In this study it is #1….

Conclusions

Systematic validation methodology outlined for a low-Mach LES DSW problem-of-interest; #1 Physics Form ε !

Remember the steps! Code verification before validation

Solution verification, although problematic for LES, should be performed (simple due diligence)

Model-form studies for LES are pedestrian (no offence)

Model-form uncertainties via eigenvalue perturbations is a novel, possibly promising area

Standard LES models within Solution verification converge rate lower than P=2 numerics....

My Thanks to...

Walt Whitkowski; kick-off 2016 VVUQ project
  Domino, PI

David Womble and the ATCC-1 committee
  ~2+ million CPU hours consumed on Cielo; dedicated Skybridge queue for CTR visiting scholar position

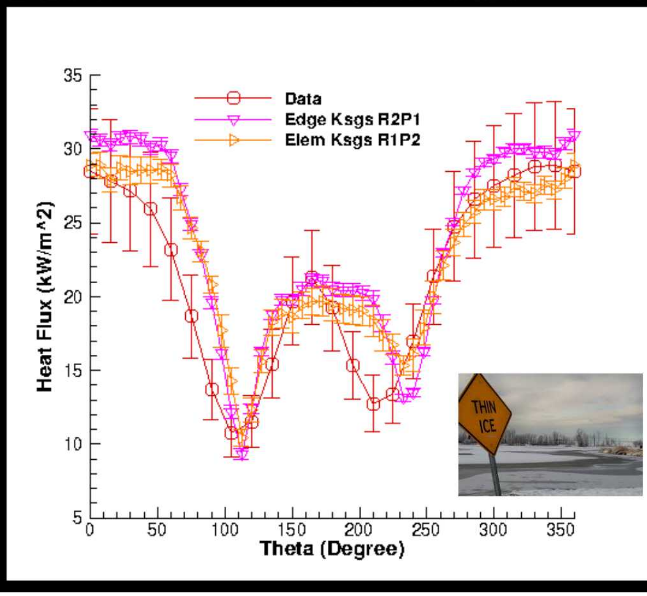
Robert Knaus

Stanford team

The SNL pioneers

https://github.com/spdomin/Nalu

Edge(P1R2)- vs Element(P2R1)-based; (Ksgs)



What about for Ksgs?

- $\mu^t \sim C\,\Delta\, Ksgs^{1/2}$
- Assuming that we are within the inertial subrange, i.e., a legitimate LES, k ~ -2/3
- Therefore, model form error is $\sim\Delta^{5/3}$
- This suggests that for P >2, solution verification will demonstrate a dominant modeling form error
- If HO methods will provide an impact on LES, novel models must be developed