SAND2015-2332C

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

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contract DE-AC04-94L85000.

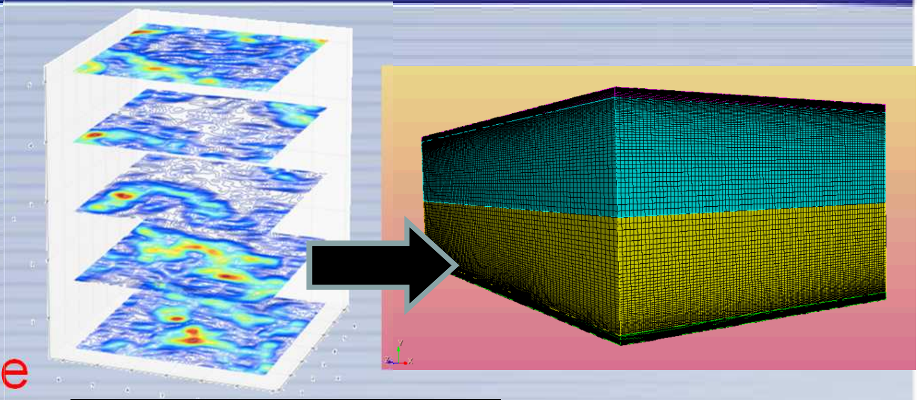
Group Effort

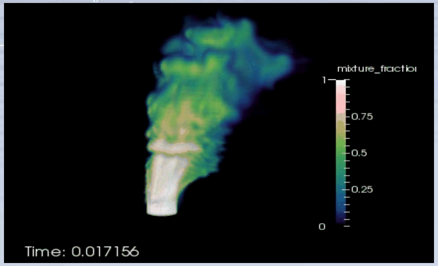
Team Members:

- Myra Blaylock
- Cosmin Safta
- Jeremy Templeton
- Stefan Domino
- John Hewson
- Habib N. Najm
- Khachik Sargsyan

Breadth 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

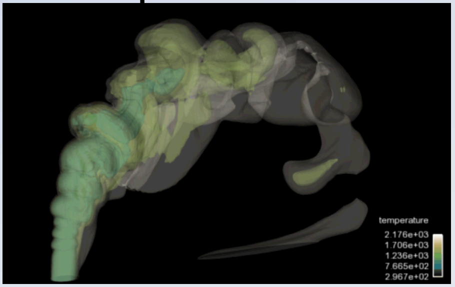


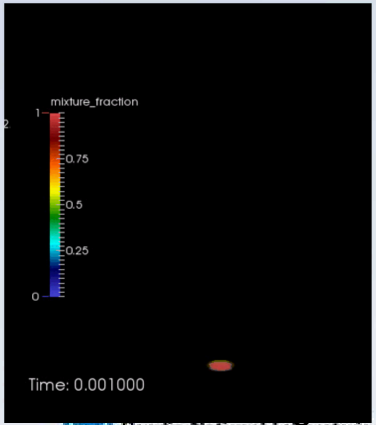


- **Reacting Flow**
  - Implement industrial and advanced combustion models
  - Infer combustion model parameters
  - UQ of reacting jet-in-crossflow

Burke Schumann Methane Combustion

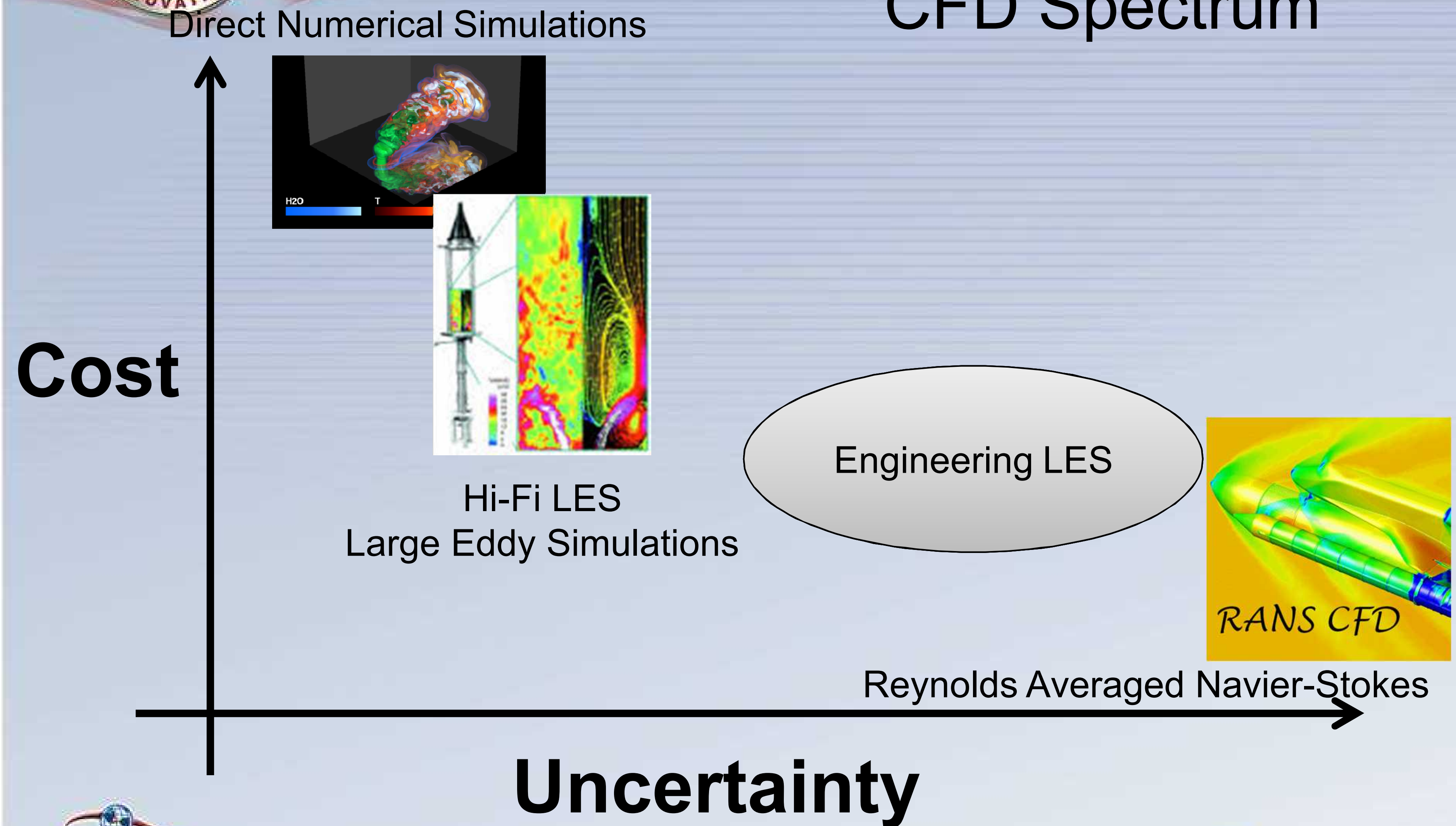
Temperature





What is Engineering LES?

CFD Spectrum



Direct Numerical Simulations

Cost

Hi-Fi LES
Large Eddy Simulations

Engineering LES

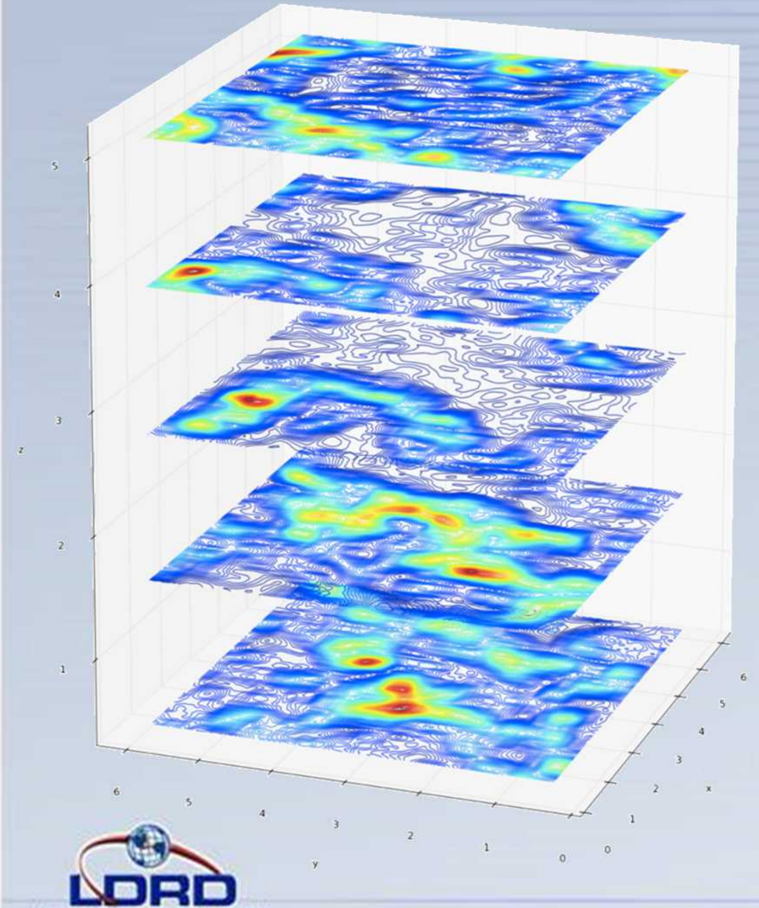
Reynolds Averaged Navier-Stokes

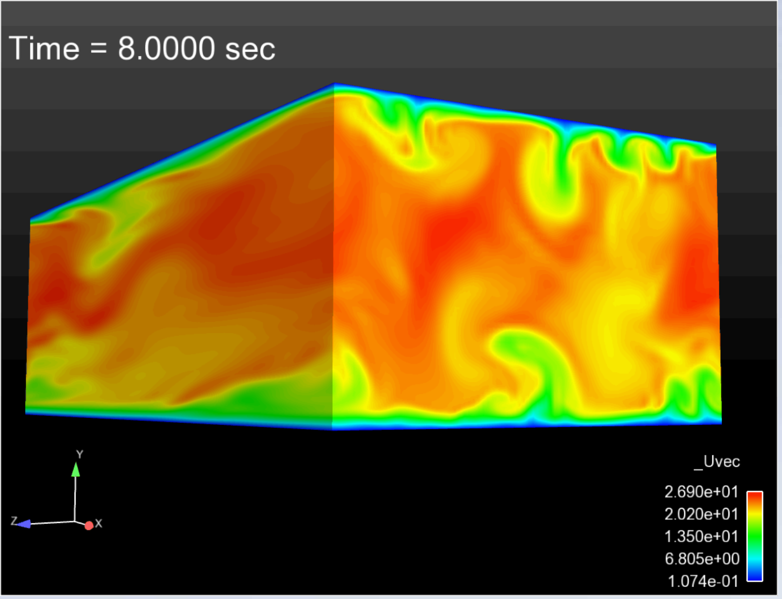
Uncertainty

Uncertainty Quantification of Channel Flow

DNS of Isotropic Turbulence (JHU)

Engineering LES for Channel Flow





Calibrate Subgrid-Scale Kinetic Energy (k^{sgs}) One-Equation LES Model

Transport Model:

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

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

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

Calibrate: C_ϵ and C_{μ_ϵ}

LDRD

LABORATORY DIRECTED RESEARCH & DEVELOPMENT

Sandia National Laboratories

Bayesian Calibration

Bayes formula:

$$\underbrace{P(\theta|D)}_{\text{posterior}} = \frac{\overbrace{P(D|\theta)}^{\text{likelihood}}\overbrace{P(\theta)}^{\text{prior}}}{\underbrace{P(D)}_{\text{evidence}}}$$

- Data *D* based on DNS of Isotropic Turbulence
- Model parameters *θ* are the k^{sgs} model constants: C_{ϵ} & $C_{\mu\epsilon}$
- The likelihood *P(D|θ)* is the probability of observing D given θ. If C_{ϵ} & $C_{\mu\epsilon}$ values are right, what are the chances of seeing D.
- The prior distribution *P(θ)* is the belief of what θ should be. Gaussians centered around the current nominal values for *θ*.
- The posterior distribution *P(θ|D)* is the probability that θ is correct after taking into account D.

