SAND2014-19999PE

Model Calibration and Forward Uncertainty Quantification for Large-Eddy Simulation of Turbulent Flows

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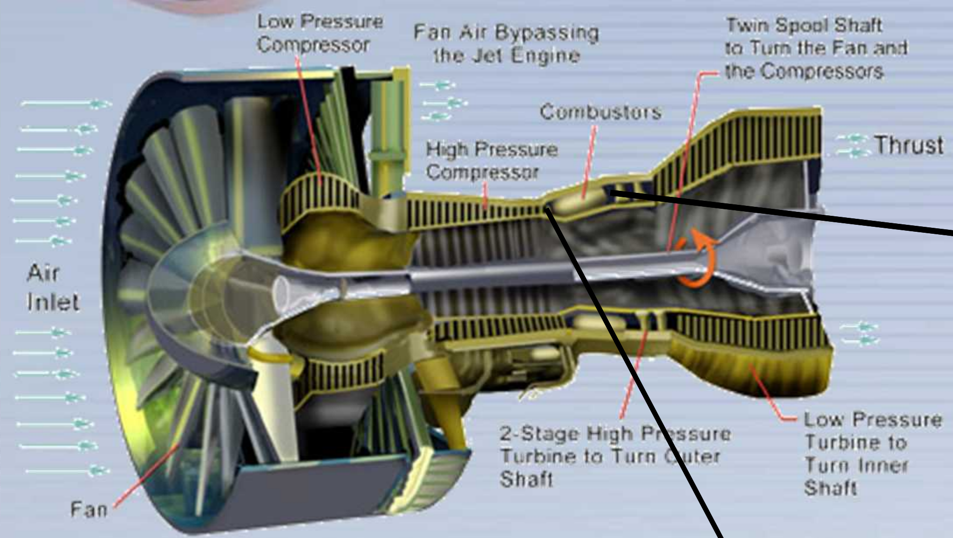
Special thanks to: Jeremy Templeton, Cosmin Safta, Stefan Domino, John Hewson

LDRD LABORATORY DIRECTED RESEARCH & DEVELOPMENT

Sandia National Laboratories

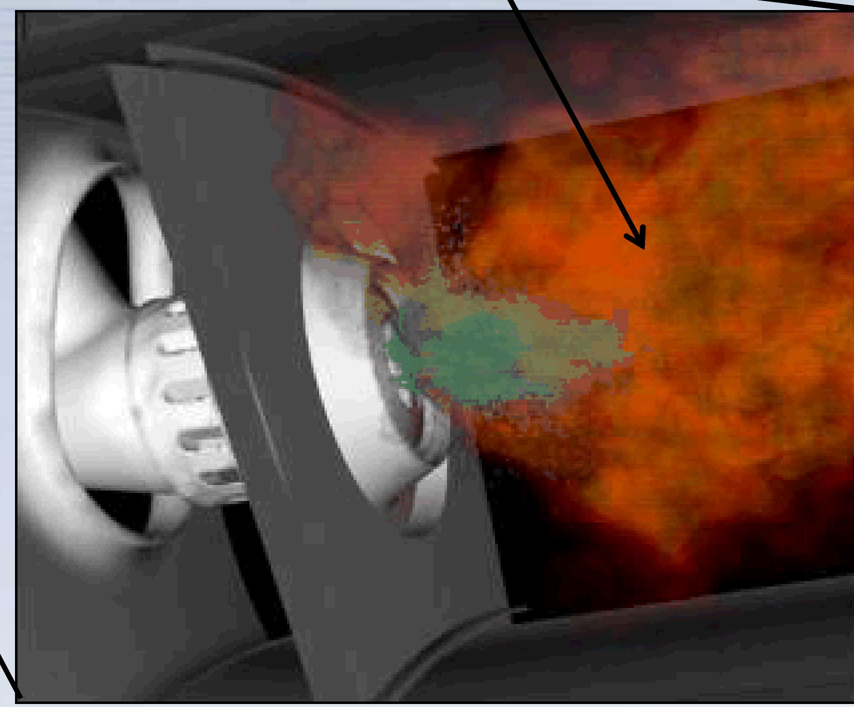
Gas Turbine Challenges



Gas Turbine Engine

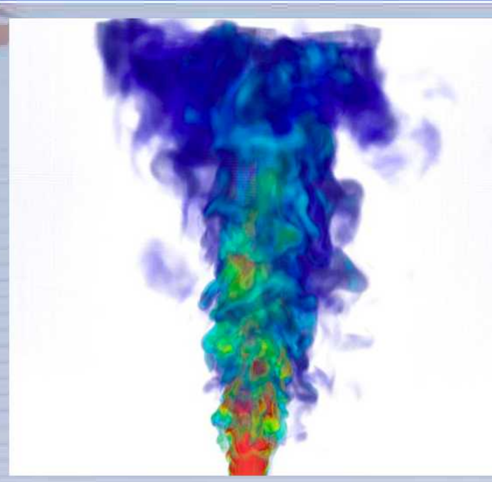
Complex flow physics coupled with chemistry drives efficiency and pollutant emissions

RANS solutions and modeling strategies are inadequate given the free flow and turbulence driven by heat release



Gas Turbine Combustor Flow
Stanford ASCI Alliance Center

Motivation

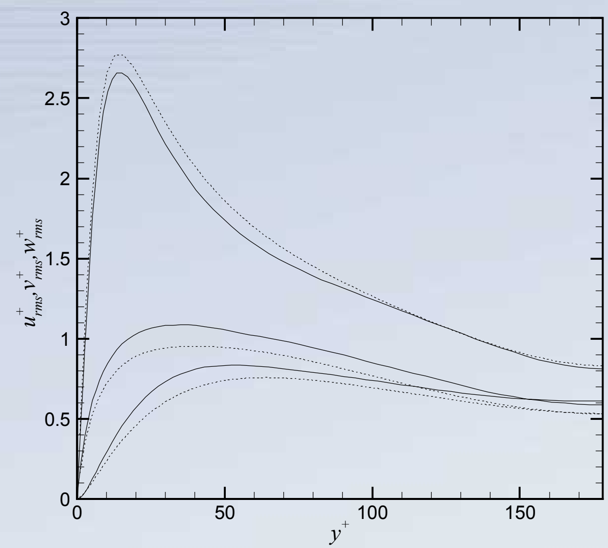


Re 6600 turbulent jet using SIERRA Fuego

Gas Turbine combustion processes offer such complexity that new approaches to enable high-fidelity calculations are needed to enable next-generation technology

High-Fidelity LES Advantages:
- Resolves many turbulent structures
- Less dependent on model form
- Verified predictivity for combustion

Engineering LES Challenges:
- Insufficient turbulence models
  Combustion models taken from RANS
- Complex interactions with mesh and models impacting mesh refinement
- Difficult to assess with UQ

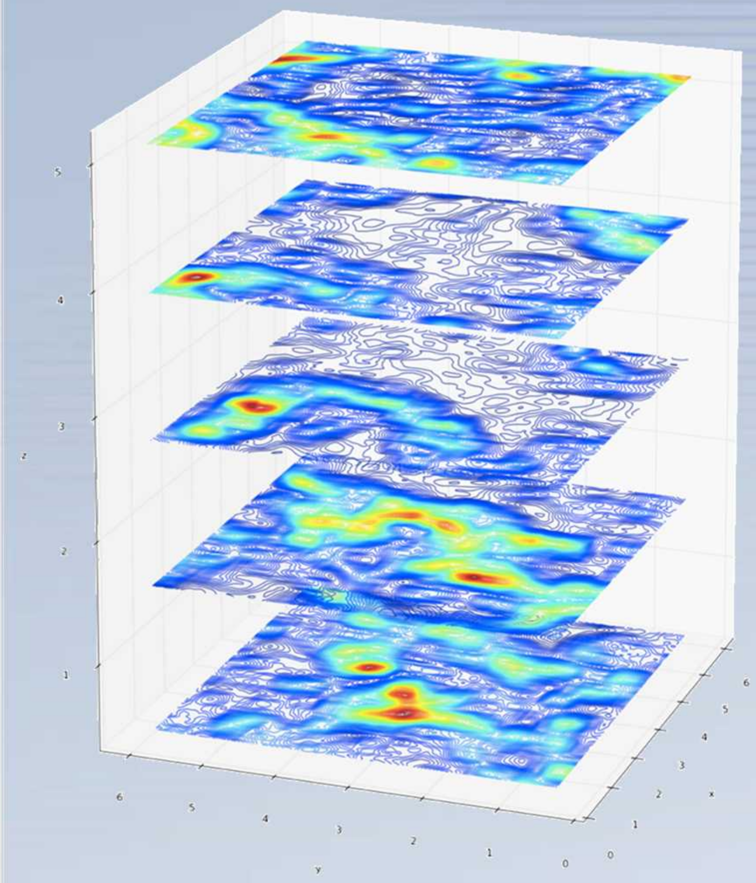


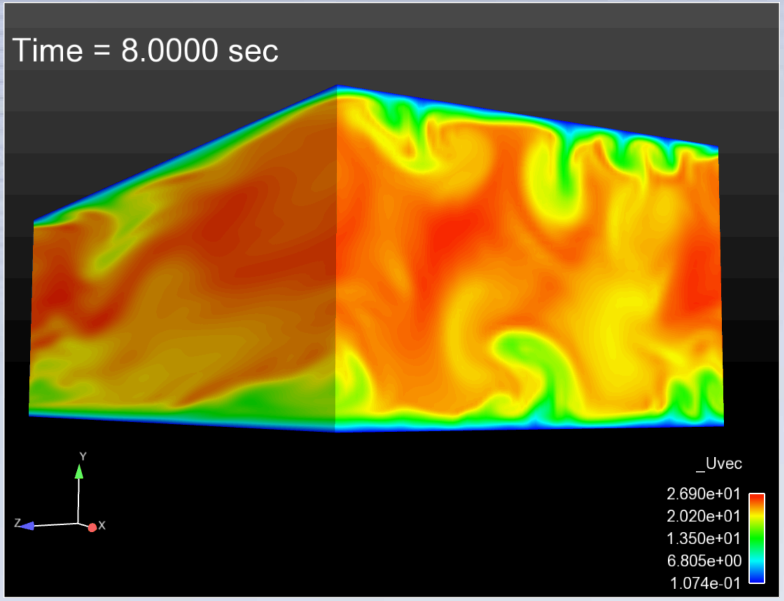
Overprediction of turbulent kinetic energy, Templeton 2006

Breath of Study

- **Cold Flow**
  - Comparison between engineering and high-fidelity LES
  - Develop UQ strategies and calibrate turbulence model parameters using channel flow
  - Application: Jet-in-Crossflow
  - *Developed approaches and are applying them to: k-SGS model calibration, wall-modeling, jet-in-crossflow*
- **Reacting Flow**
  - Implement industrial and advanced combustion models
  - Infer combustion model parameters
  - UQ of reacting jet-in-crossflow and complex geometry flow
  - *Currently implementing Burke-Schumann with mixture fraction table look up*

UQ of Channel Flow





Calibrate Subgrid-Scale Kinetic Energy One-Equation LES Model

Model:

$$\int \frac{\partial \bar{\rho} k^{sgs}}{\partial t} dv + \int \bar{\rho} k^{sgs} \bar{u}_j n_j dS = \int \frac{\mu_t}{\sigma_k} \frac{\partial k^{sgs}}{\partial x_j} n_j dS + \int \left(P_k^{sgs} - D_k^{sgs} \right) dv$$

Production: $$P_k^{sgs} = \left[2\mu_t \left(\tilde{S}_{ij} - \frac{1}{3} \tilde{S}_{kk} \delta_{ij} \right) - \frac{2}{3} \bar{\rho} k^{sgs} \delta_{ij} \right] \frac{\partial \tilde{u}_i}{\partial x_j}$$

$$\mu_t = C_{\mu_\epsilon} \Delta \sqrt{k^{sgs}}$$

Dissipation: $$D_k^{sgs} = C_\epsilon \frac{\sqrt{\left(k^{sgs}\right)^3}}{\Delta}$$

Calibrate: C_ϵ and C_{μ_ϵ}

Bayesian Calibration

Bayes formula:

likelihood prior

$$P(\theta|D) = \frac{P(D|\theta)P(\theta)}{P(D)}$$

posterior evidence

- Data *D* based on DNS of Isotropic Turbulence
- Model parameters θ are the k^{sgs} model constants
- The prior distribution $P(\theta)$ is set to MVN with diagonal covariance, centered around the current nominal values for θ.
- The likelihood $P(D|\theta)$ is assumes a Gaussian discrepancy between the data and the model
- The posterior distribution $P(\theta|D)$ is sampled via and adaptive Markov Chain Monte Carlo algorithm