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
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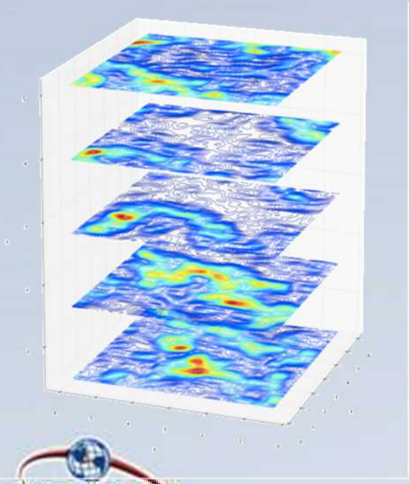
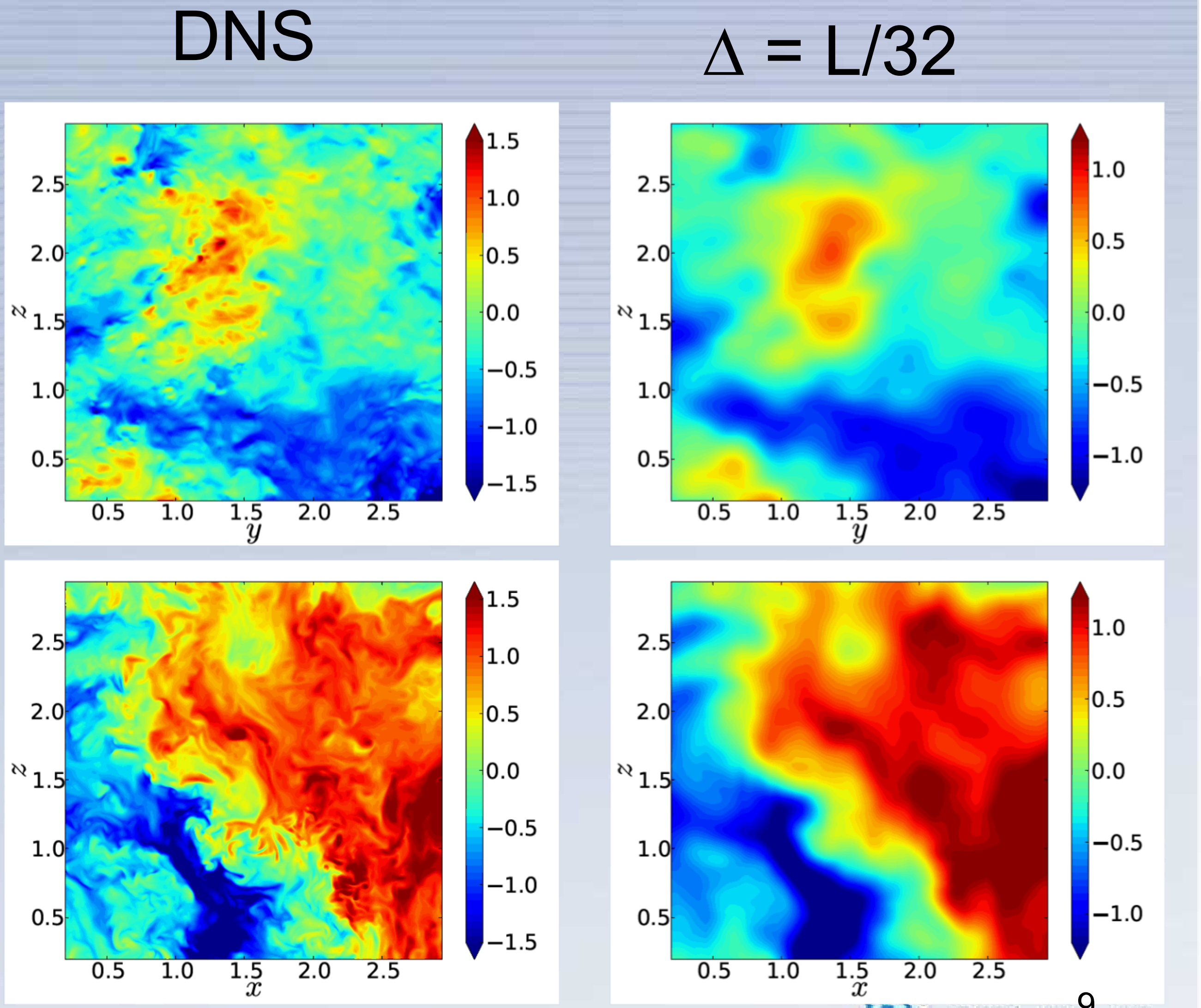
Data is Filtered DNS to LES scale

3 Filter sizes:

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



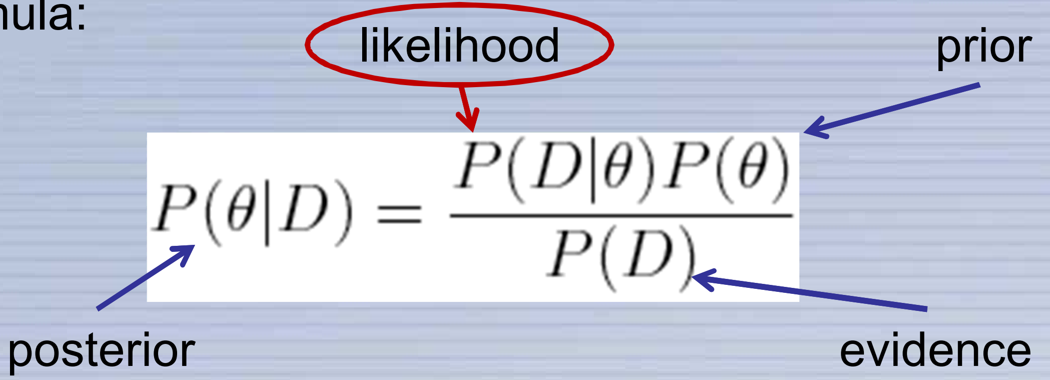


DNS

$\Delta = L/32$

Bayesian Calibration: Likelihood

Bayes formula:



likelihood

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

posterior

evidence

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Likelihood

$$z = m(\boldsymbol{x};\boldsymbol{\theta}) + \epsilon_z$$

$$z = m(\boldsymbol{x_a};\boldsymbol{\theta}) + \epsilon_z$$
$$\boldsymbol{x_o} = \boldsymbol{x_a} + \epsilon_x$$

$$p(\boldsymbol{\theta},\boldsymbol{\theta}_{\epsilon,z},\boldsymbol{\theta}_{\epsilon,x},\boldsymbol{x_a}|z,\boldsymbol{x_o}) \propto \underbrace{p(z|\boldsymbol{\theta},\boldsymbol{\theta}_{\epsilon,z},\boldsymbol{x_a})p(\boldsymbol{x_o}|\boldsymbol{\theta}_{\epsilon,x},\boldsymbol{x_a})}_{\text{Likelihood}} \times \underbrace{p(\boldsymbol{\theta},\boldsymbol{\theta}_{\epsilon,z})p(\boldsymbol{\theta}_{\epsilon,x},\boldsymbol{x_a})}_{\text{Prior}}$$

Likelihood Depends on Model Assumptions

- **Additive Error (Classical) Model (AEM)**

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

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

$\theta = \{C_{\mu\epsilon},\ C_\epsilon\}$

Embedded Error Model (EEM)

- **Hermite-Gauss PCEs**

$$C_{\mu_\epsilon} = \sum_k \alpha_{1,k}\Psi_k(\xi),\ C_\epsilon = \sum_k \alpha_{2,k}\Psi_k(\xi)$$

$$C_{\mu_\epsilon} = \alpha_{10} + \alpha_{11}\xi_1$$
$$C_\epsilon = \alpha_{20} + \alpha_{21}\xi_1 + \alpha_{22}\xi_2$$

- **Data model**

$$f_k = C_{\mu_\epsilon}(\boldsymbol{\alpha}_1) f_P - C_\epsilon(\boldsymbol{\alpha}_2) f_D$$

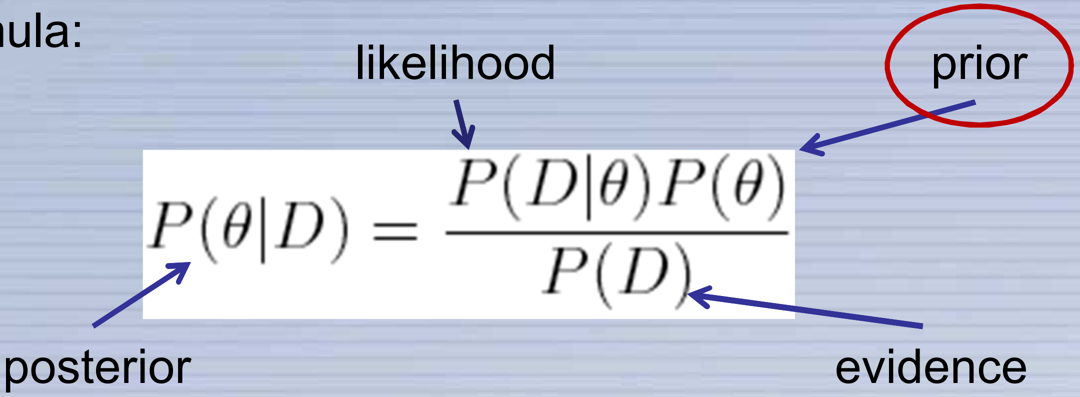
$$L_{\mathcal{D}}(\boldsymbol{\alpha}_1, \boldsymbol{\alpha}_2) = \prod_{i=1}^{N_t} p(f_{k,i} | \boldsymbol{\alpha}_1, \boldsymbol{\alpha}_2, \boldsymbol{x}_{\boldsymbol{a}})$$

$$\mu_f = \alpha_{10} f_P^a - \alpha_{11} f_D^a$$
$$\sigma_f^2 = \left(\alpha_{20} f_P^a - \alpha_{21} f_D^a\right)^2 + \left(\alpha_{22} f_D^a\right)^2$$

(Sargsyan, Najm, Ghanem - 2015)

Bayesian Calibration: Prior

Bayes formula:



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

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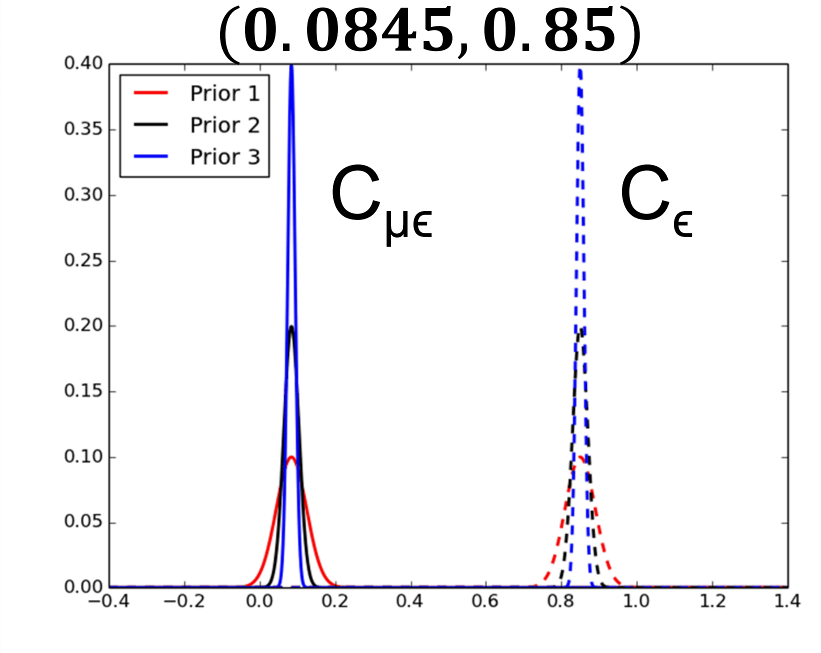
Independent Gaussian Priors

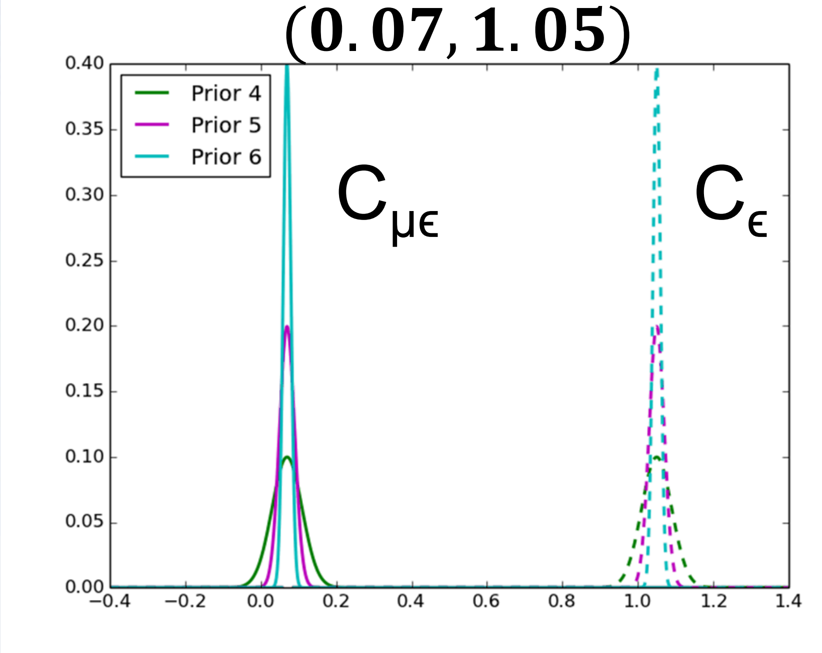
- **Centered at values from the literature ($C_{\mu\epsilon}$, C_{ϵ})**

  $\mathbf{(0.0845, 0.85)}$ $\mathbf{(0.07, 1.05)}$

- **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
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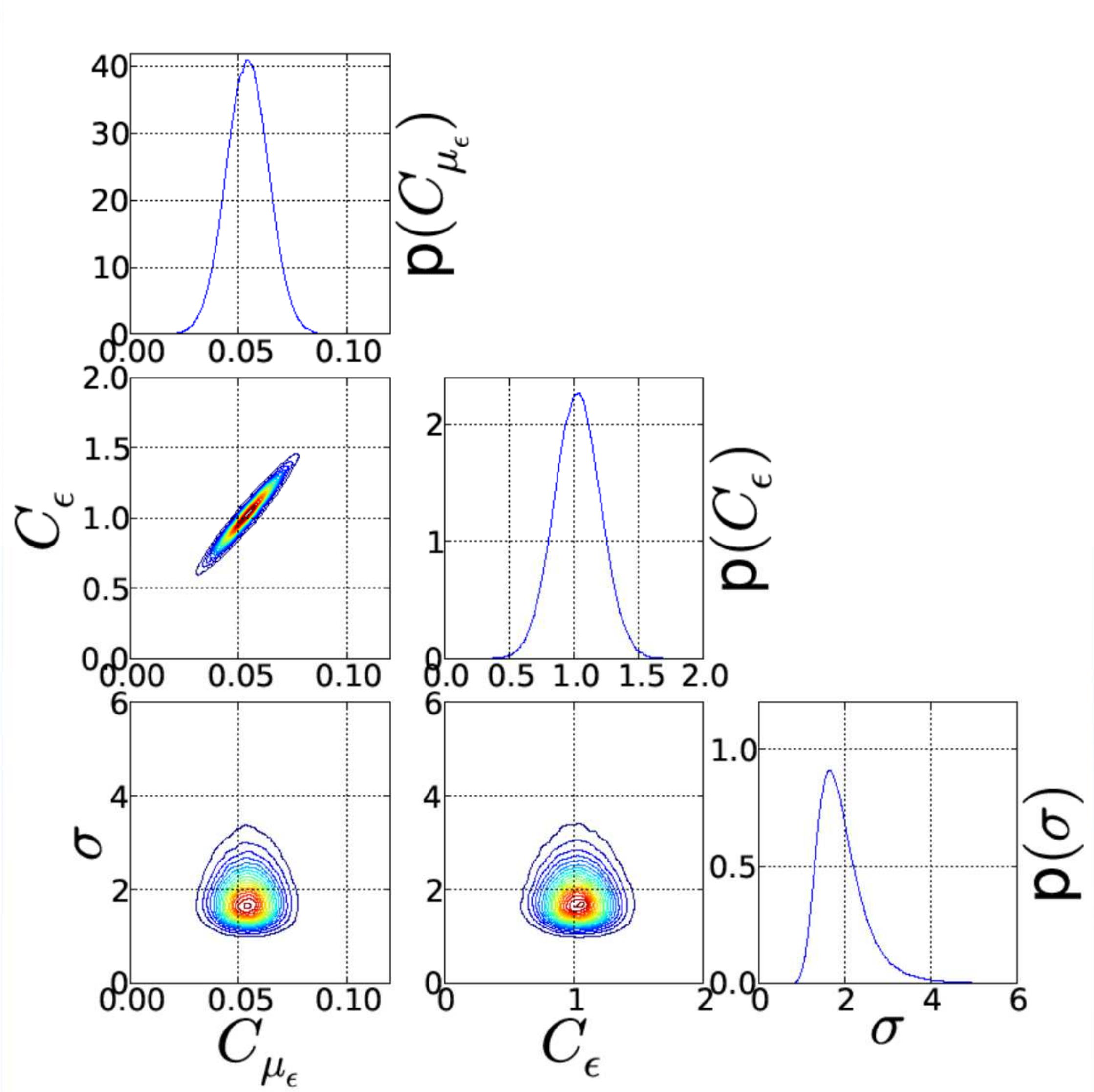
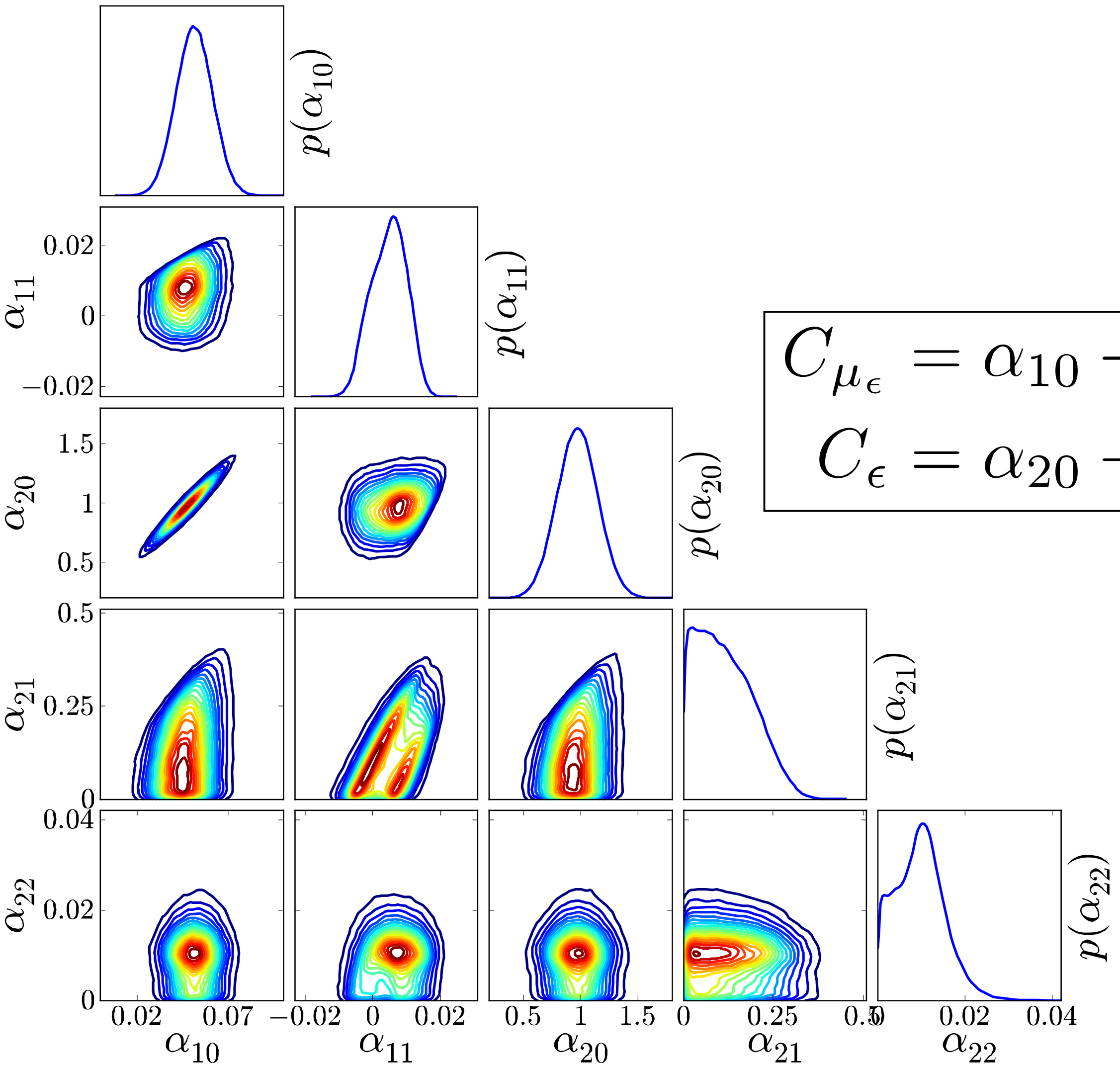
C_ϵ and $C_{\mu\epsilon}$ are Highly Correlated



Filter:
- Δ = L/16

Prior:
- (0.0845,0.85)
- σ = (0.01, 0.1)

Both Error Assumptions Recover Production to Dissipation Ratio



Filter:

- Δ = L/16

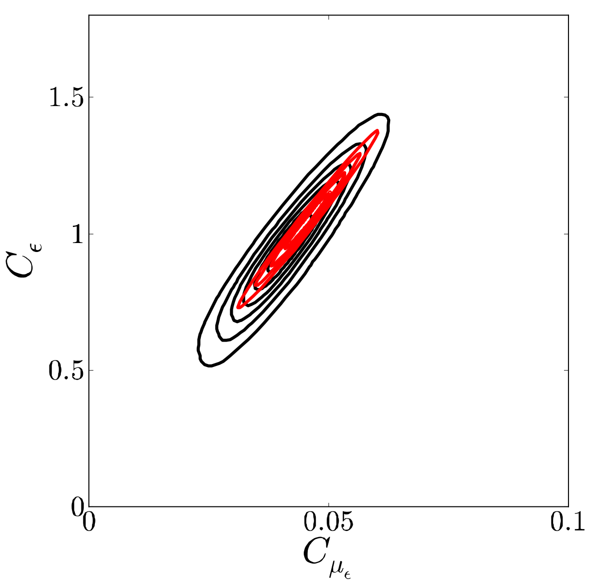
Prior:

- (0.0845,0.85)
- σ = (0.01, 0.1)

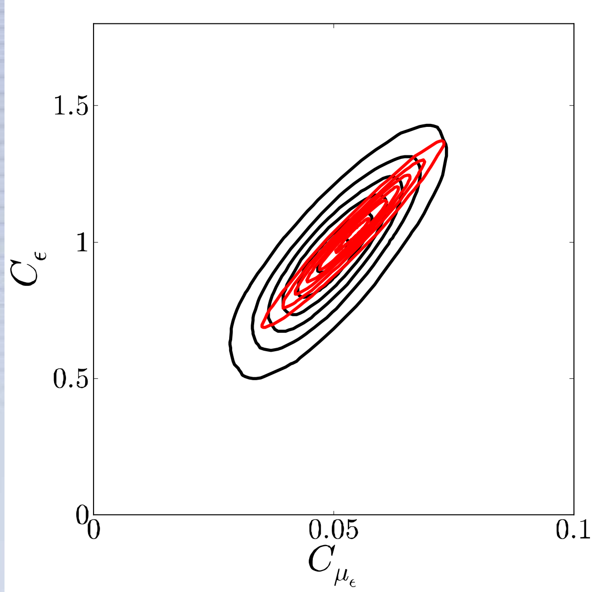
$$C_{\mu_\epsilon} = \alpha_{10} + \alpha_{11}\xi_1$$
$$C_\epsilon = \alpha_{20} + \alpha_{21}\xi_1 + \alpha_{22}\xi_2$$