Data

Bayes formula:

likelihood prior

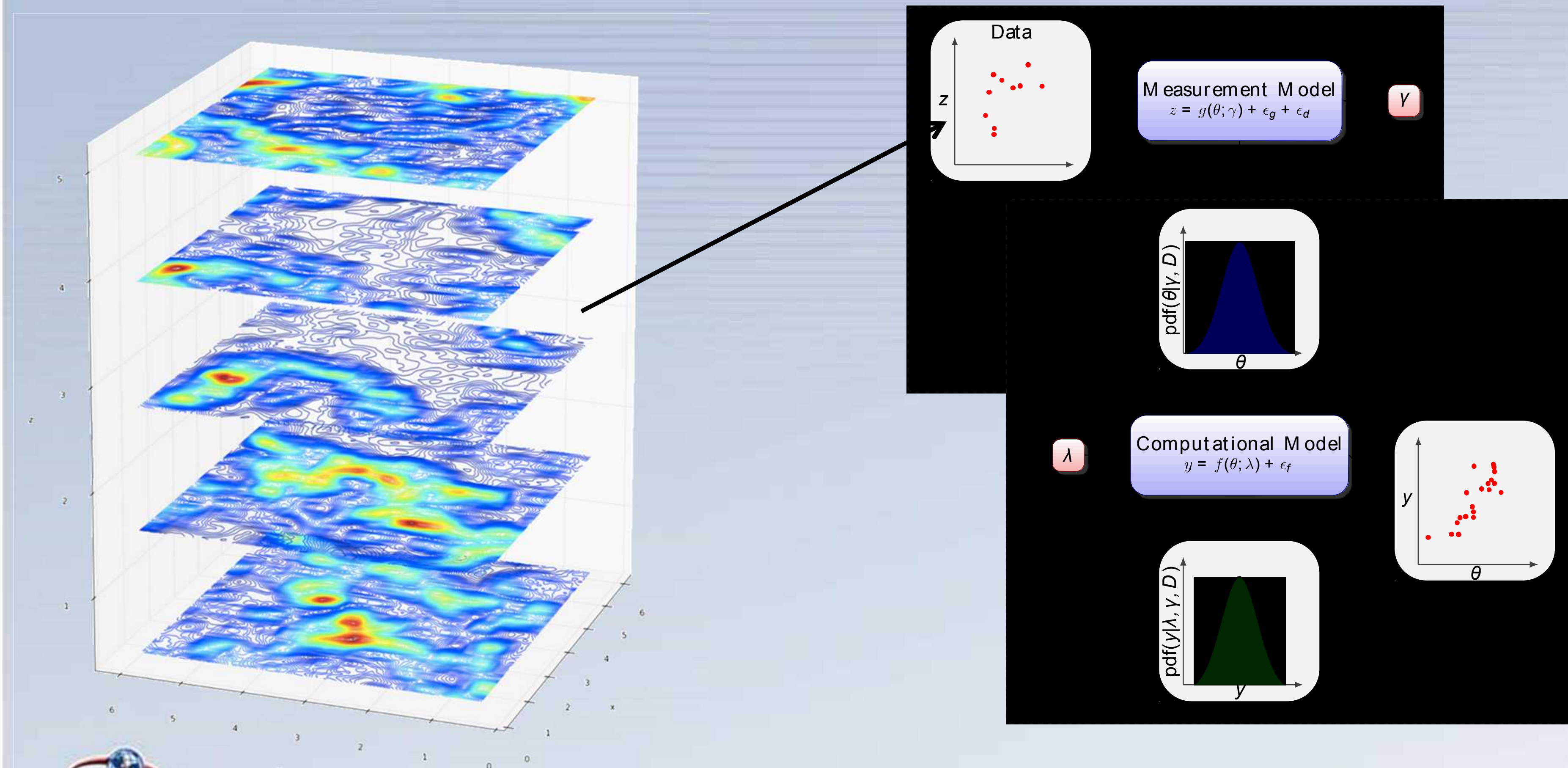
$$P(\theta|D) = \frac{P(D|\theta)P(\theta)}{P(D)}$$

posterior evidence

- Data *D* based on DNS of Isotropic Turbulence
- Model parameters *θ* are the k^{sgs} model constants
- The prior distribution *P(θ)* is set to MVN with diagonal covariance, centered around the current nominal values for *θ*.
- The likelihood *P(D|θ)* is assumes a Gaussian discrepancy between the data and the model
- The posterior distribution *P(θ|D)* is sampled via and adaptive Markov Chain Monte Carlo algorithm

DNS-Informed Calibration

Filtered DNS k^{sgs} (JHU)

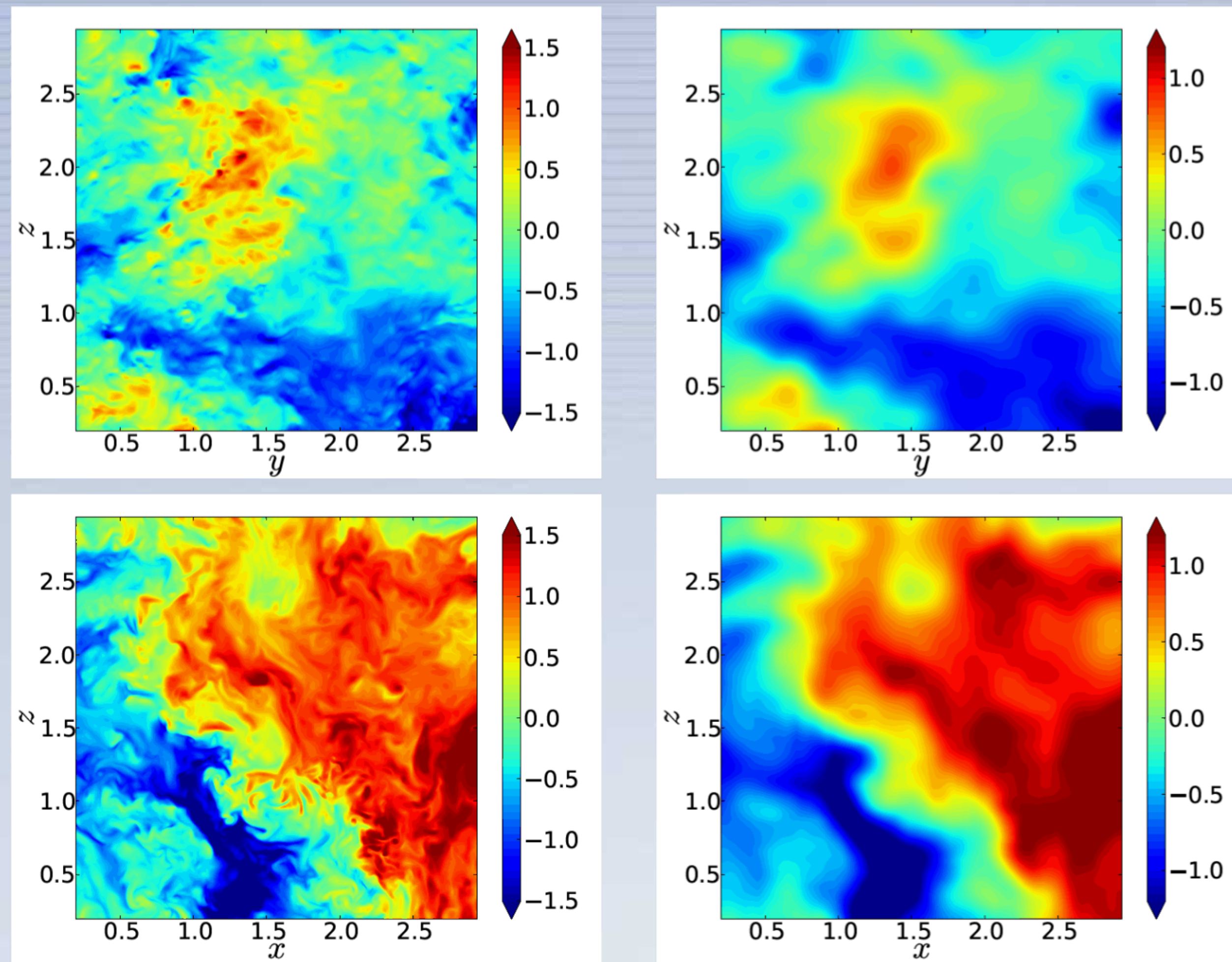


Data is Filtered DNS to LES scale

3 Filter sizes:

- $\Delta = L/64$
- $\Delta = L/32$
- $\Delta = L/16$

DNS | $\Delta = L/32$



Bayesian Calibration: Likelihood

Bayes formula:

likelihood, prior

$$P(\theta|D) = \frac{P(D|\theta)P(\theta)}{P(D)}$$

posterior, evidence

- Data *D* based on DNS of Isotropic Turbulence
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Likelihood

- **Classical Approach**

$$f_k(t;\Delta) = C_{\mu_\epsilon} f_P(t;\Delta) - C_\epsilon f_D(t;\Delta) + \epsilon_m + \epsilon_d.$$

$$L_{\mathcal{D}}(\theta) = \prod_{i=1}^{N_t} \frac{1}{\sqrt{2\pi}\sigma_i} \exp\left(-\frac{(f_{k,i} - C_{\mu_\epsilon} f_{P,i} + C_\epsilon f_{D,i})^2}{2\sigma_i^2}\right)$$

- **Embedded Error (K. Sargsyan, H.N. Najm, and R. Ghanem - 2014)**

Bayesian Calibration: Prior

Bayes formula:

$$P(\theta|D) = \frac{P(D|\theta)P(\theta)}{P(D)}$$

likelihood: $P(D|\theta)$; prior: $P(\theta)$; posterior: $P(\theta|D)$; evidence: $P(D)$

- Data *D* based on DNS of Isotropic Turbulence
- Model parameters θ are the k^{sgs} model constants
- The prior distribution *P(θ)* is set to MVN with diagonal covariance, centered around the current nominal values for θ.
- The likelihood *P(D|θ)* is assumes a Gaussian discrepancy between the data and the model
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Independent Gaussian Priors

- **Centered at values from the literature ($C_{\mu\epsilon}$, C_{ϵ})**

$$\mu_1^{pr} = (0.0845, 0.85) \qquad \mu_2^{pr} = (0.07, 1.05)$$

- **Range of Marginal Standard Deviations**

$$\sigma_1^{pr} = (0.04, 0.4),\ \sigma_2^{pr} = (0.02, 0.2),\ \sigma_3^{pr} = (0.01, 0.1)$$

Bayesian Calibration: Posterior

Bayes formula:

likelihood prior

$$P(\theta|D) = \frac{P(D|\theta)P(\theta)}{P(D)}$$

posterior evidence

- Data *D* based on DNS of Isotropic Turbulence
- Model parameters θ are the k^{sgs} model constants
- The prior distribution $P(\theta)$ is set to MVN with diagonal covariance, centered around the current nominal values for θ.
- The likelihood $P(D|\theta)$ is assumes a Gaussian discrepancy between the data and the model
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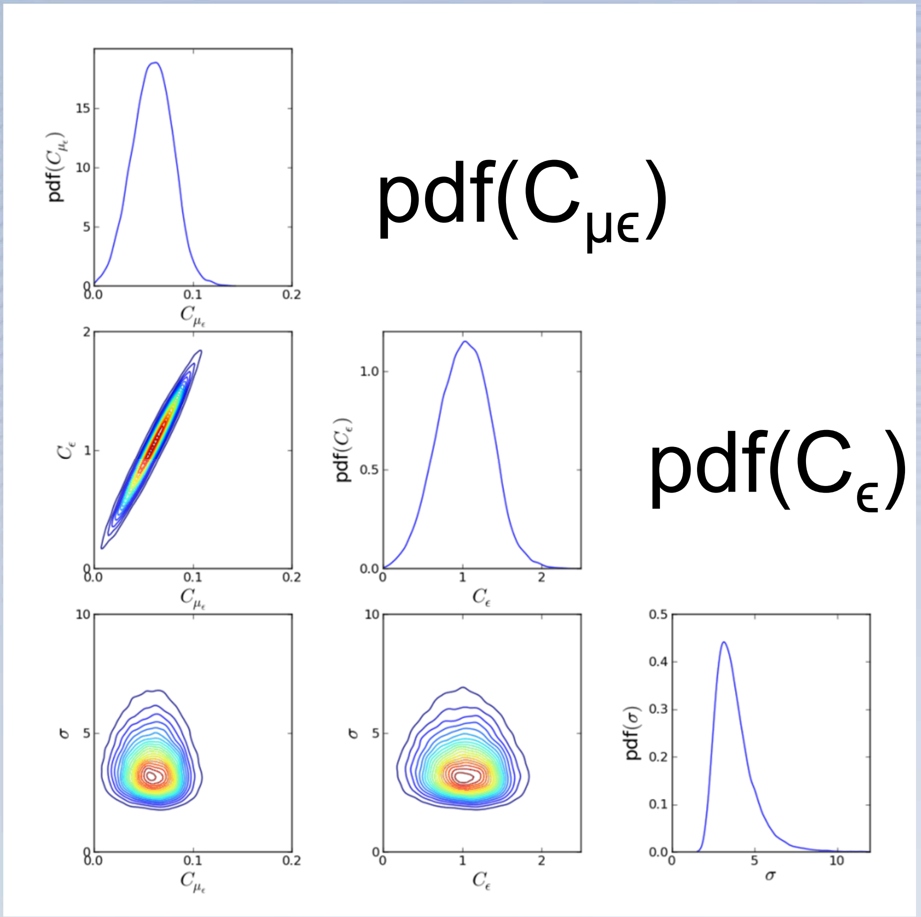
Sample Posterior Distributions



pdf($C_{\mu\epsilon}$)

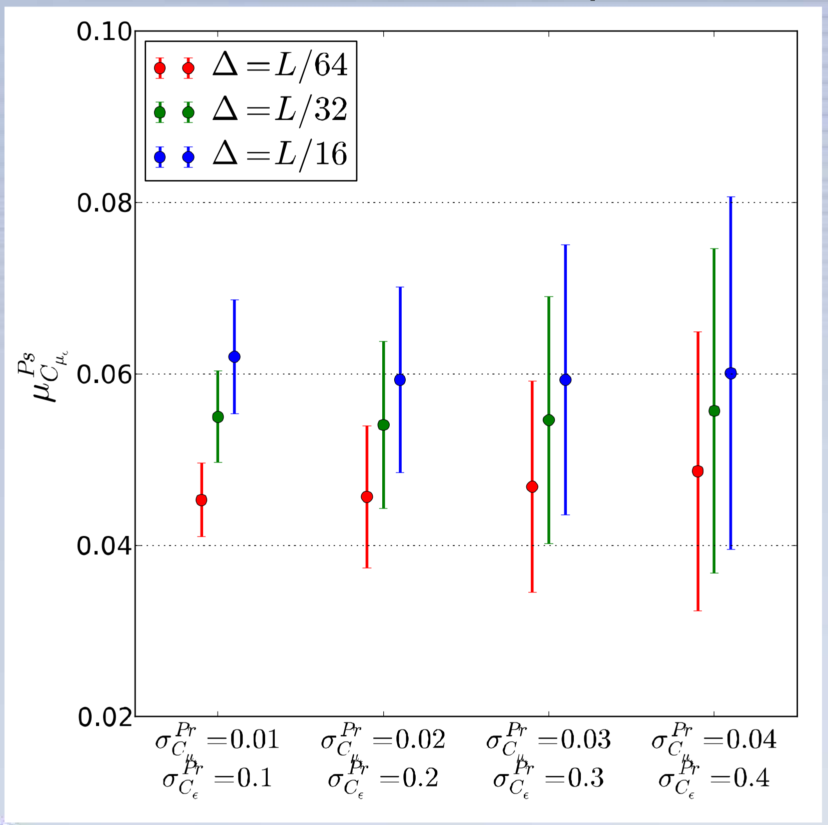
pdf(C_ϵ)

pdf(σ)

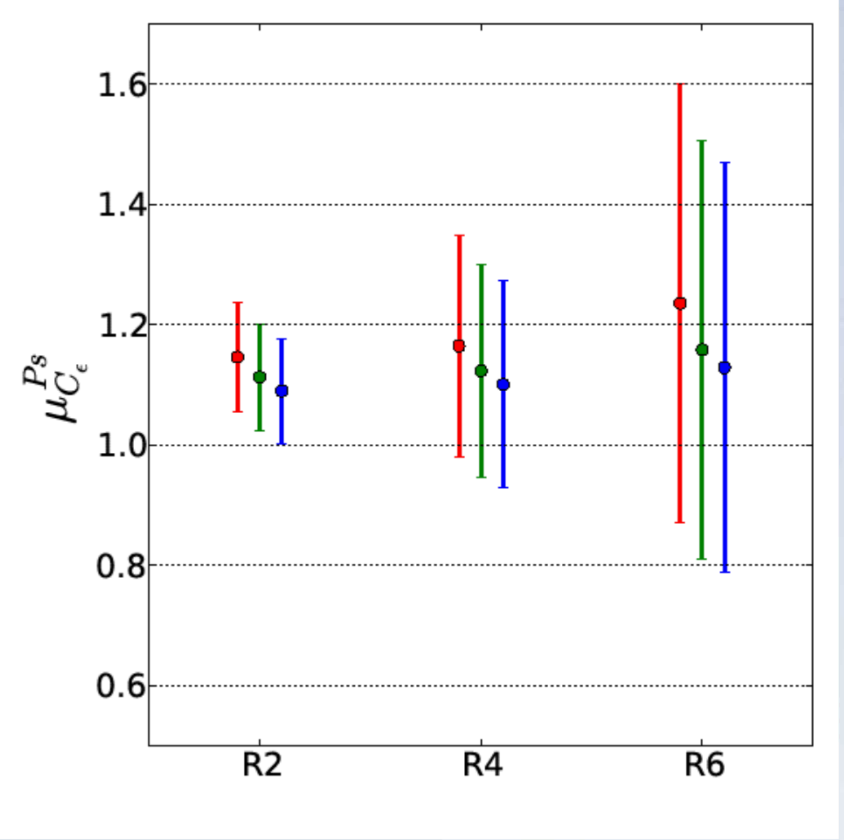
$C_{\mu\epsilon}$ C_ϵ σ

Effect of Filter Size and Prior

Posterior for $C_{\mu\epsilon}$



Posterior for C_ϵ



Forward UQ – Predictive Assessment

Employ Polynomial Chaos (PC) Expansion to propagate uncertainties from input parameters to output Quantities of Interest

$$M\left(C_\epsilon, C_{\mu_e}\right) \approx \sum_{k=0}^{P} c_k \Psi_k\left(\xi_1, \xi_2\right)$$

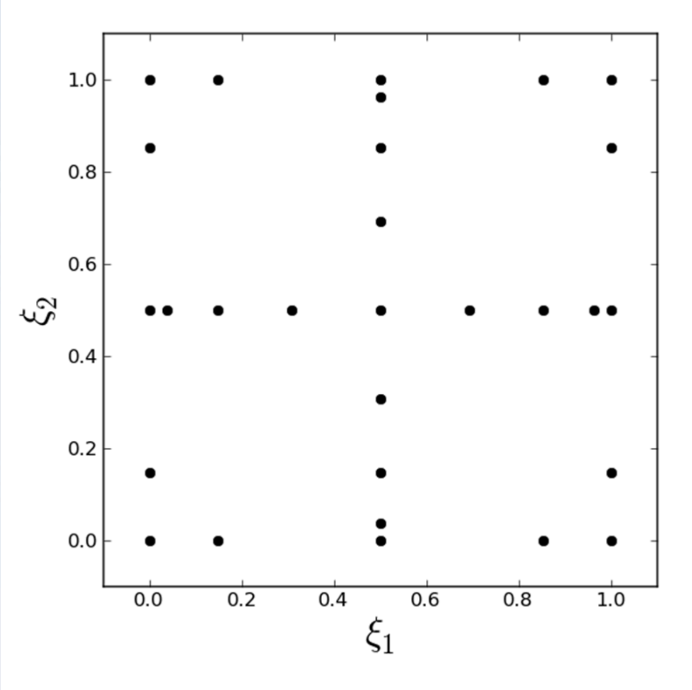
$$C_\epsilon = C_\epsilon\left(\xi_1, \xi_2\right), \; C_{\mu_e} = C_{\mu_e}\left(\xi_1, \xi_2\right)$$

Employ quadrature to compute PC coefficients

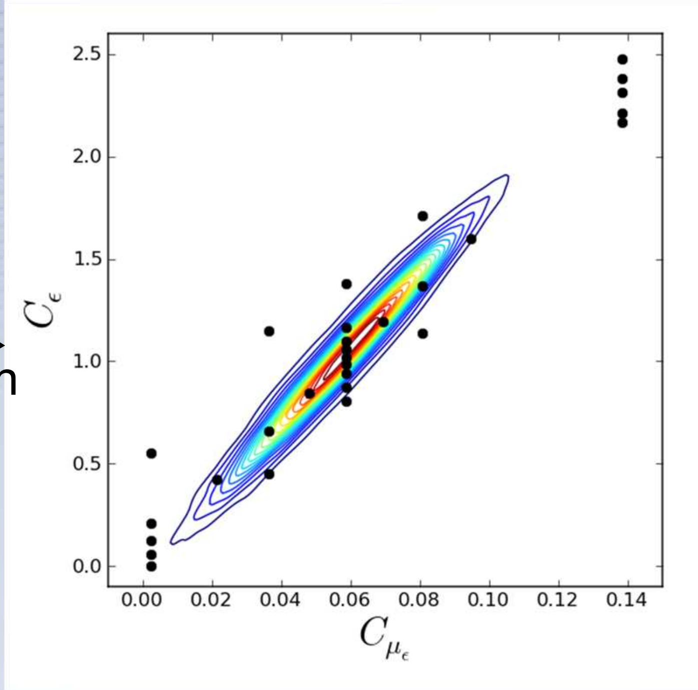
$$c_k = \frac{\left\langle M\left(C_\epsilon, C_{\mu_e}\right) \Psi_k\left(\xi_1, \xi_2\right)\right\rangle}{\left\langle \Psi_k^2\left(\xi_1, \xi_2\right)\right\rangle}$$

Sparse Quadrature to Construct PC Expansion for Model Output

$$C_\epsilon = C_\epsilon(\xi_1, \xi_2)\,,\; C_{\mu_\epsilon} = C_{\mu_\epsilon}(\xi_1, \xi_2)$$

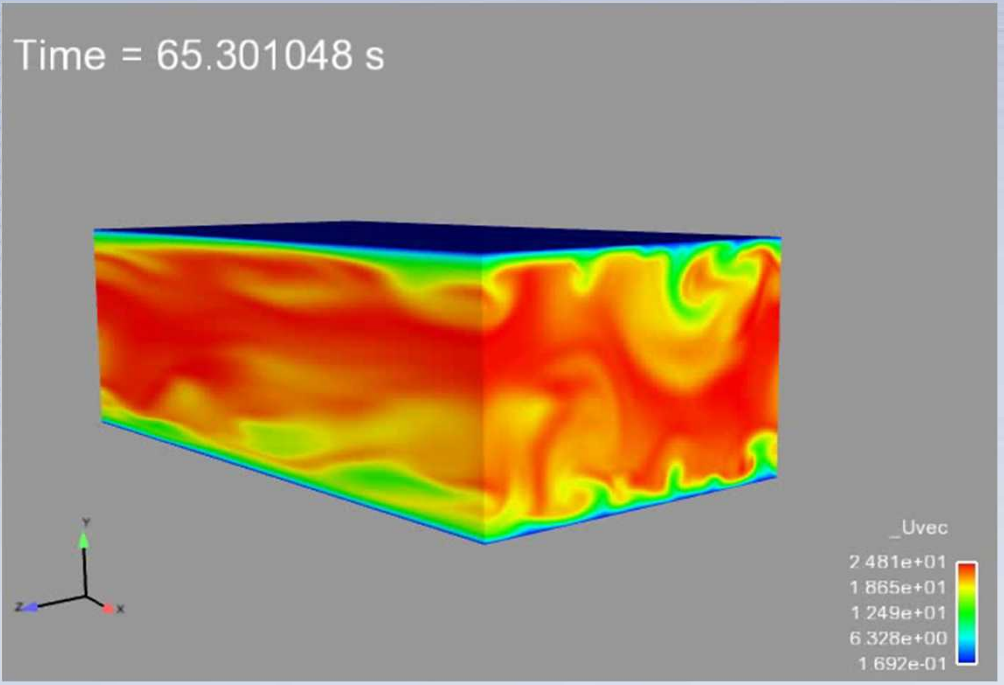


Rosenblatt
Transformation



Fuego LES Simulations with Calibrated Parameters

- k^{sgs} Turbulence Model with various C_ϵ and $C_{\mu\epsilon}$ corresponding to quadrature points
- Normalized Input Parameters
  - $\rho = 1.0$
  - $\mu = 1/Re_\tau = 1/590$
- No slip walls at top and bottom
- Periodic in x and z
- Body force in x-direction to produce flow