EEM Approach Results in Greater Model Uncertainty

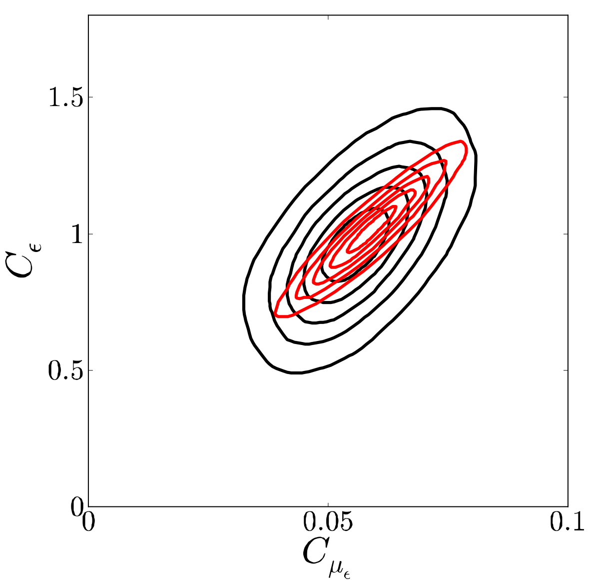
Small Prior Uncertainty



Medium Prior Uncertainty



High Prior Uncertainty

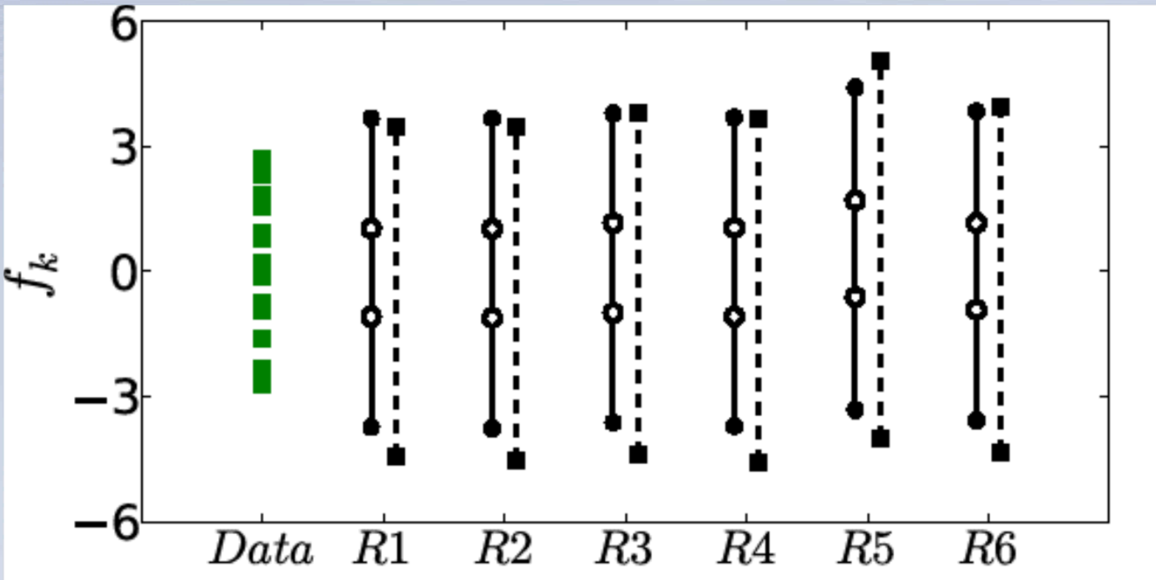


Joint Posterior Density Distributions

- Black – AEM
- Red – EEM

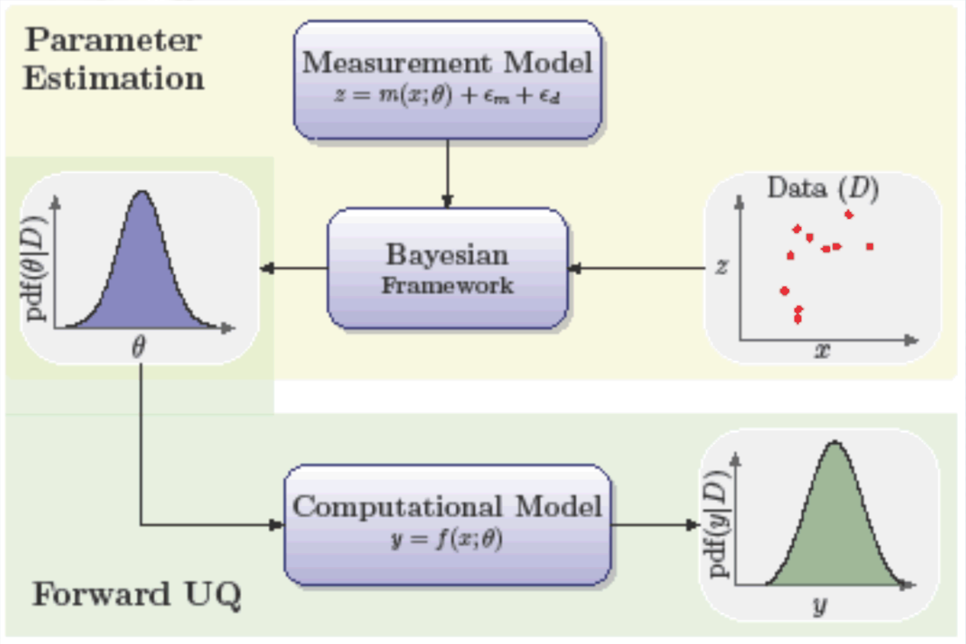
A Posteriori Test Shows EEM Recovers Data Uncertainty

- **Green – Medium filtered DNS data**
- **Dashed – EEM**
- **Solid – AEM : ○ -no error ● - including error model**



Different Prior Means and Standard Deviations

Forward UQ – Predictive Assessment



Parameter Estimation

Measurement Model
$z = m(x;\theta) + \epsilon_m + \epsilon_d$

Bayesian Framework

Data (D)

Computational Model
$y = f(x;\theta)$

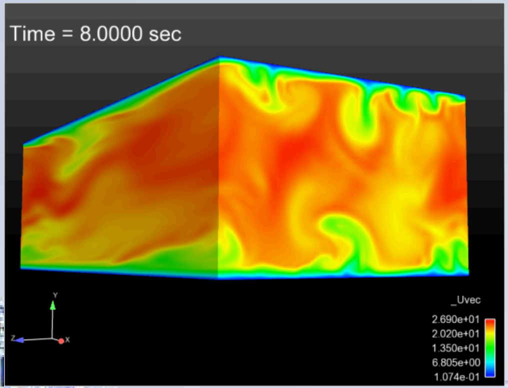
Forward UQ

- y – quantity of interest: mean x velocity, rms, $\dot{m}$
- Modeled by Polynomial Chaos Expansion

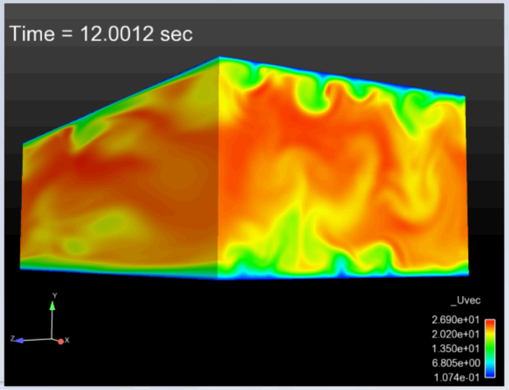
$$y(C_\epsilon,C_{\mu\epsilon}) = \Sigma\, c_k \Psi_k(\xi_1,\xi_2)$$

- Galerkin projection:

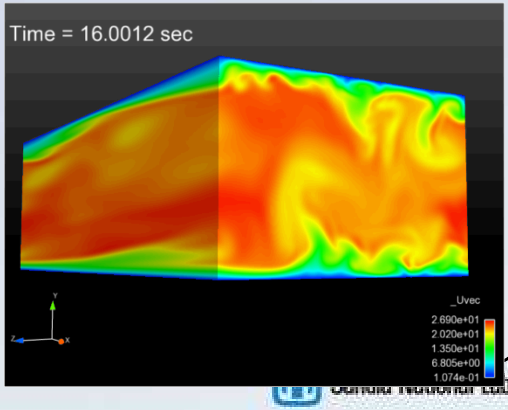
$$c_k = \frac{\langle y(C_\epsilon, C_{\mu\epsilon})\Psi_k(\xi_1,\xi_2)\rangle}{\langle \Psi_k{}^2(\xi_1,\xi_2)\rangle}$$



Time = 8.0000 sec



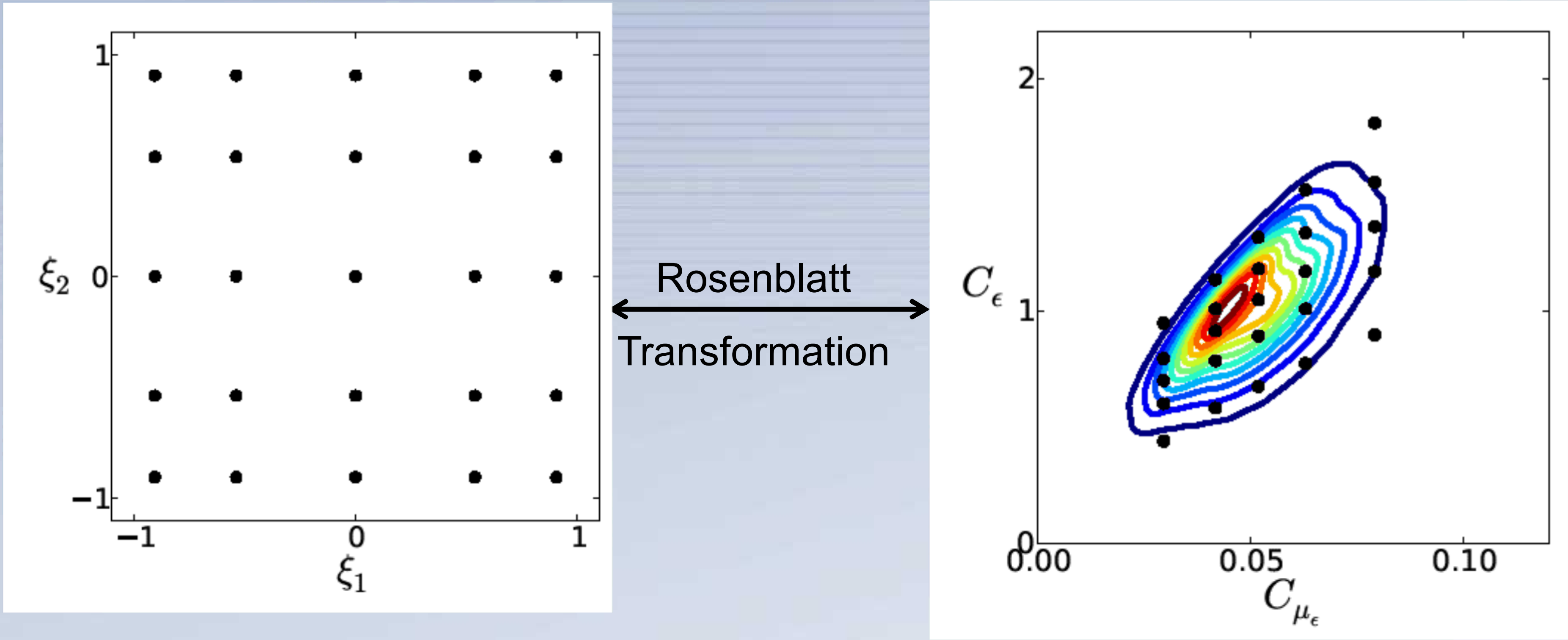
Time = 12.0012 sec



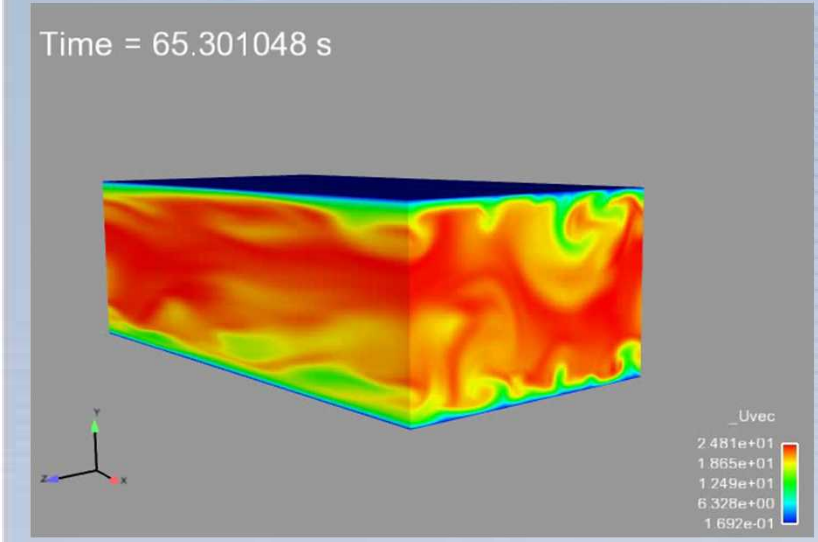
Time = 16.0012 sec

Quadrature to Construct PC Expansion for Model Output

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



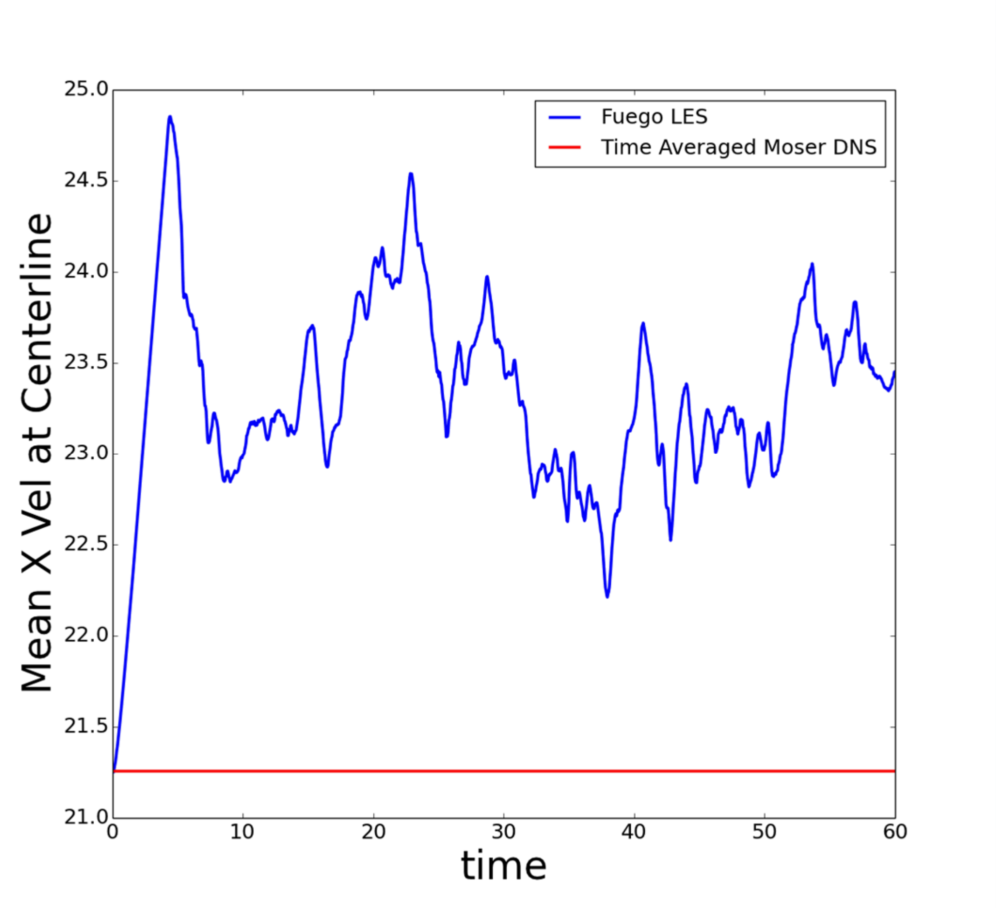
Fuego LES Simulations with Calibrated Parameters