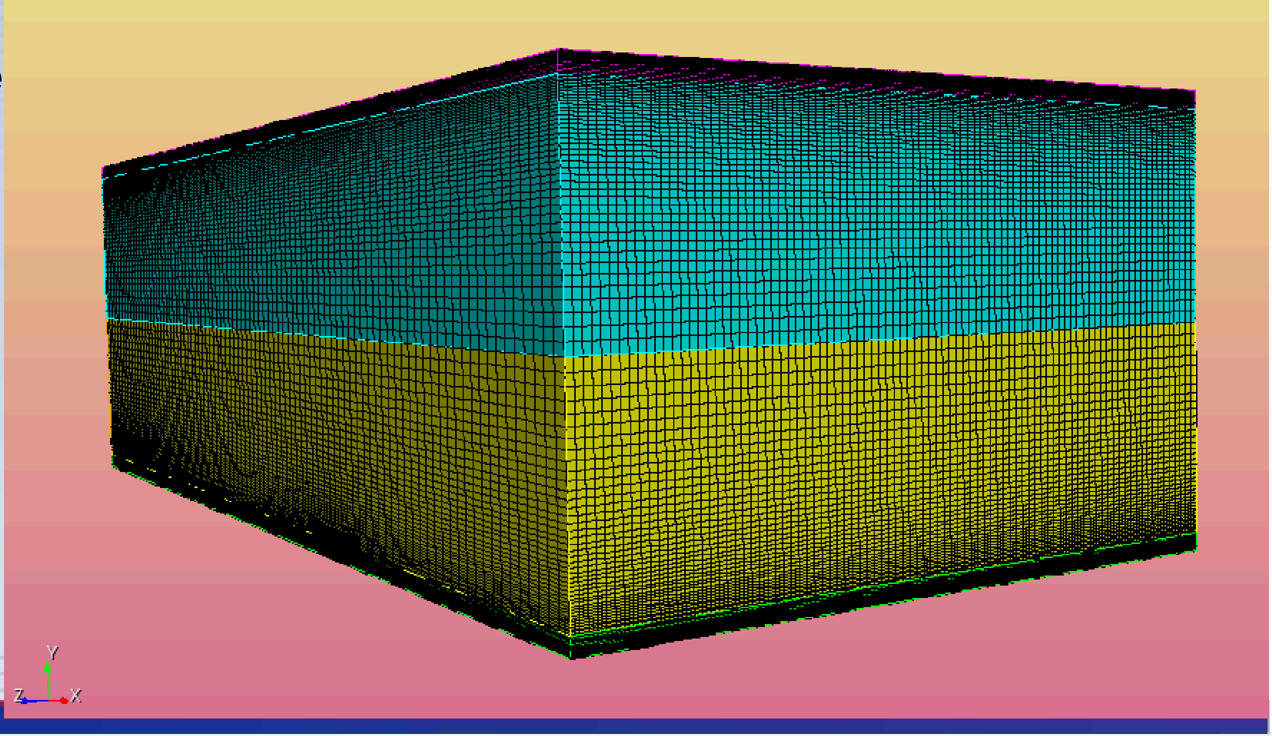


Mesh

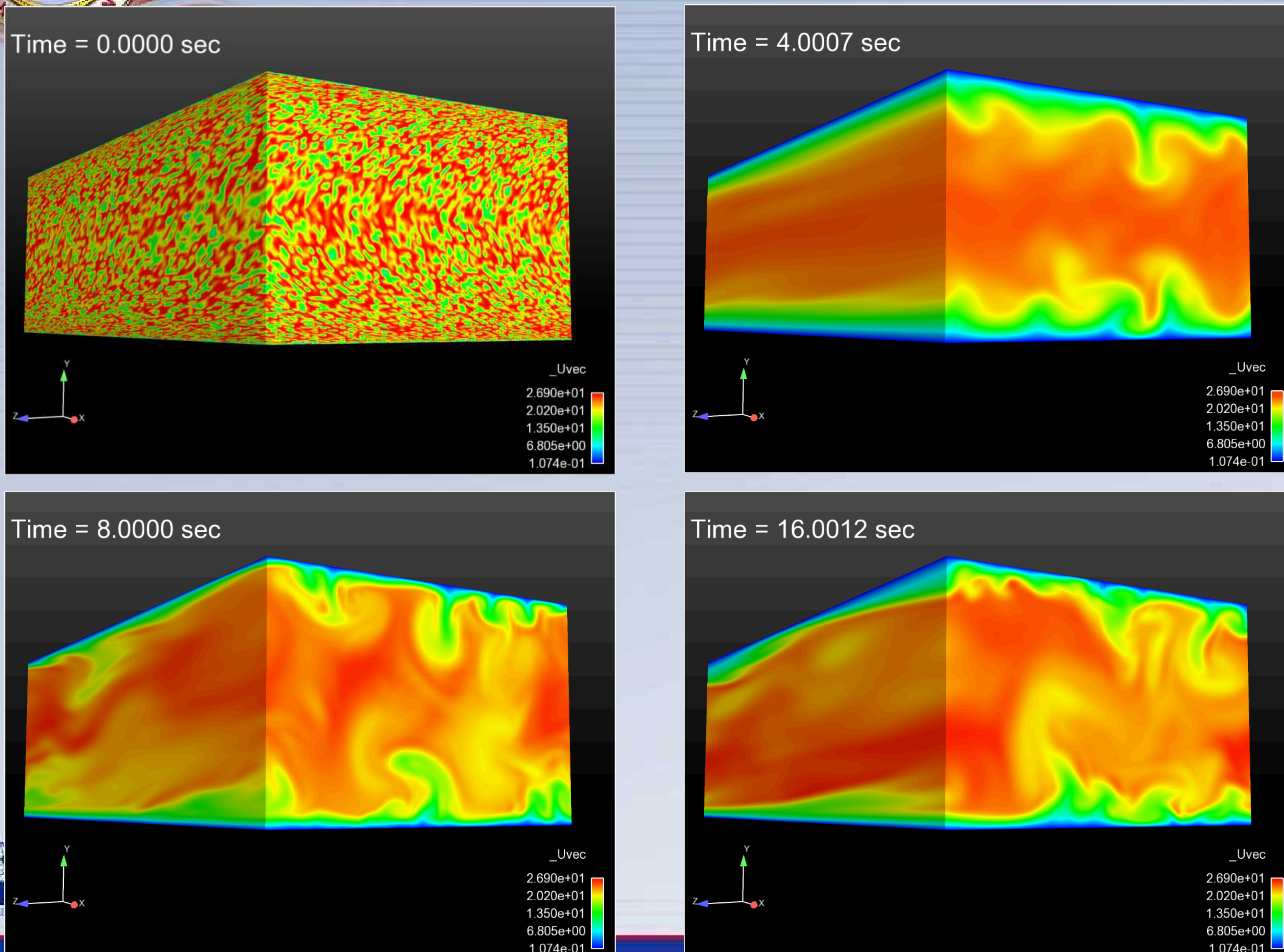
- **Dimensions:**
  - Flow direction: $x = 2\pi$ (periodic)
  - Wall normal direction: $y = 2$
  - Cross flow direction: $z = \pi$ (periodic)
- **Grid size:**

90 × 116 × 90 = 931500 points

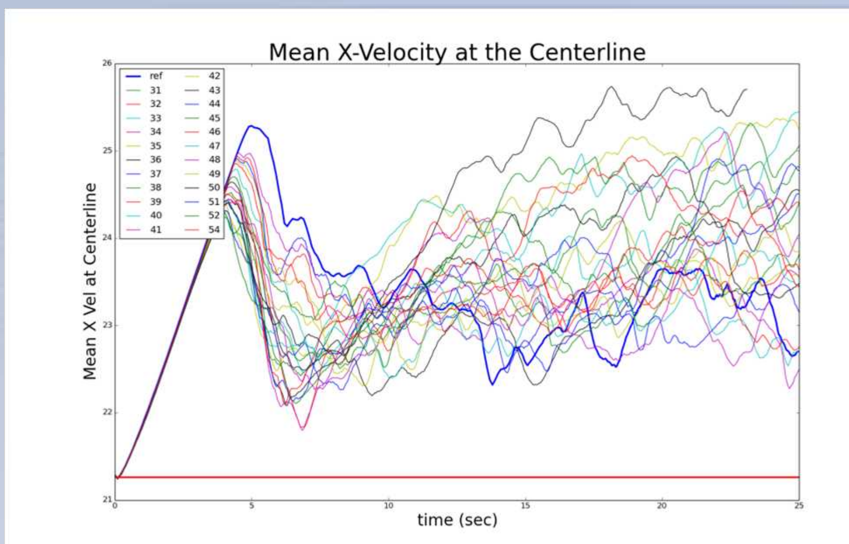
- **$y^+ \approx 1.15$ at walls**
- **Hyperbolic tan to same spaceing as in z**

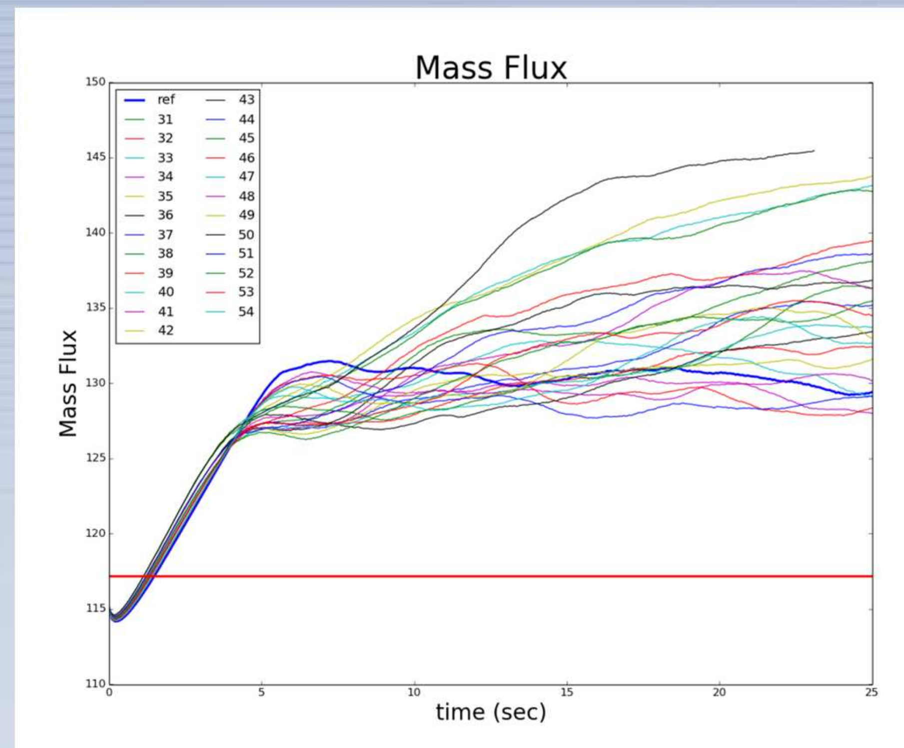


Fuego LES Simulations

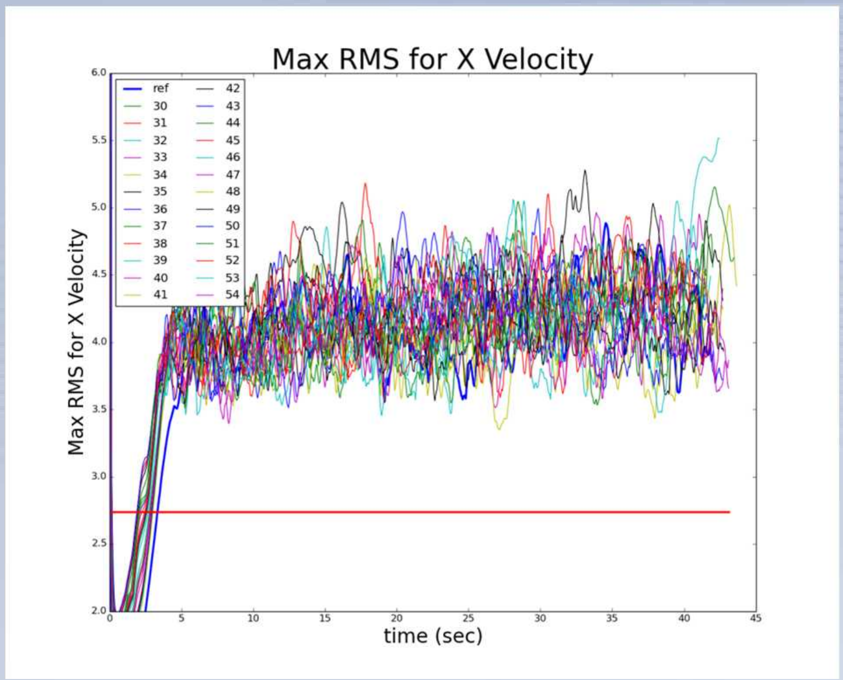


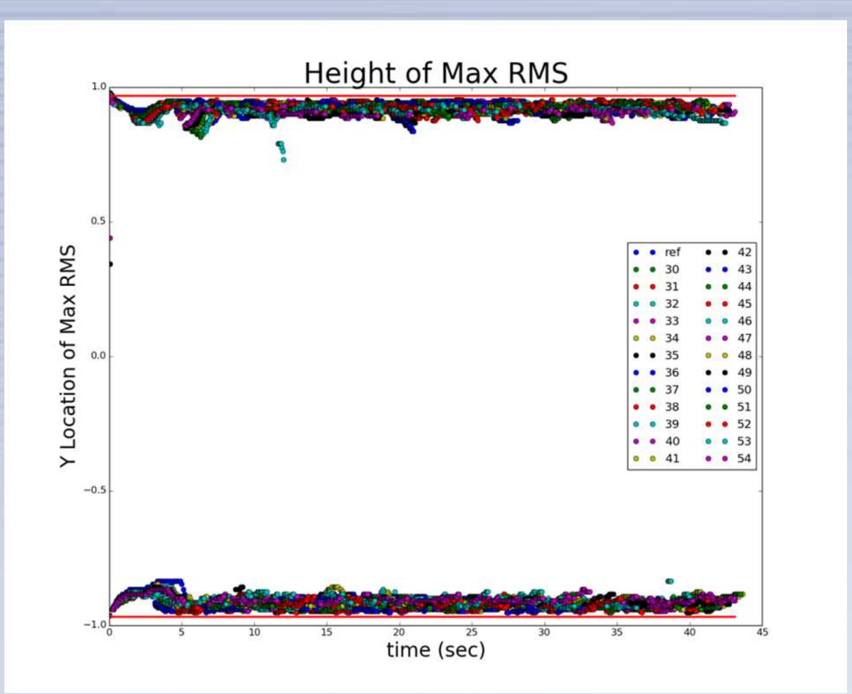
QoIs: Velocity and Mass Flux





QoI: RMS of Centerline Velocity





Forward UQ – Predictive Assessment

Evaluate weights with values from LES

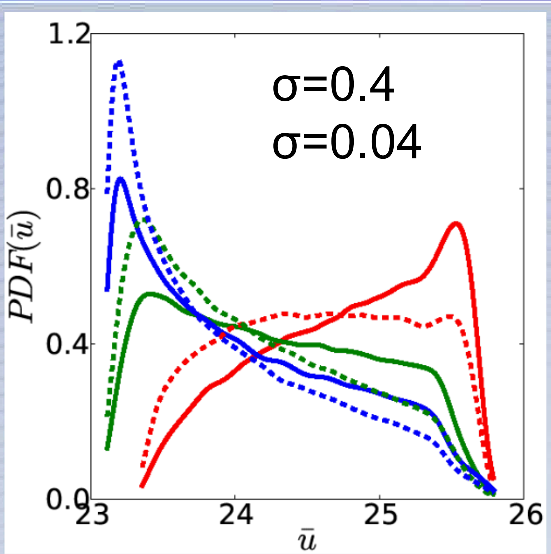
$$c_k = \frac{\langle M\left(C_\epsilon, C_{\mu_e}\right)\Psi_k\left(\xi_1, \xi_2\right)\rangle}{\langle \Psi_k^2\left(\xi_1, \xi_2\right)\rangle}$$