- 250k nodes
  - $y^+ \approx 1.15$ at walls
  - Hyperbolic tan to same spacing as in z
  - 40 processors ~ 780 hours
- DNS (Moser *et al.*)
  ~ 37 M points

- 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
- Body force in *x*-direction to produce flow
- Dimensions:
  - Flow direction: $x = 2\pi$ (periodic)
  - Wall normal direction: $y = 2$
  - Cross flow direction: $z = \pi$ (periodic)

Average Velocity at the Centerline



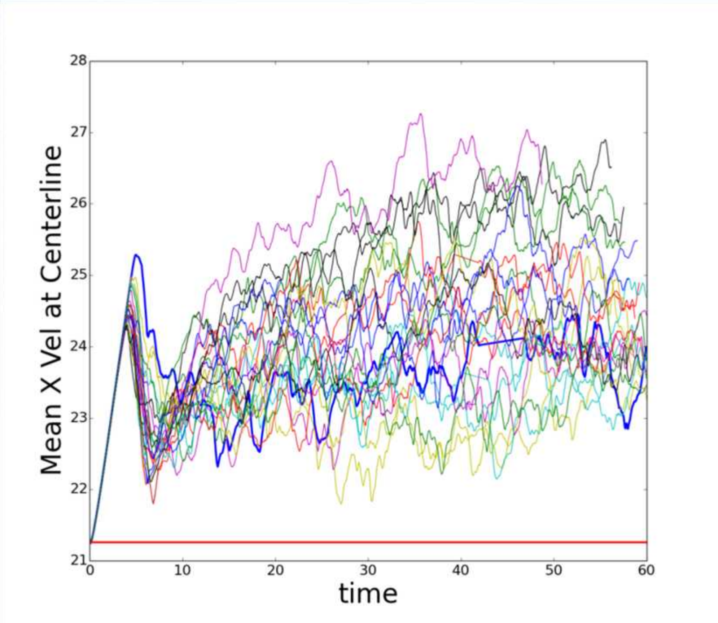
Moser DNS time averaged value: 21.26

- 15% off

Average Velocity at the Centerline

- 250k nodes
  - $y^+ \approx 1.15$ at walls
  - Hyperbolic tan to same spacing as in z
  - 40 processors ~ 780 hours
- DNS (Moser *et al.*)

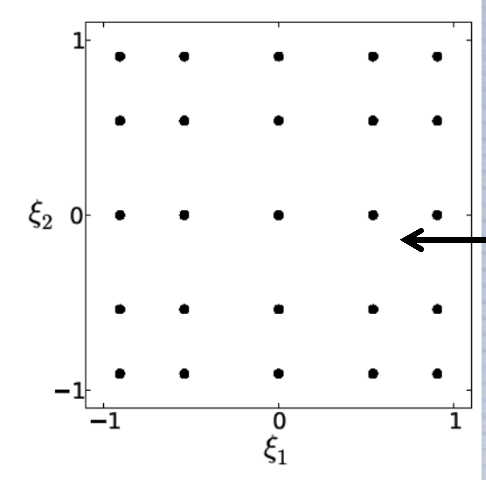
  ~ 37 M points

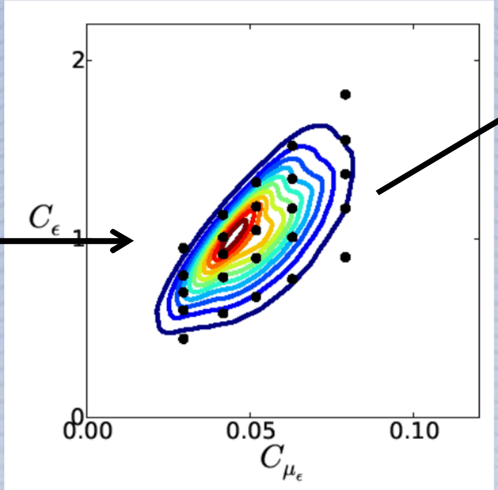


Moser DNS time averaged value: 21.26

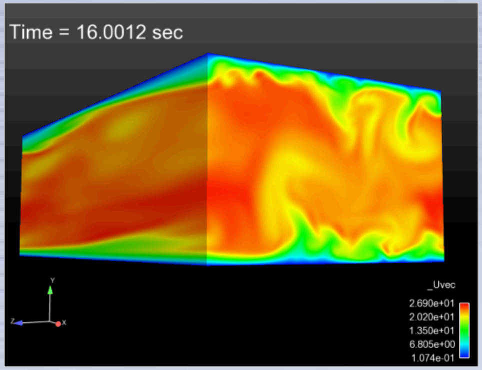
- 15% off

Creating the Polynomial Chaos Expansions





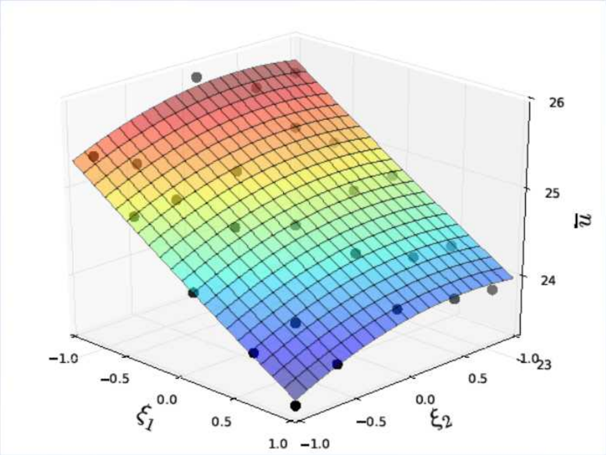
Run LES 25 times



Calculate weighting coefficient

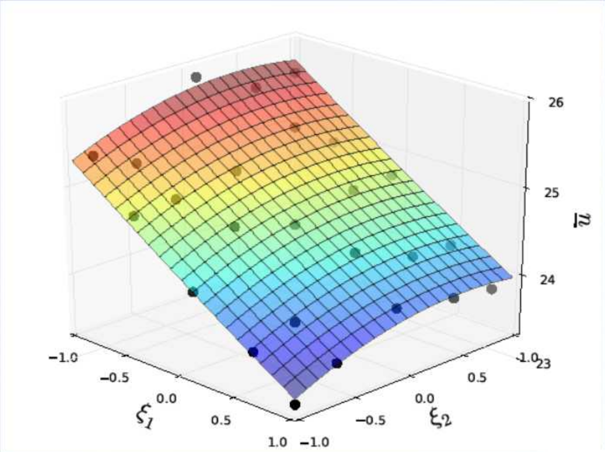
$$c_k = \frac{\langle y(C_\epsilon, C_{\mu\epsilon})\Psi_k(\xi_1,\xi_2)\rangle}{\langle {\Psi_k}^2(\xi_1,\xi_2)\rangle}$$

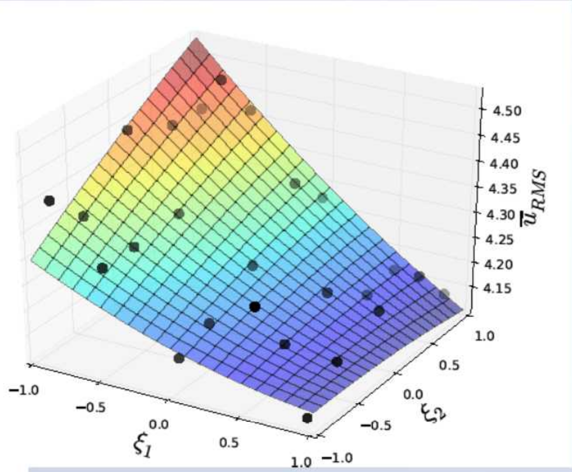
Create PCE

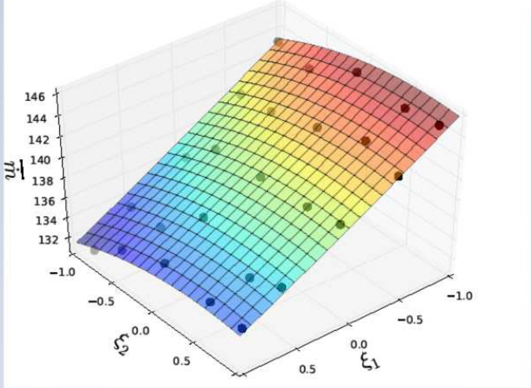


$$y(C_\epsilon(\xi_1,\xi_2), C_{\mu\epsilon}(\xi_1,\xi_2)) = \Sigma\, c_k\, \Psi_k(\xi_1,\xi_2)$$

Creating the Polynomial Chaos Expansions

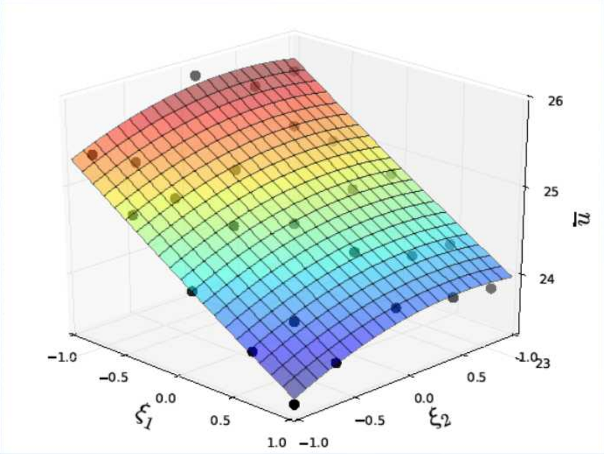






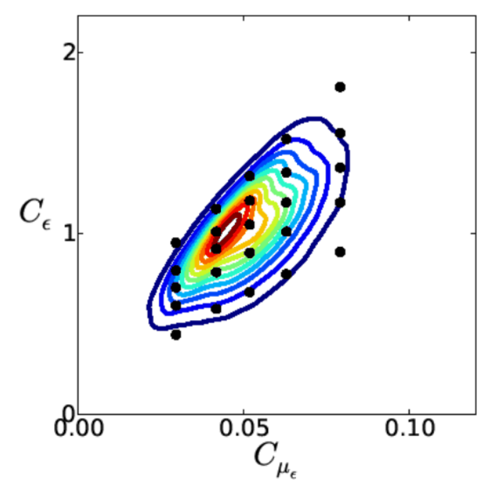
Sample Mean Velocity with PCE

$$\overline{u_x}(C_\epsilon(\xi_1,\xi_2),C_{\mu\epsilon}(\xi_1,\xi_2)) = \Sigma\ c_k \Psi_k(\xi_1,\xi_2)$$

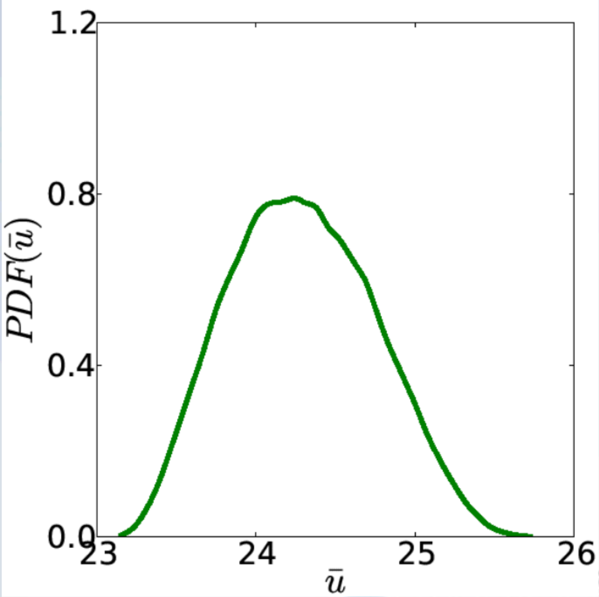


- **For one prior and filter width**

Sample many times

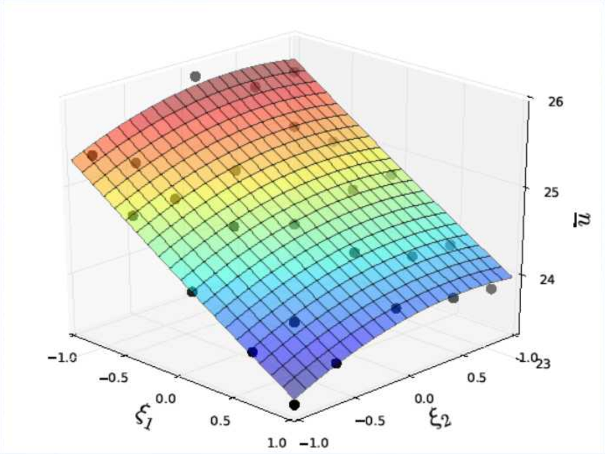


For each pair of $C_\epsilon, C_{\mu\epsilon}$, get $\overline{u_x}$



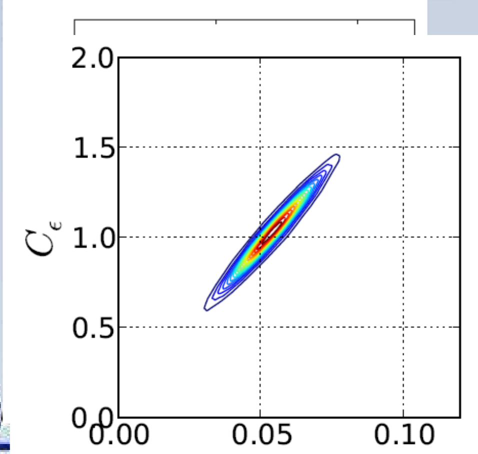
Sample Different Mean Velocity with PCE

$$\overline{u_x}(C_\epsilon(\xi_1,\xi_2),C_{\mu\epsilon}(\xi_1,\xi_2)) = \Sigma\ c_k \Psi_k(\xi_1,\xi_2)$$

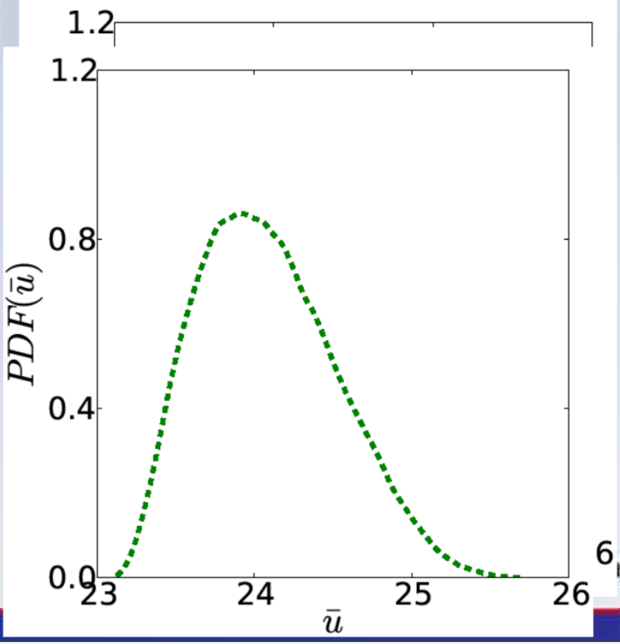


- **Same PCE**
- **Different prior and filter width**

Sample many times



For each pair of C_ϵ,$C_{\mu\epsilon}$, get $\overline{u_x}$

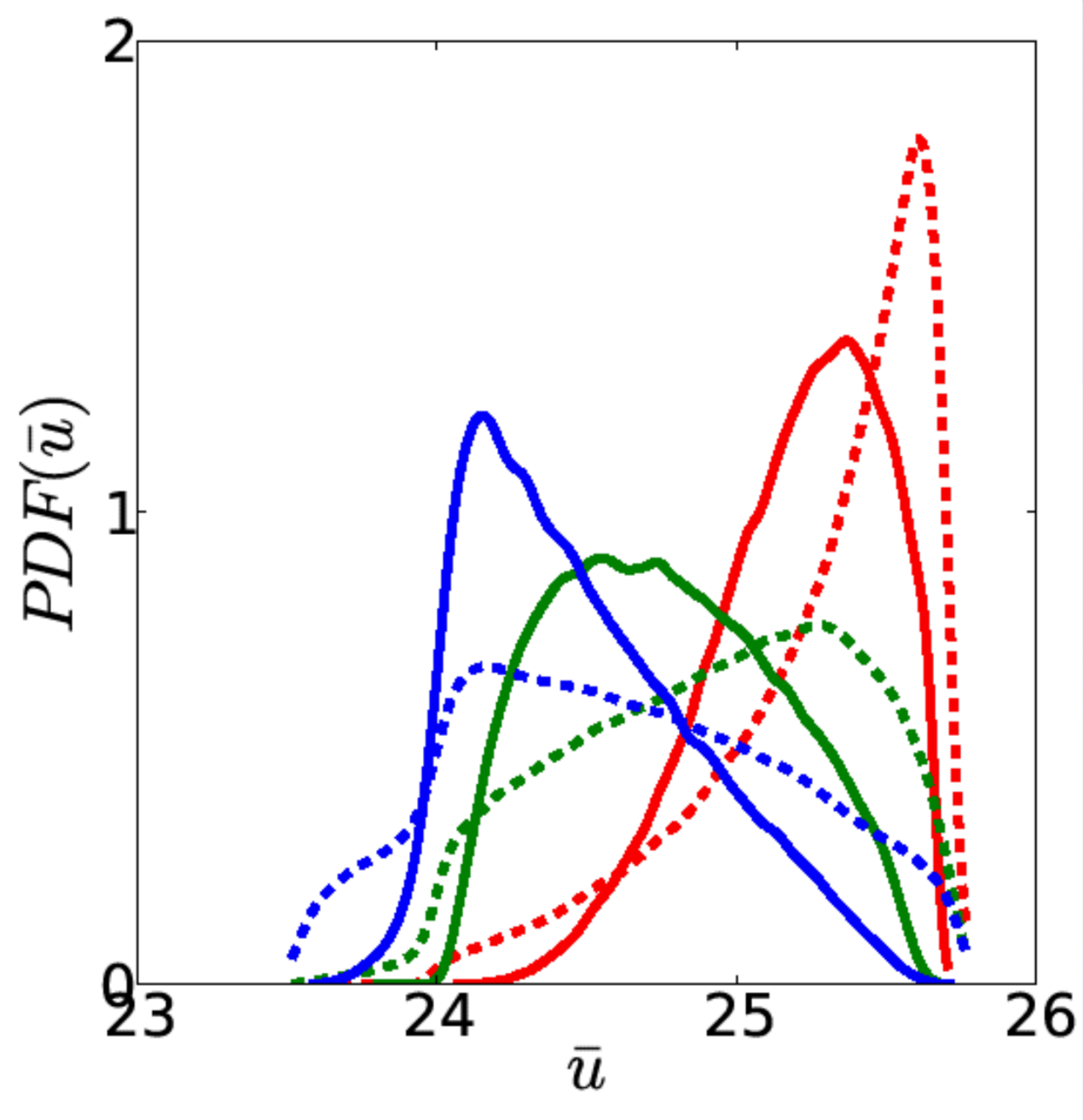


Midline Average Velocity – AEM vs EEM

- Red - Δ = L/64
- Green - Δ = L/32
- Blue - Δ = L/16

- Solid –AEM
- Dashed – EEM

- Moser DNS = 21.2



Conclusions

- **Used DNS isotropic turbulence to predict engineering LES channel flow Quantities of Interest**
- **Production and dissipation terms for the k^{sgs} model are highly correlated**
- **Filter width matters in the construction of the Posterior**
- **AEM vs. EEM**
  - EEM enables posterior checks without need to account for extra error information
- **Discrepancy in QoI values from Channel flow DNS**
  - “engineering level”
  - Filter size is too small

Thank You

&

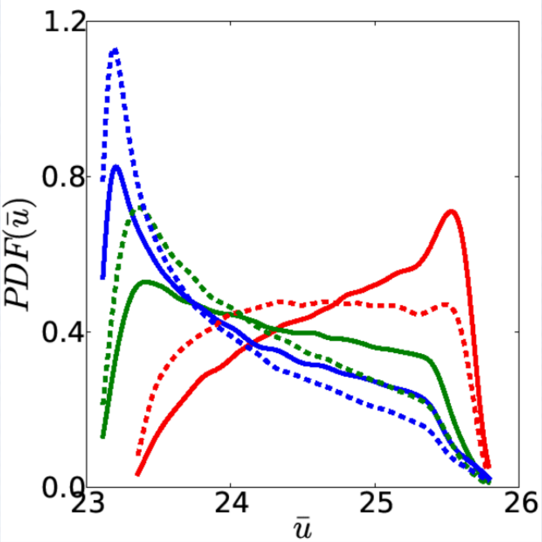
Questions

Midline Average Velocity - AEM

- **6 Prior and 3 Filter widths**
- **Red - Δ = L/64**
- **Green - Δ = L/32**
- **Blue - Δ = L/16**

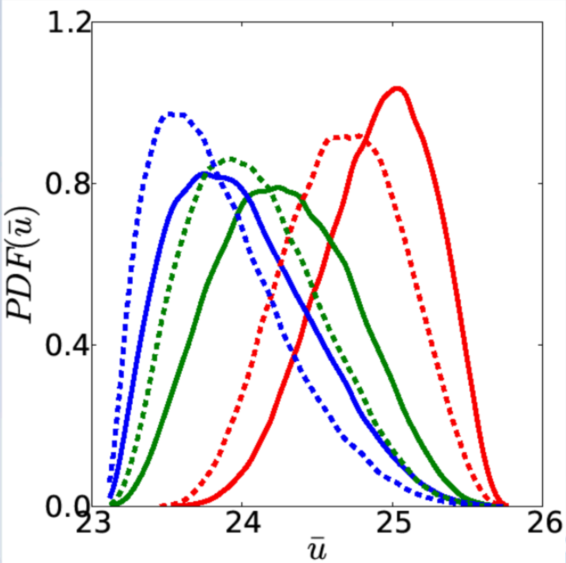
- **Solid = (0.0845, 0.85)**
- **Dashed = (0.07, 1.05)**