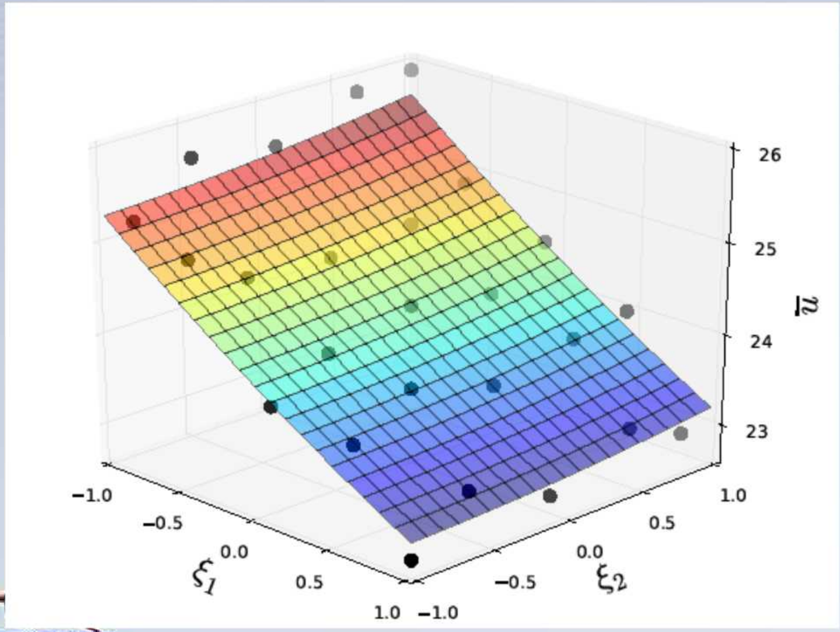
Employ Polynomial Chaos (PC) Expansion to propagate uncertainties from input parameters to output Quantities of Interest

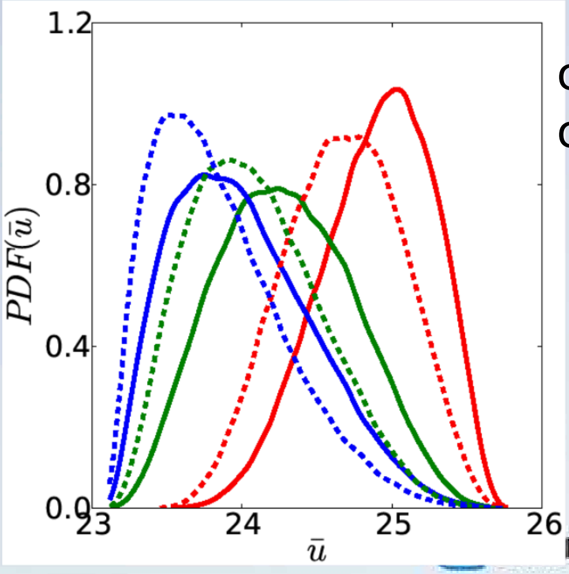
$$M\left(C_\epsilon, C_{\mu_e}\right) \approx \sum_{k=0}^{P} c_k \Psi_k\left(\xi_1, \xi_2\right)$$

Midline Average Velocity

- **DNS = 21.26**
- **Solid =** $\mu_1^{pr} = (0.0845, 0.85)$
- **Dashed =** $\mu_2^{pr} = (0.07, 1.05)$



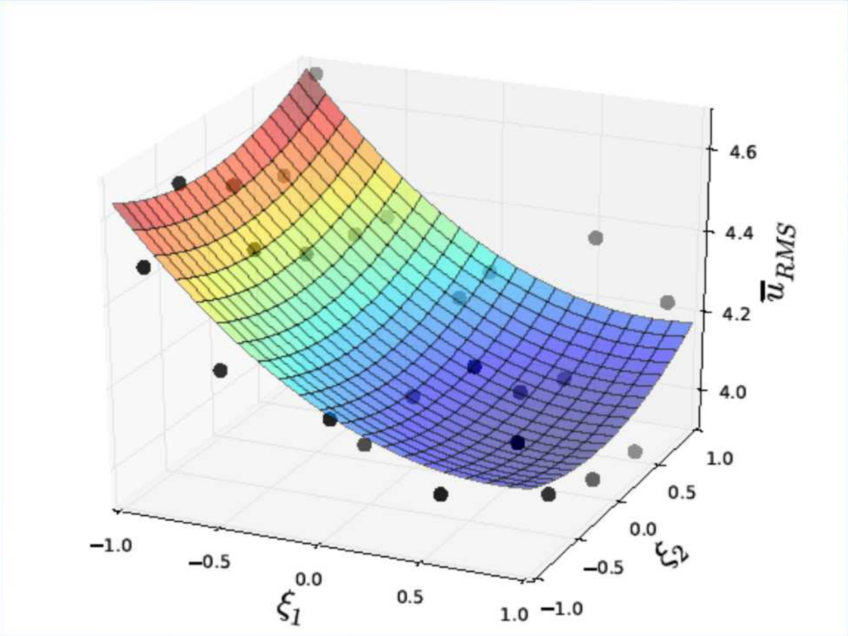


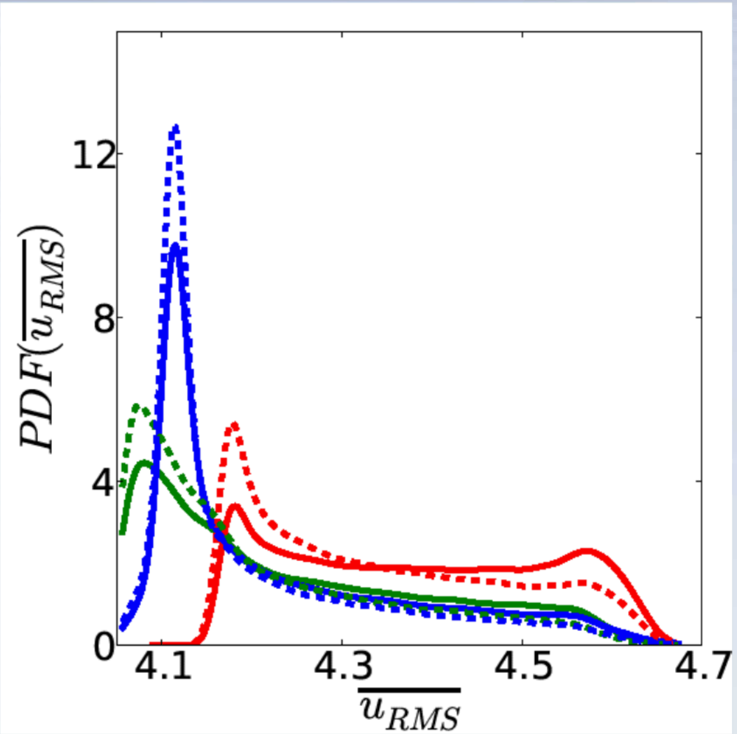


σ=0.2
σ=0.02

RMS of Centerline Velocity

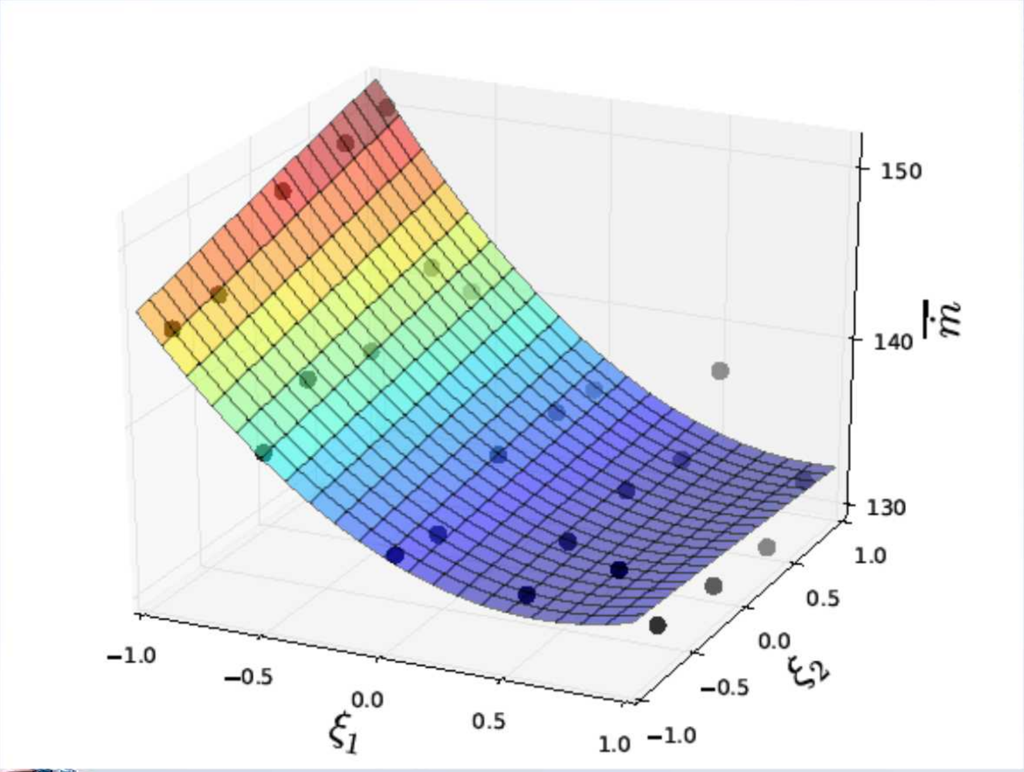
- **DNS = 2.7**

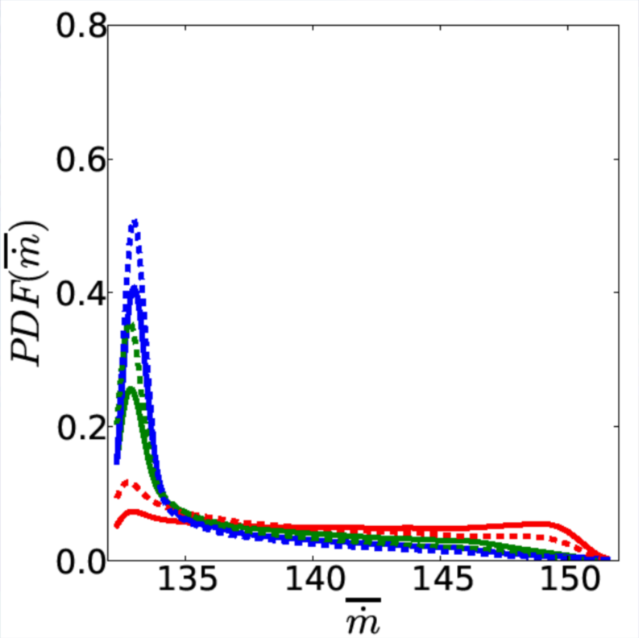




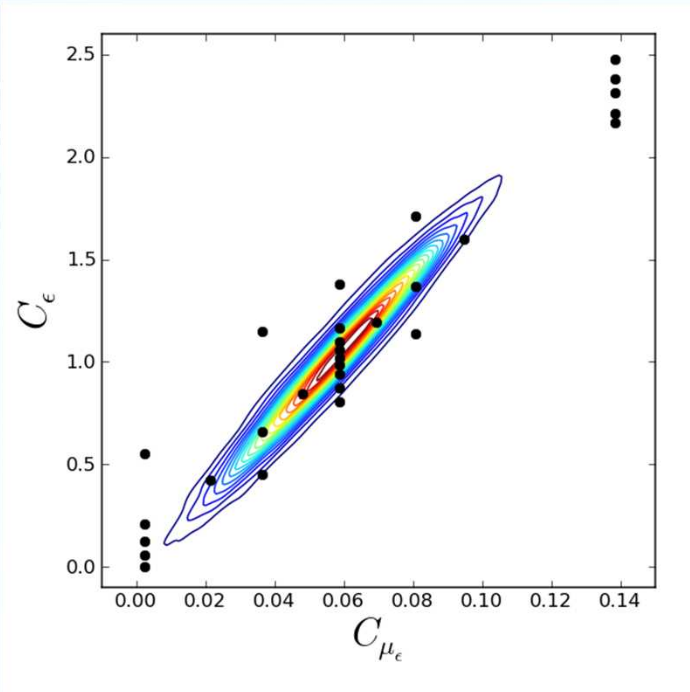
Mean Mass Flux

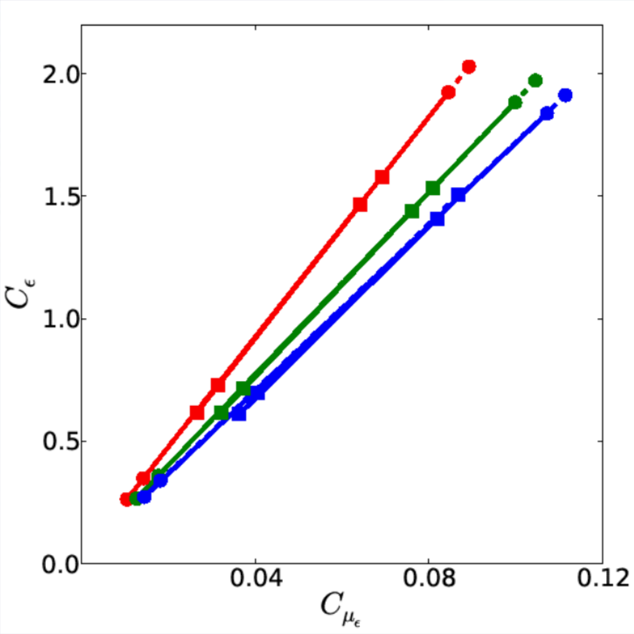
- **DNS = 117**





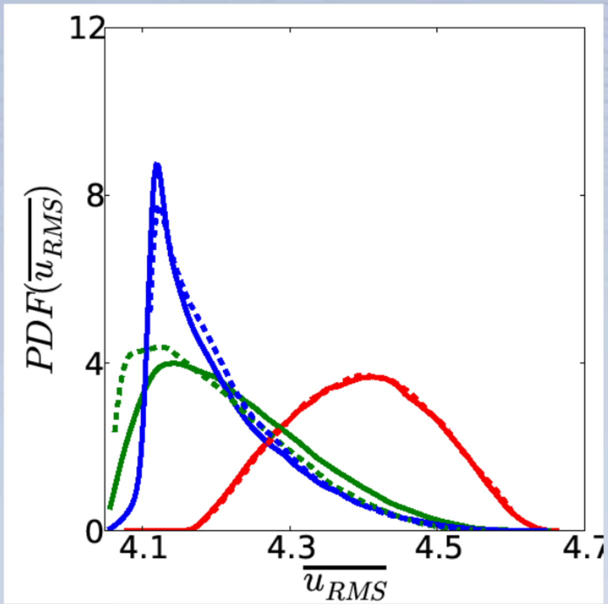
Principal Component Analysis of Joint PDF's