- **Moser DNS = 21.26**



Less confident in prior

σ=0.4
σ=0.04

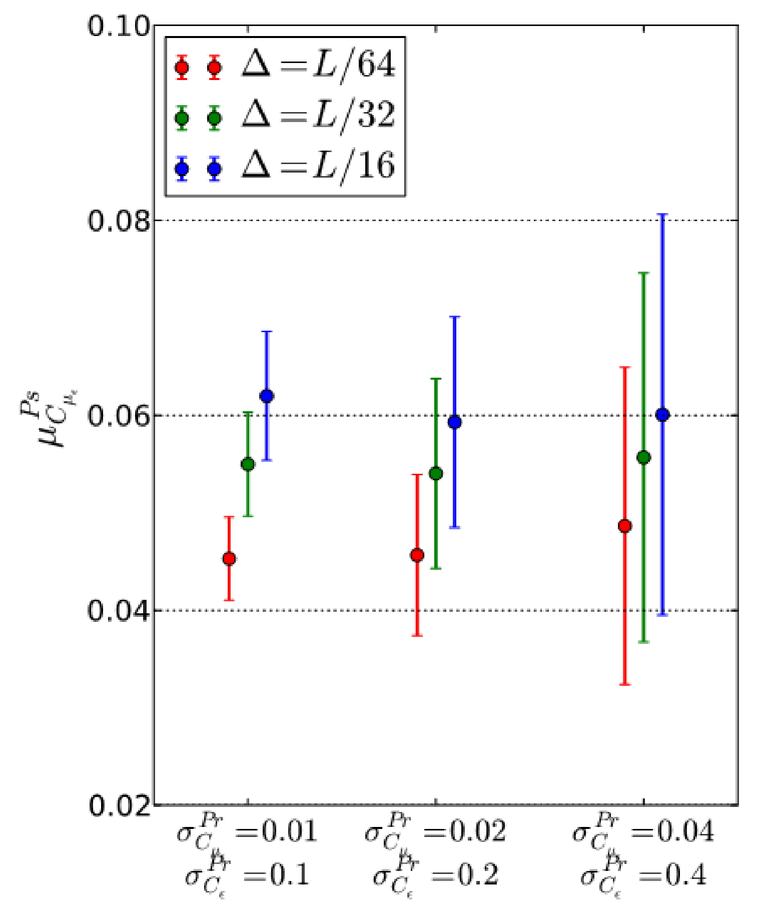


More confident in prior

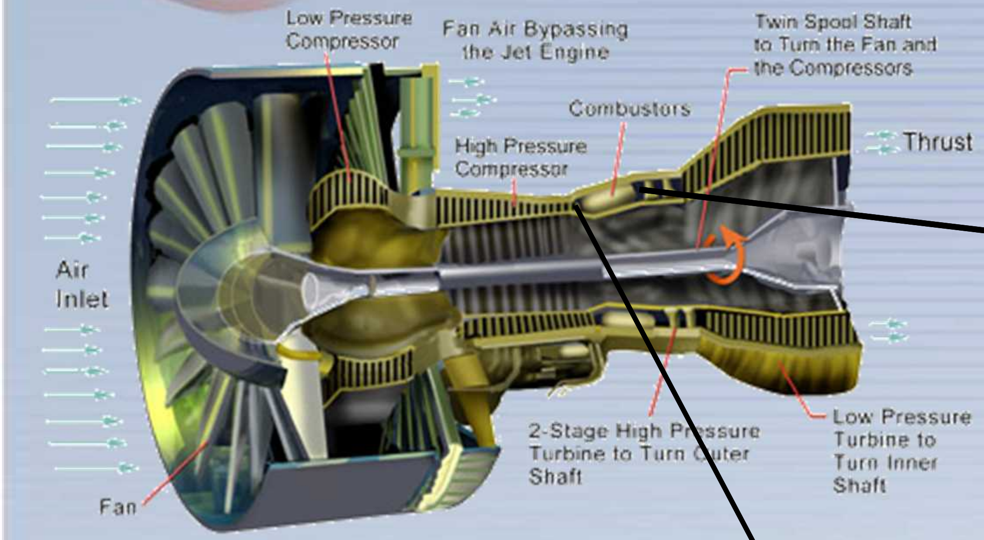
σ=0.2
σ=0.02

Effect of Filter Size and Prior

Posterior for $C_{\mu\epsilon}$



Gas Turbine Challenges

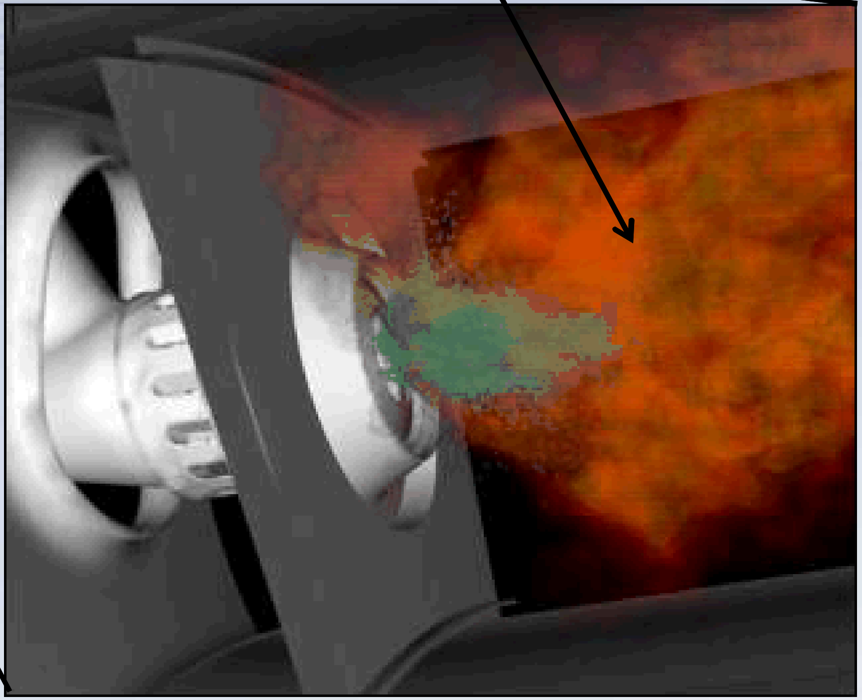


RANS solutions and modeling strategies are inadequate given the free flow and turbulence driven by heat release

Gas Turbine Engine

Complex flow physics coupled with chemistry drives efficiency and pollutant emissions

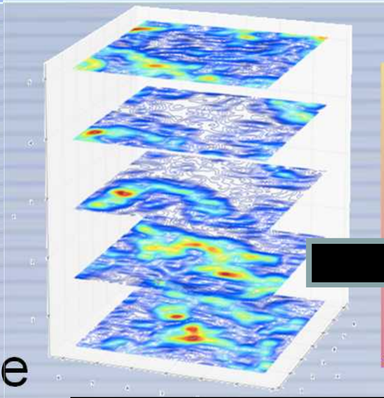
High Fidelity LES vs Engineering LES

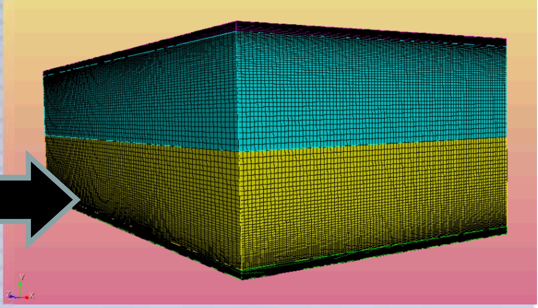


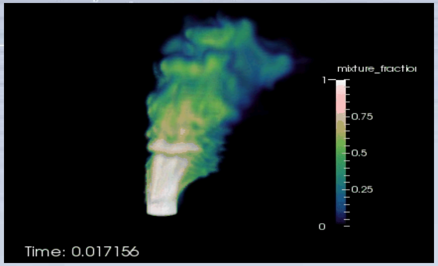
Gas Turbine Combustor Flow
Stanford ASCI Alliance Center

Breadth 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



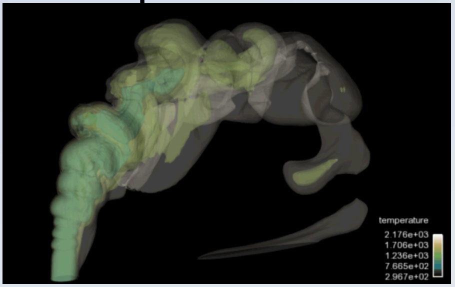


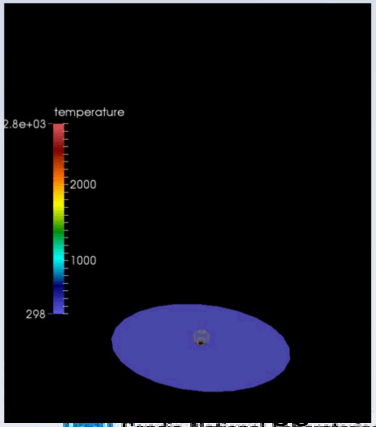


- **Reacting Flow**
  - Implement industrial and advanced combustion models
  - Infer combustion model parameters
  - UQ of reacting jet-in-crossflow and complex geometry flow

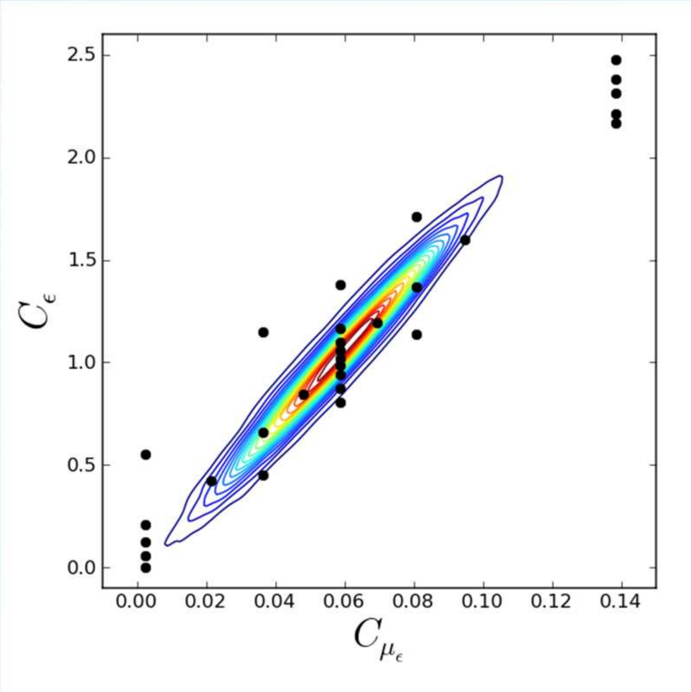
Burke Schumann Methane Combustion

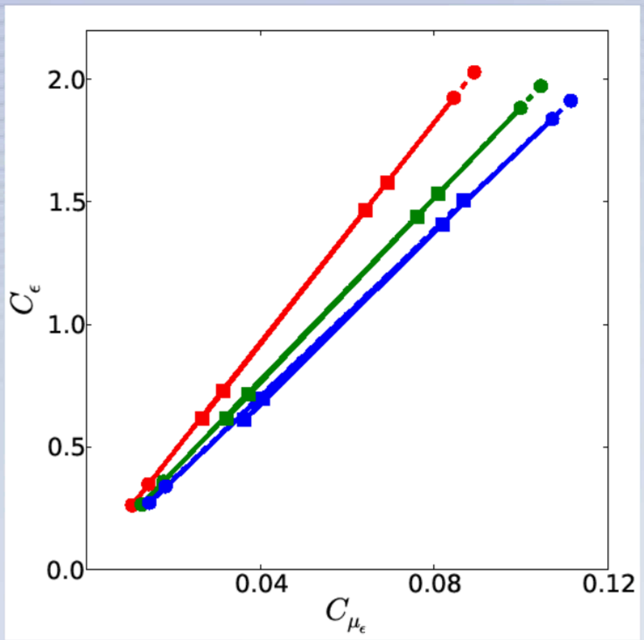
Temperature





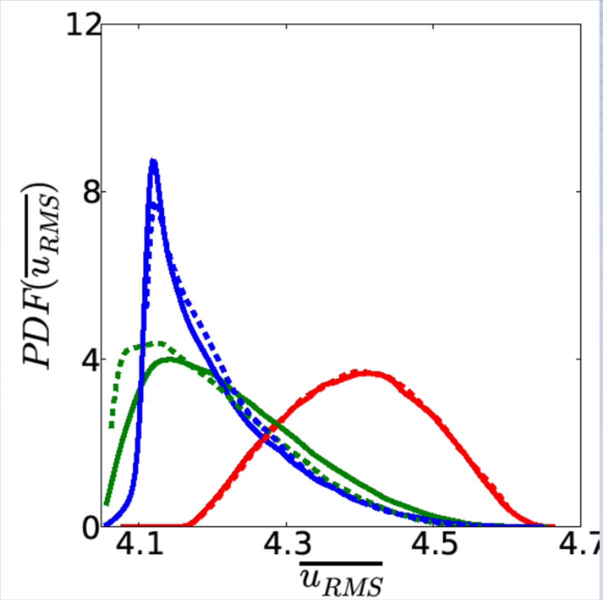
Principal Component Analysis of Joint PDF's

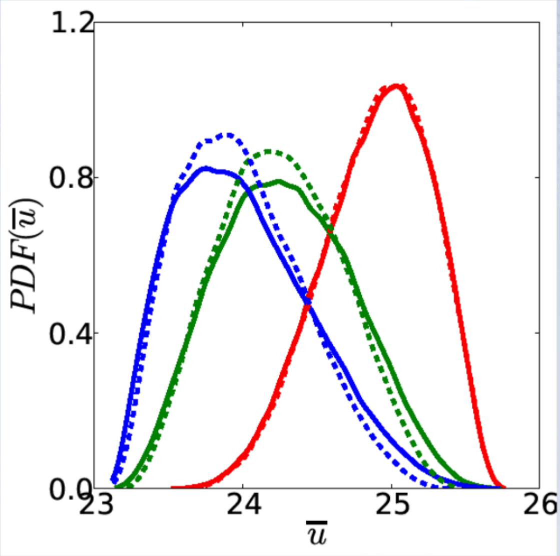


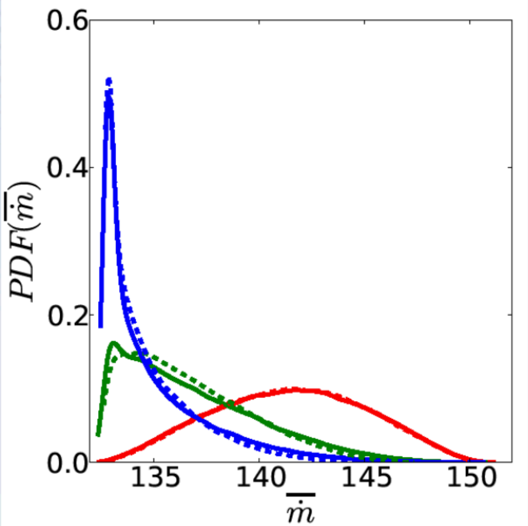


First Principal Component yields similar results to Joint PDF

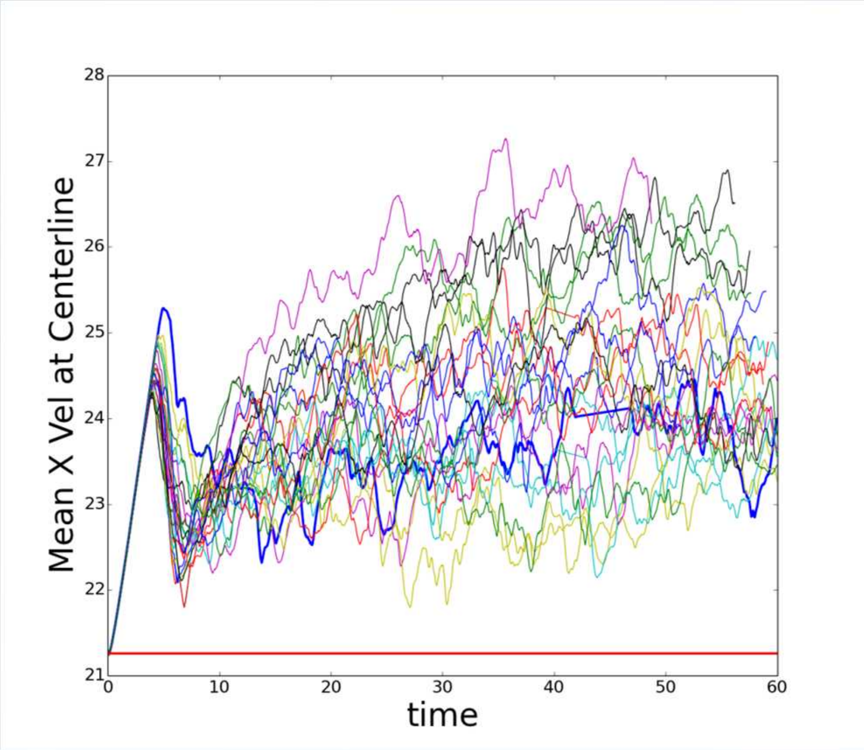
- **Solid – Joint PDF**
- **Dashed – 1st PC**

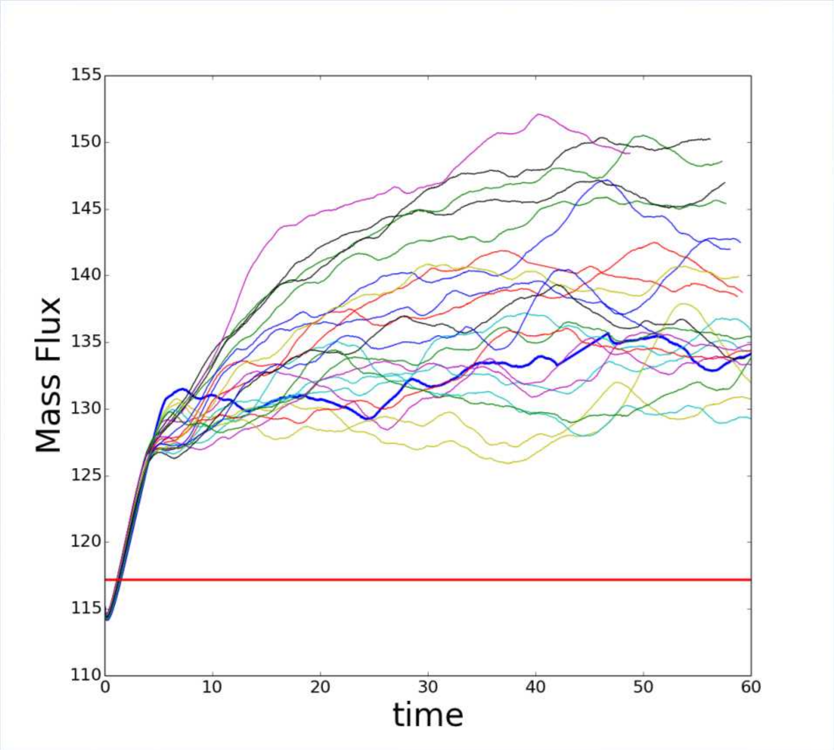






Velocity and Mass Flux





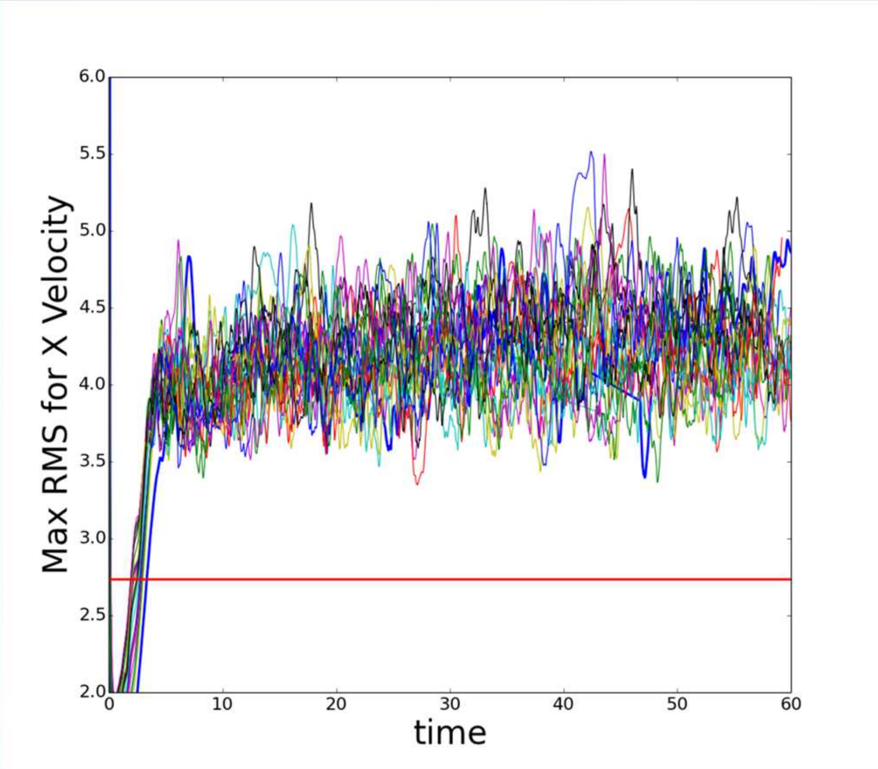
Moser DNS time averaged value: 21.26

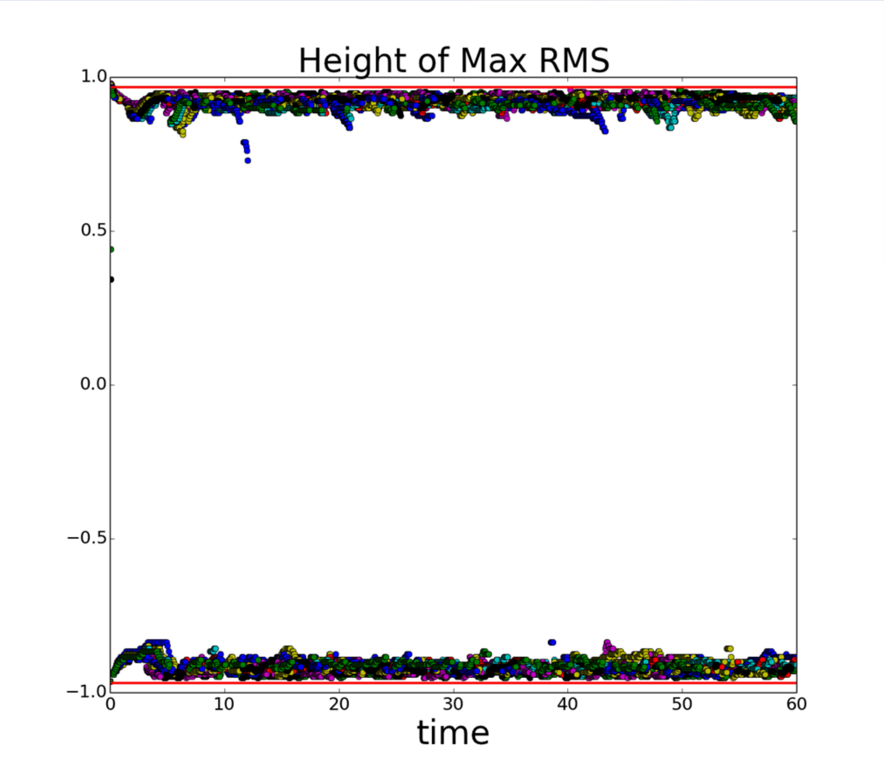
- 15% off

Moser: 117

16% off

Max RMS Velocity

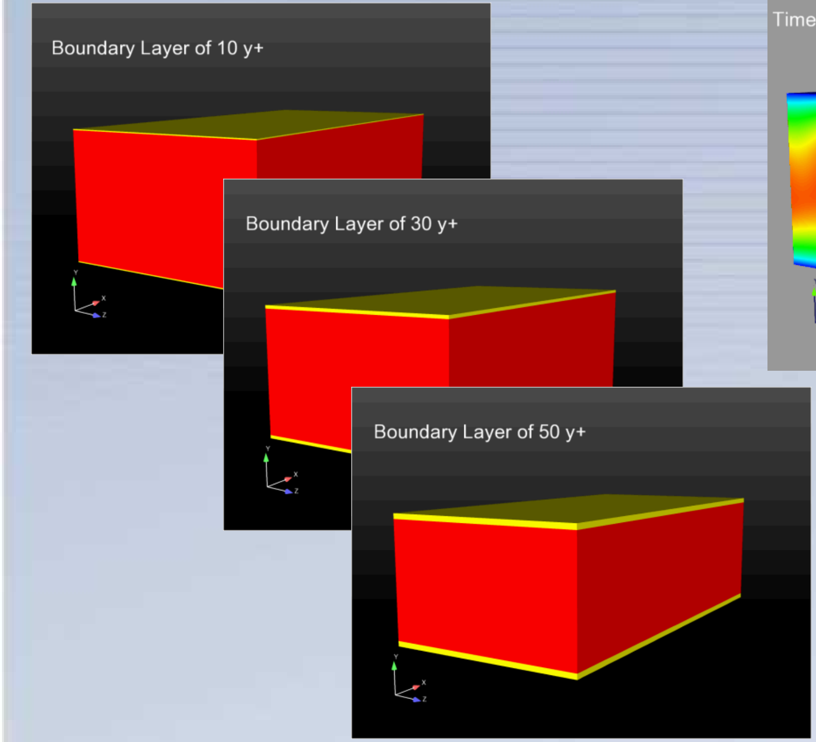


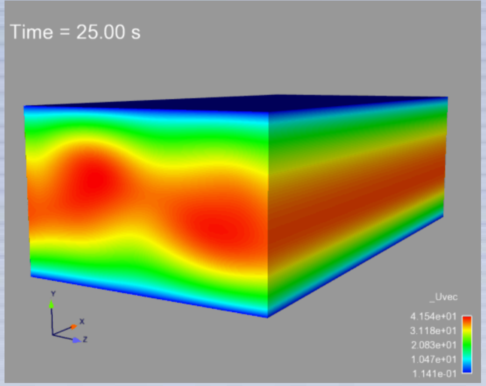


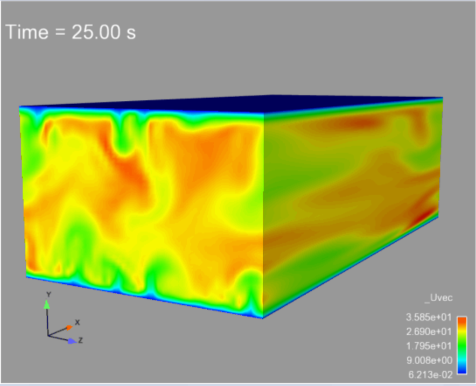
Moser: 2.7
60% off

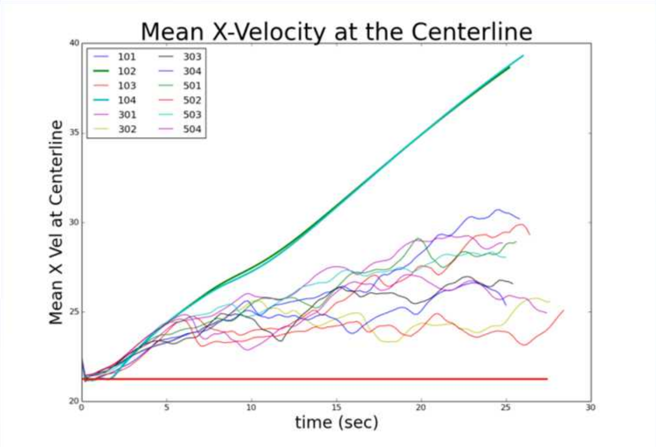
Wall-Model Calibration (in progress)

Calibrate boundary layer and bulk model parameters









Likelihood Depends on Model Assumptions

- **Presumed Error (Classical) Model (PEM)**

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

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

- **Embedded Error Model (EEM)**
  - (Sargsyan, Najm, Ghanem - 2014)

$$\begin{aligned} C_{\mu_\epsilon} &= \alpha_{10} + \alpha_{11}\xi_1 \\ C_\epsilon &= \alpha_{20} + \alpha_{21}\xi_1 + \alpha_{22}\xi_2 \end{aligned}$$