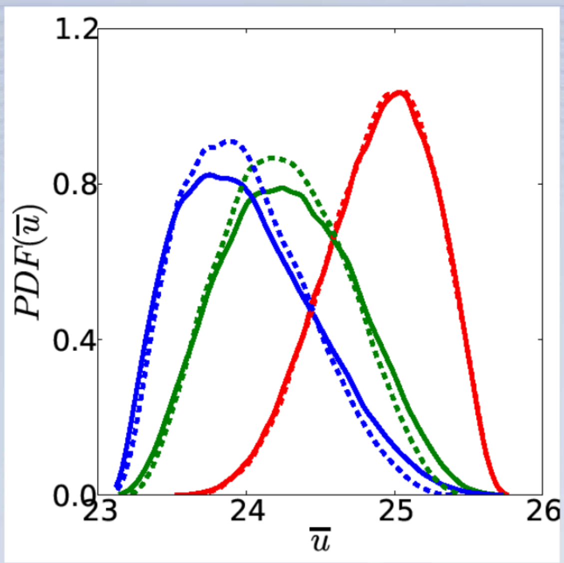


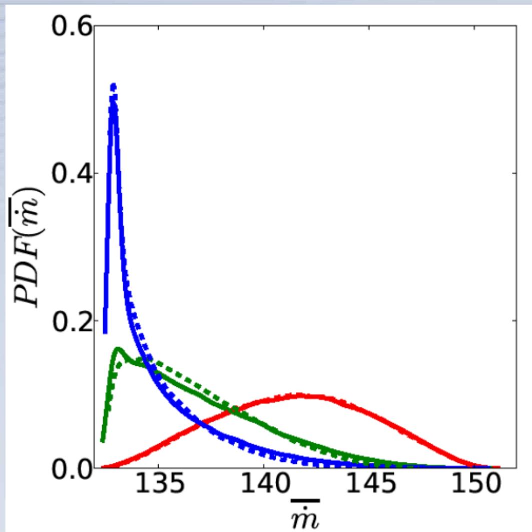


First Principal Component yields similar results to Joint PDF

- **Solid – Joint PDF**
- **Dashed – 1st PC**







Conclusions

- **Used DNS isotropic turbulence to predict engineering LES channel flow QoI**
- **Production and dissipation terms for the k_{sgs} model are highly correlated**
- **Discrepancy in QoI values from DNS**
  - Isentropic turbulence to channel flow
  - “engineering level”
  - Errors in k_{sgs}

Path Forward in FY15

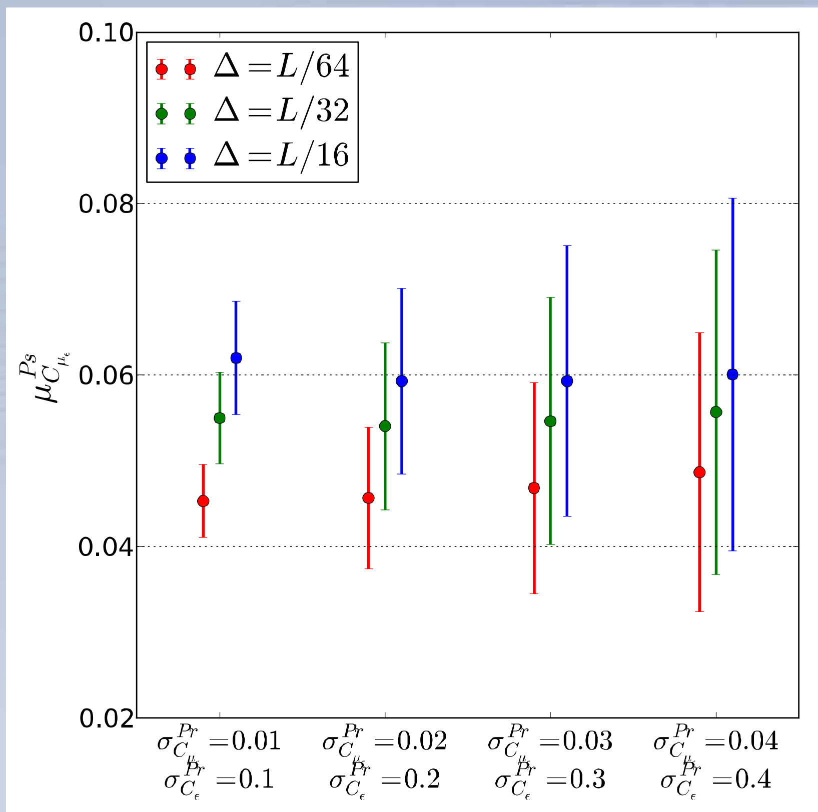
- **Complete combustion model implementation in Nalu**
  - Coordinate reaction flow case with J. Oefelein et al
  - Extra development effort from Blaylock & Hewson
- **Calibrate combustion model coefficients**
- **Tie reacting flow simulation with ODT-informed PCE model to estimate probability of extinction**
- **UQ of reacting flow simulation**
- **UQ of wall model for channel flow and backward facing step**
- **Make UQ/calibration tools available through SNL git repository**

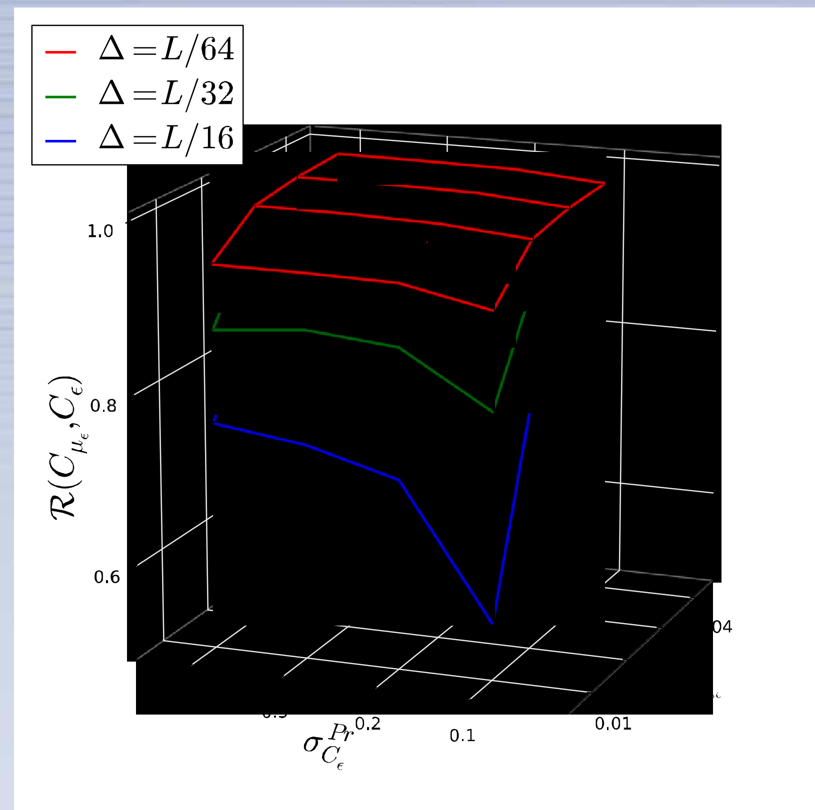
Thank You

&

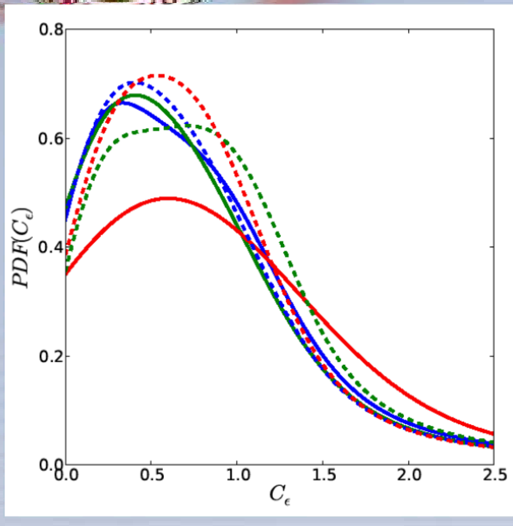
Questions

Effect of Filter Size and Prior

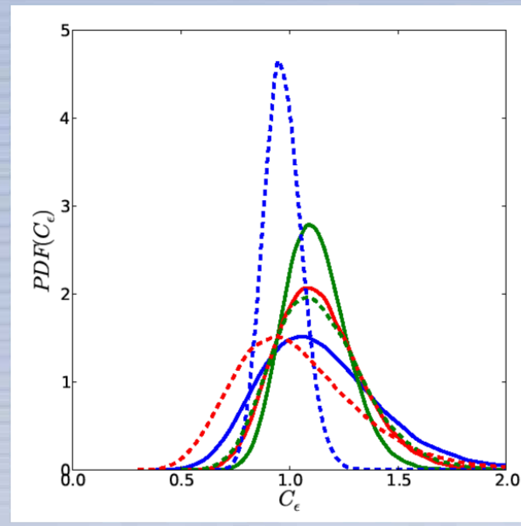




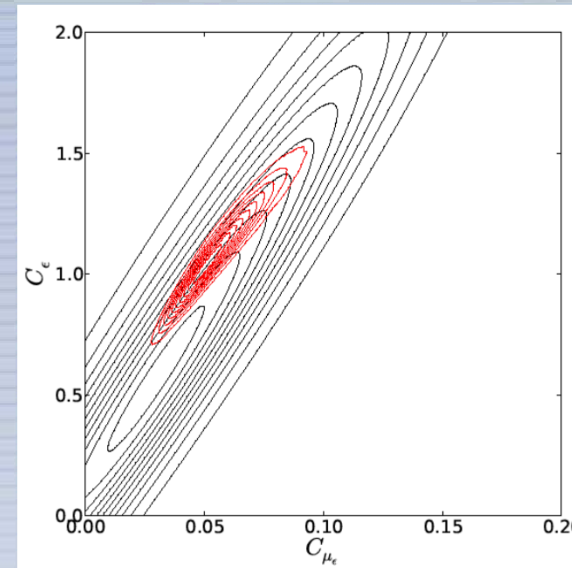
Posterior



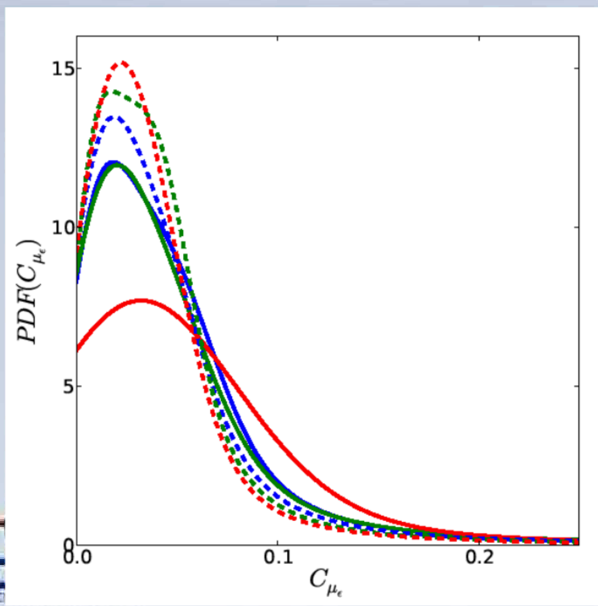
0.8
0.6
0.4
0.2
0.0
$PDF(C_\epsilon)$
0.0
0.5
1.0
1.5
2.0
2.5
C_ϵ



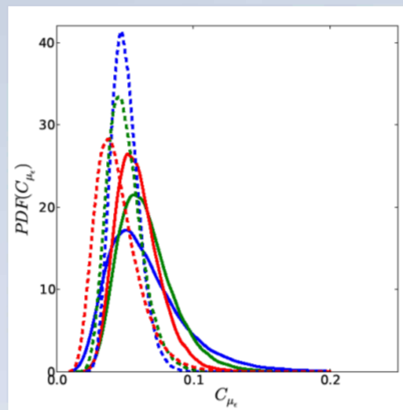
5
4
3
2
1
0
$PDF(C_\epsilon)$
0.0
0.5
1.0
1.5
2.0
C_ϵ



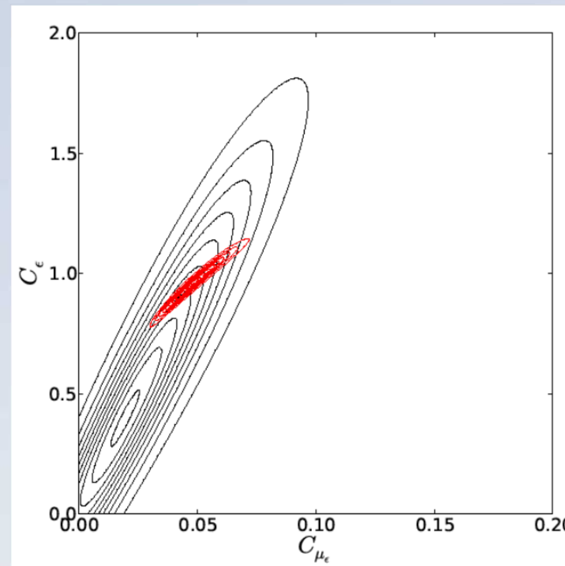
2.0
1.5
1.0
0.5
0.0
C_ϵ
0.00
0.05
0.10
0.15
0.20
C_{μ_ϵ}



15
10
5
0
$PDF(C_{\mu_\epsilon})$
0.0
0.1
0.2
C_{μ_ϵ}

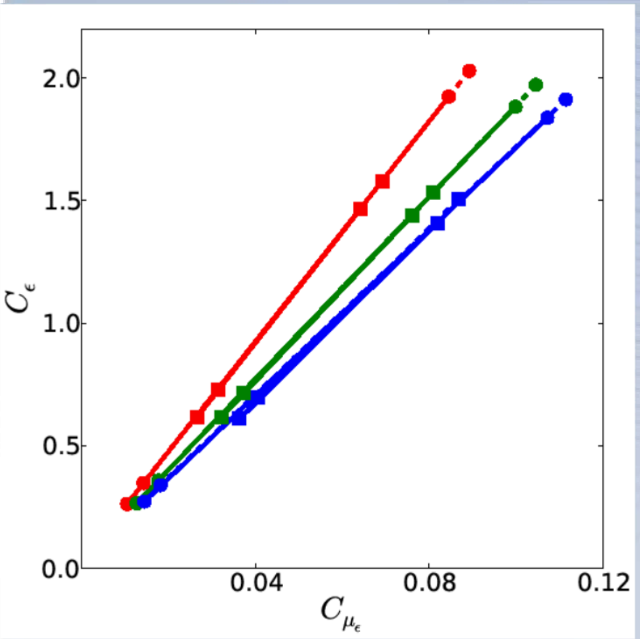


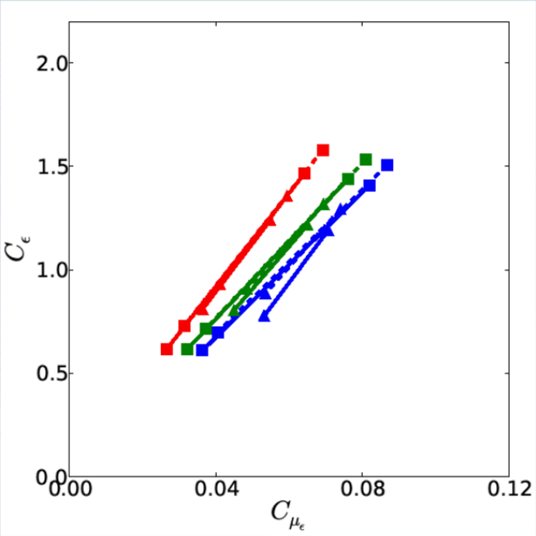
40
30
20
10
0
$PDF(C_{\mu_\epsilon})$
0.0
0.1
0.2
C_{μ_ϵ}

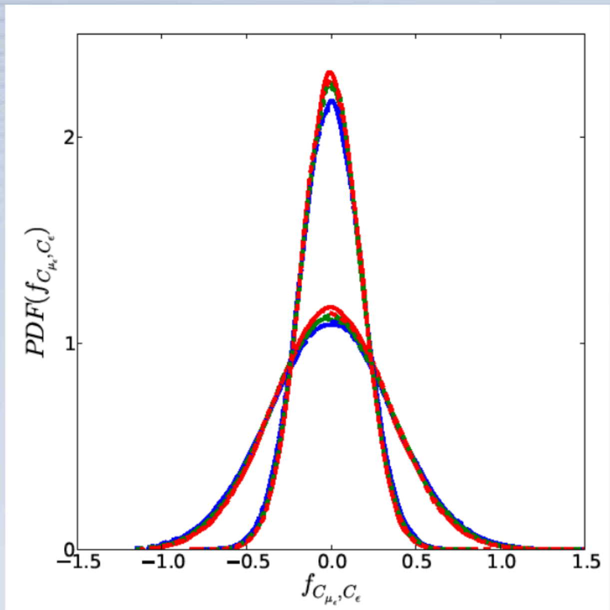


2.0
1.5
1.0
0.5
0.0
C_ϵ
0.00
0.05
0.10
0.15
0.20
C_{μ_ϵ}

Principal Component Analysis of Joint PDF's

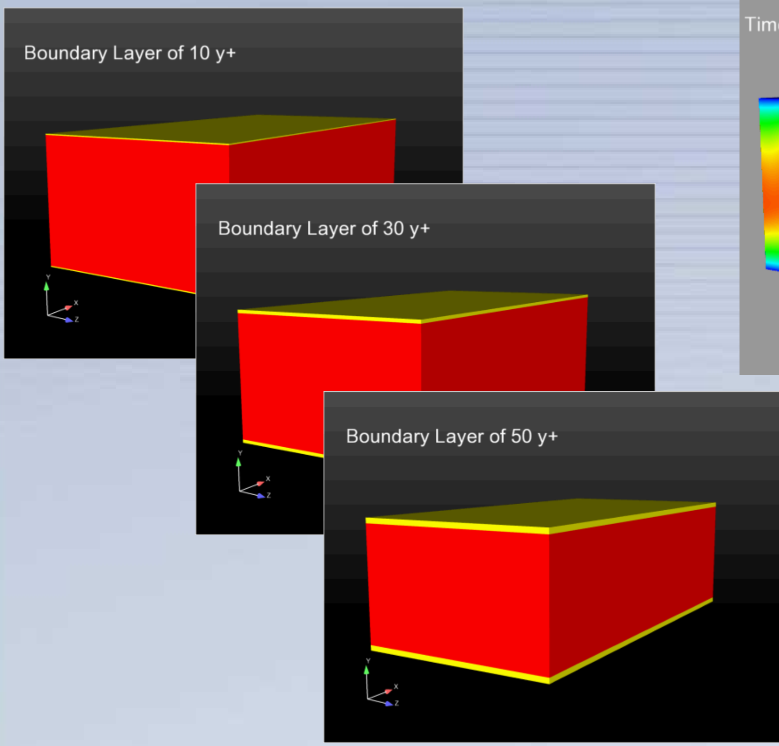


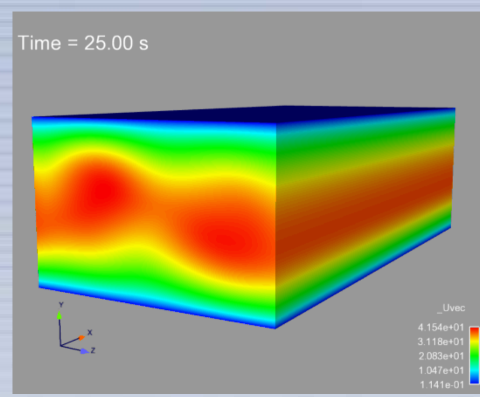


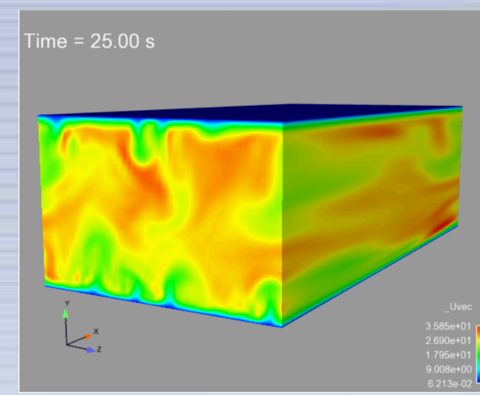


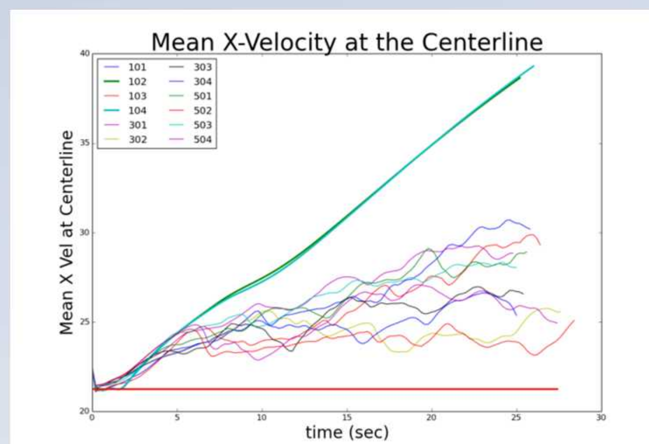
Wall-Model Calibration (in progress)

Calibrate boundary layer and bulk model parameters

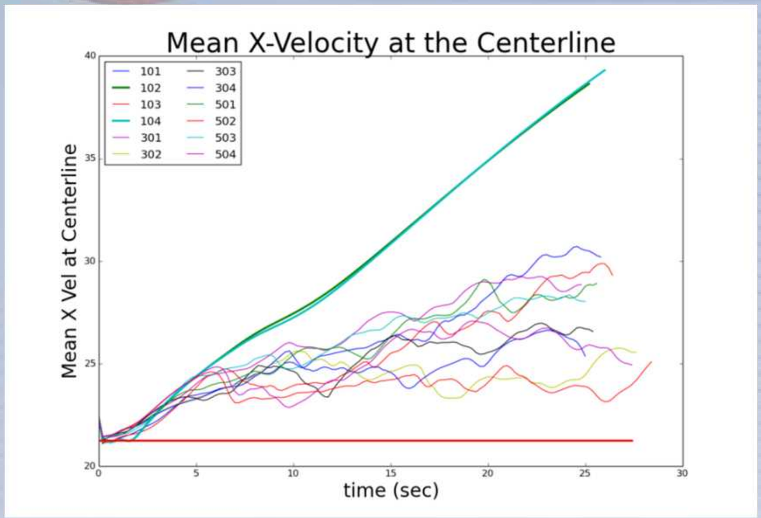


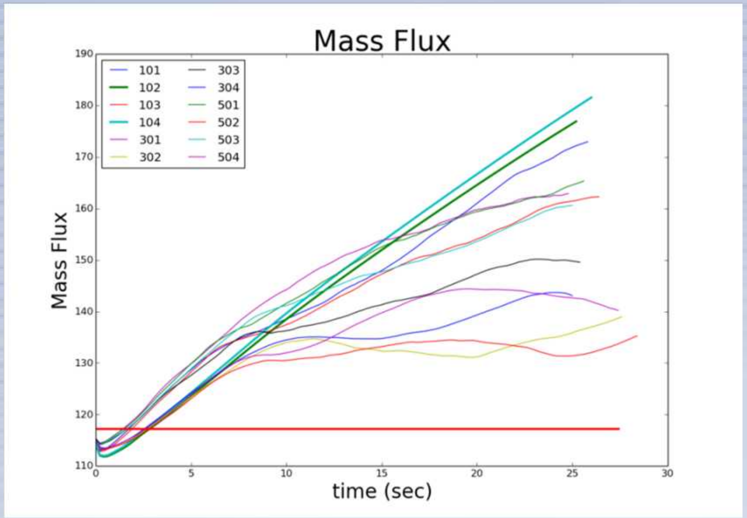


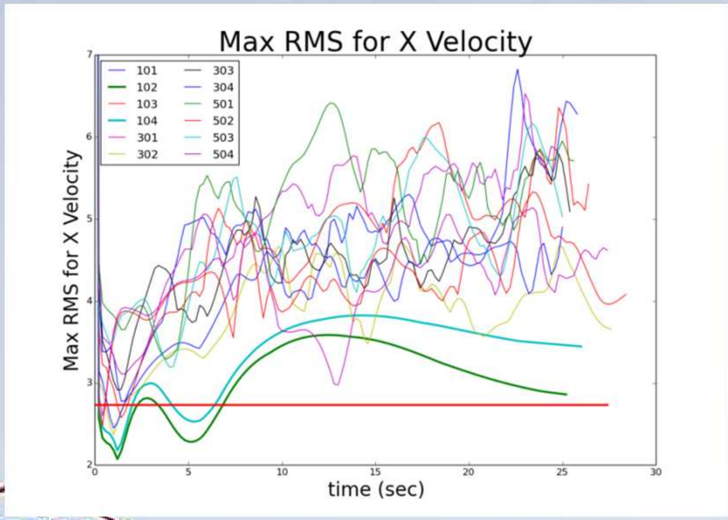


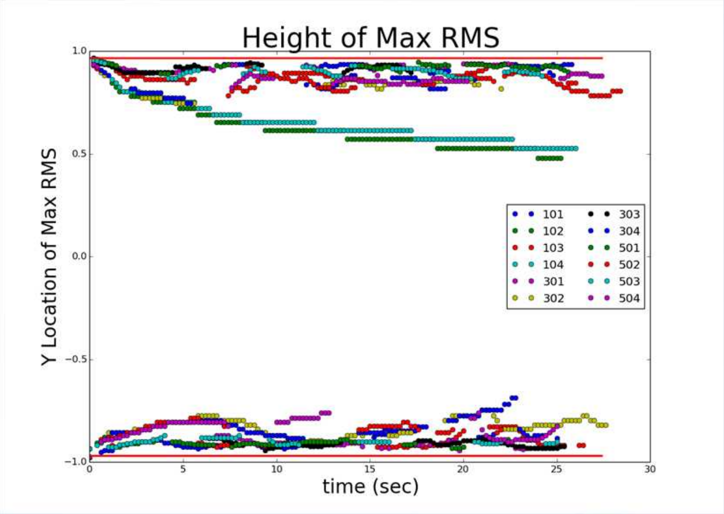


Wall Model Results



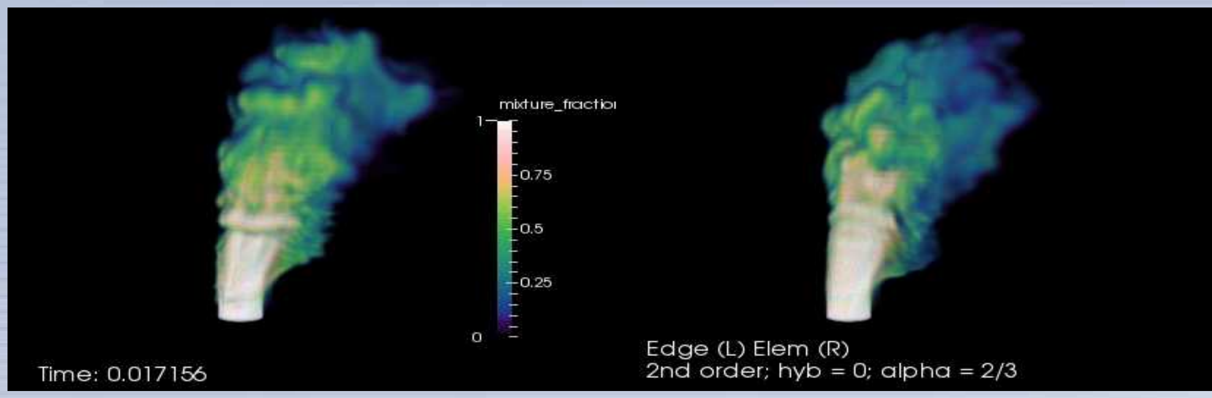


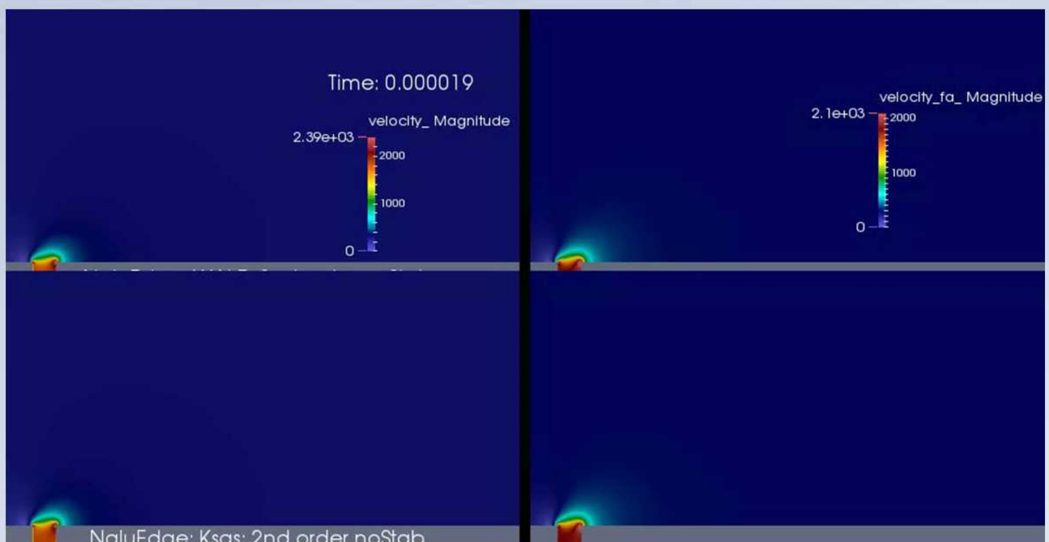




Jet-in-Crossflow UQ (in progress)

Simulation capability implemented in Nalu
Validate against Su & Mungal Re 5K case

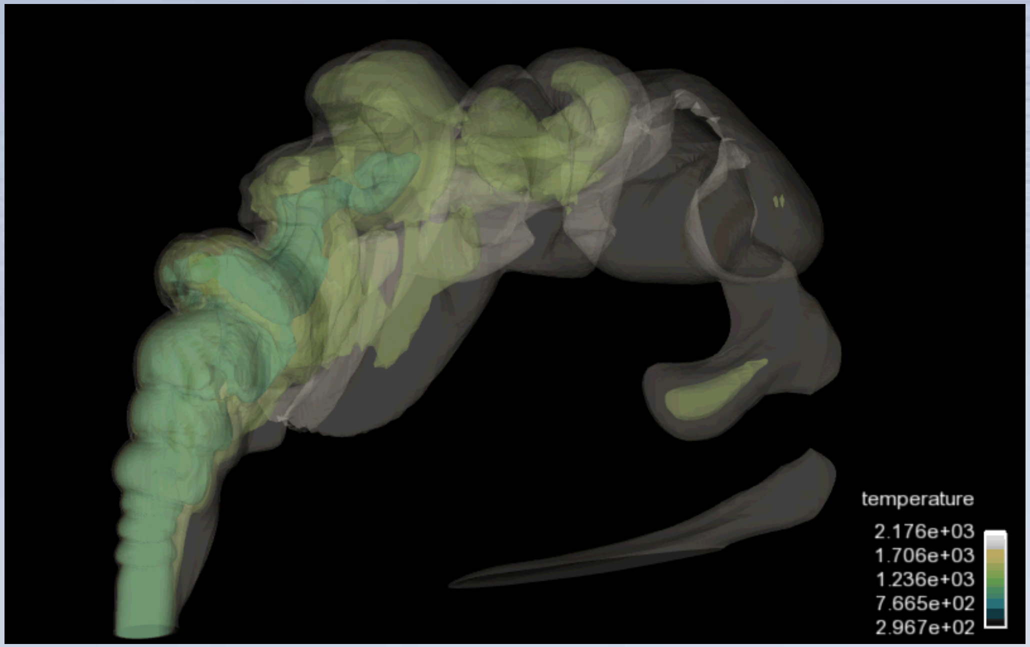




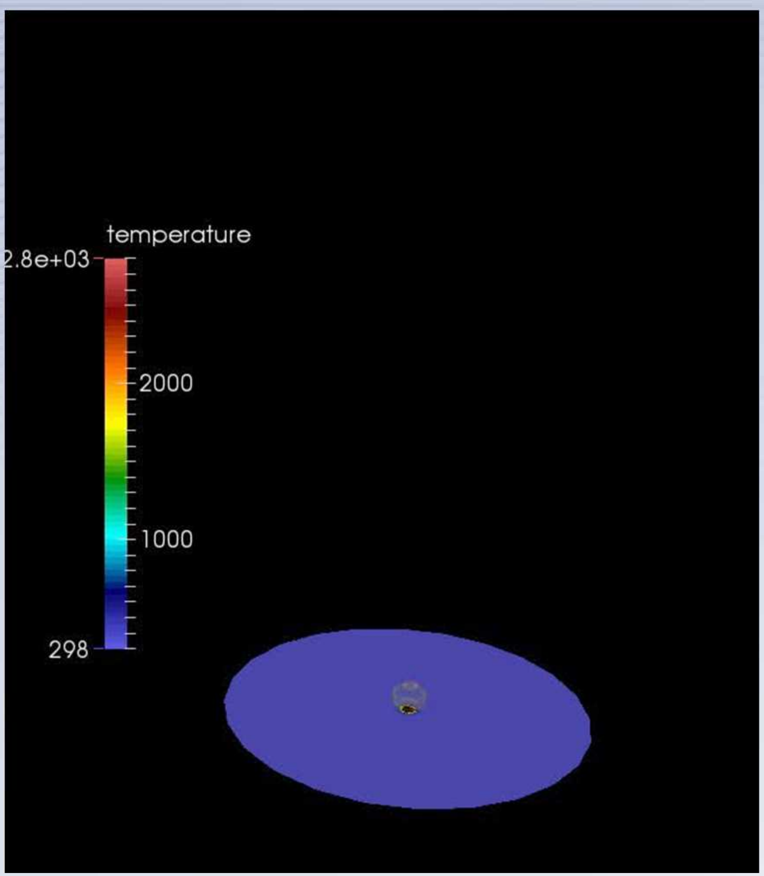
Collaborating with Ruiz, Lacaze, Oefelein, "Assessing the accuracy of Large Eddy Simulation in a Jet In Cross Flow Configuration," *(in prep)*

Combustion Model Implementation

Re ~25,000; Burke Schumann Methane Combustion

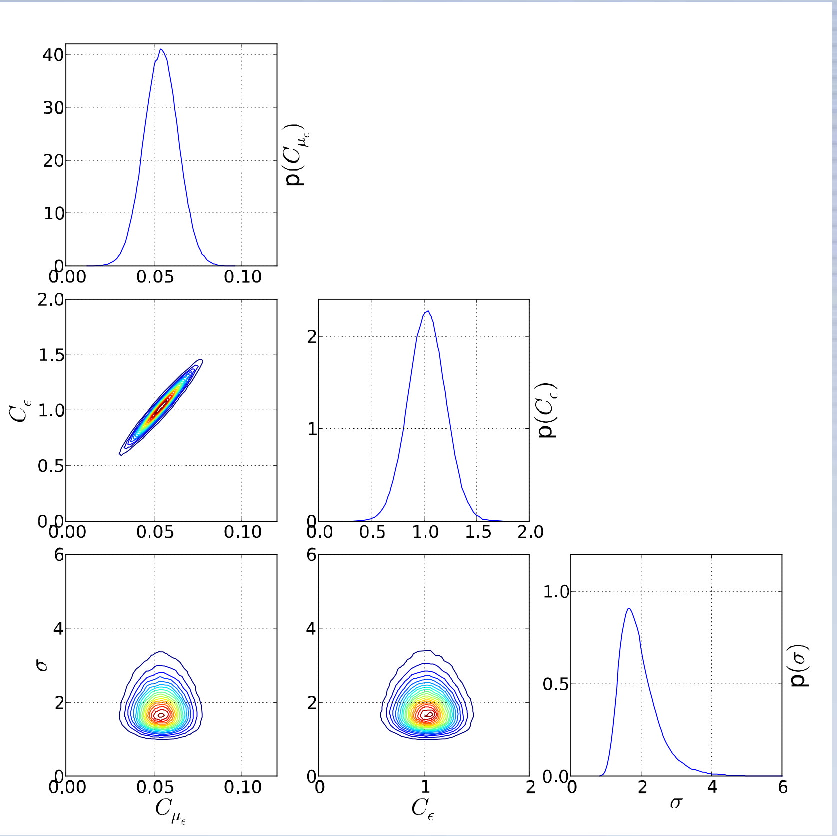


Mixture fraction iso-surfaces colored by temperature



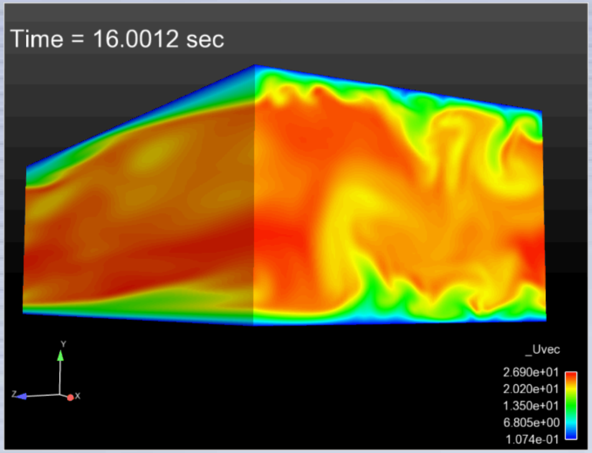
Forward UQ

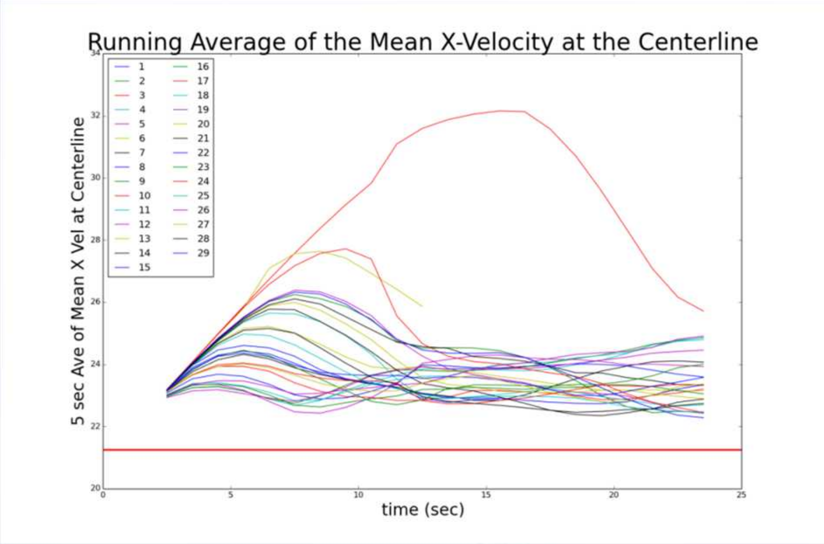
Joint PDF of Model Parameters



Safta, Blaylock, Templeton, Domino, “Parameter Uncertainty in LES of Channel Flow,” *(in prep.)*

Propagation in Turbulent Channel





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