SAND2015-6034C

Calibration and Forward Uncertainty Propagation of Turbulence Models for Coarse-Grid Large-Eddy Simulation

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Interdisciplinary Team


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Combustion Models


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Infrastructure


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UQ/Calibration


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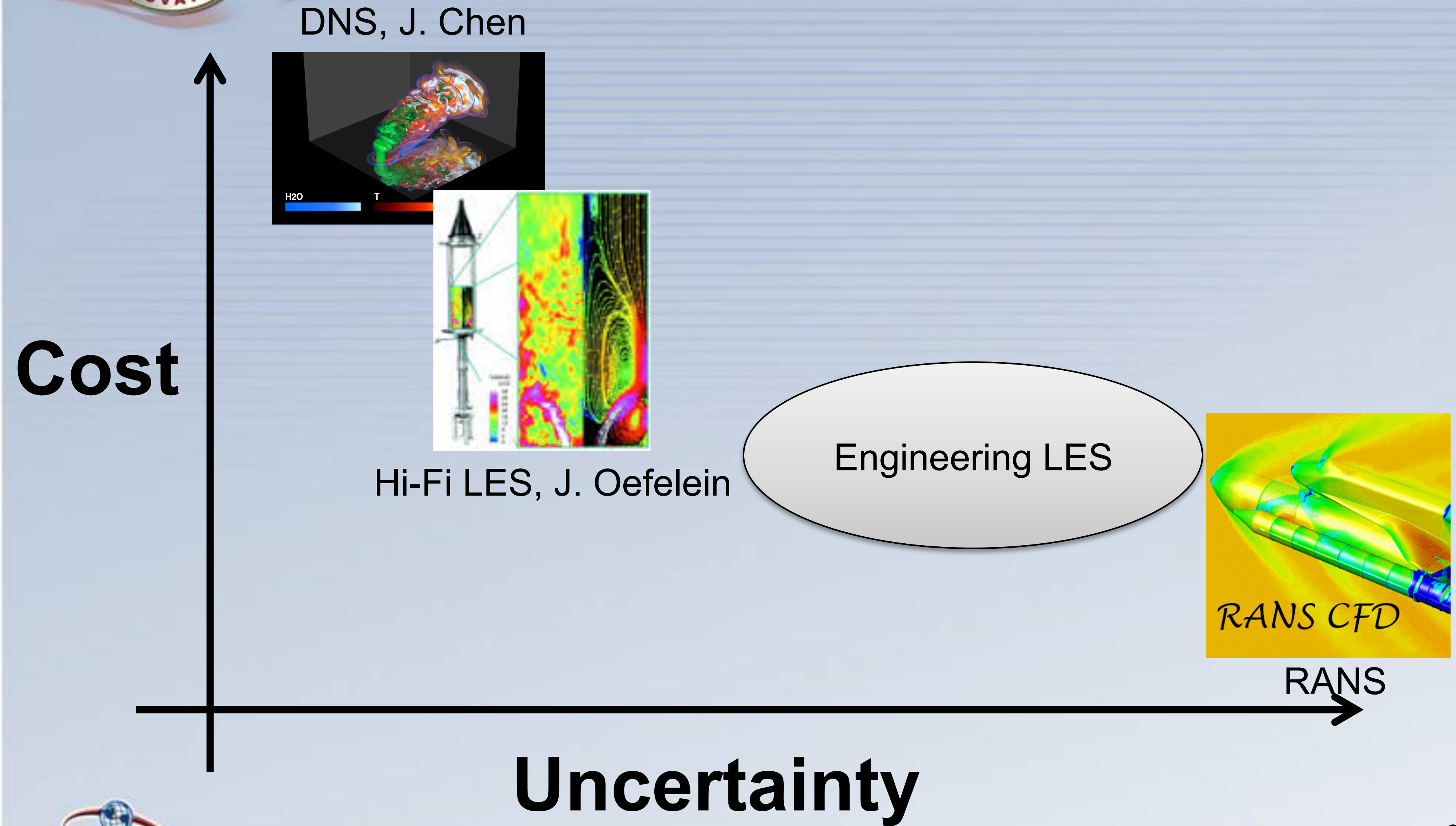
UQ Methods


Khachik Sargsyan
UQ Methods

How/Can High Fidelity Simulations to Enable Engineering LES?



DNS, J. Chen

Cost

Hi-Fi LES, J. Oefelein

Engineering LES

RANS

Uncertainty

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

Transport Model:

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

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} Safta *et al.*, submitted

LDRD LABORATORY DIRECTED RESEARCH & DEVELOPMENT

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Bayesian Calibration

Bayes formula:

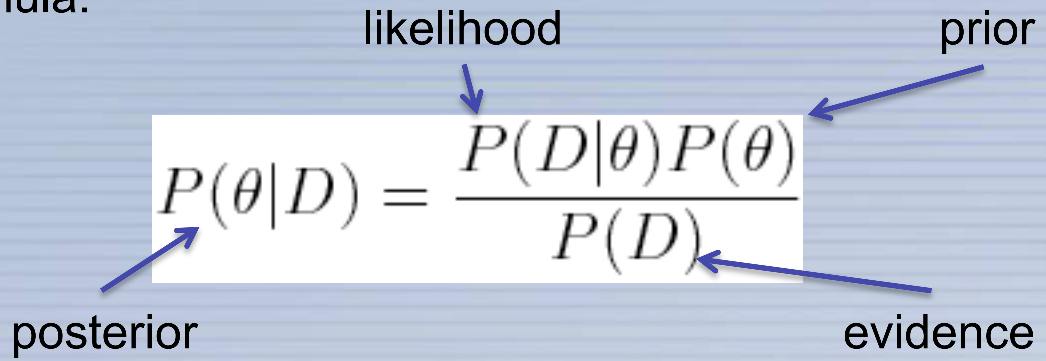
$$\underbrace{P(\theta|D)}_{\text{posterior}} = \frac{\overbrace{P(D|\theta)}^{\text{likelihood}}\,\overbrace{P(\theta)}^{\text{prior}}}{\underbrace{P(D)}_{\text{evidence}}}$$

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

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

Bayesian Calibration: Data

Bayes formula:



likelihood

prior

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

posterior

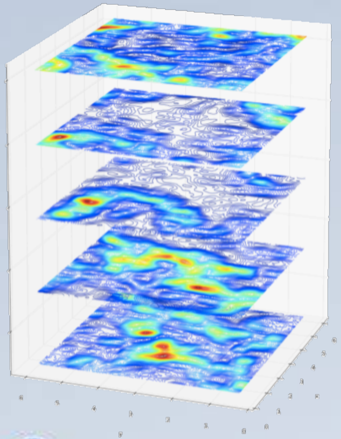
evidence

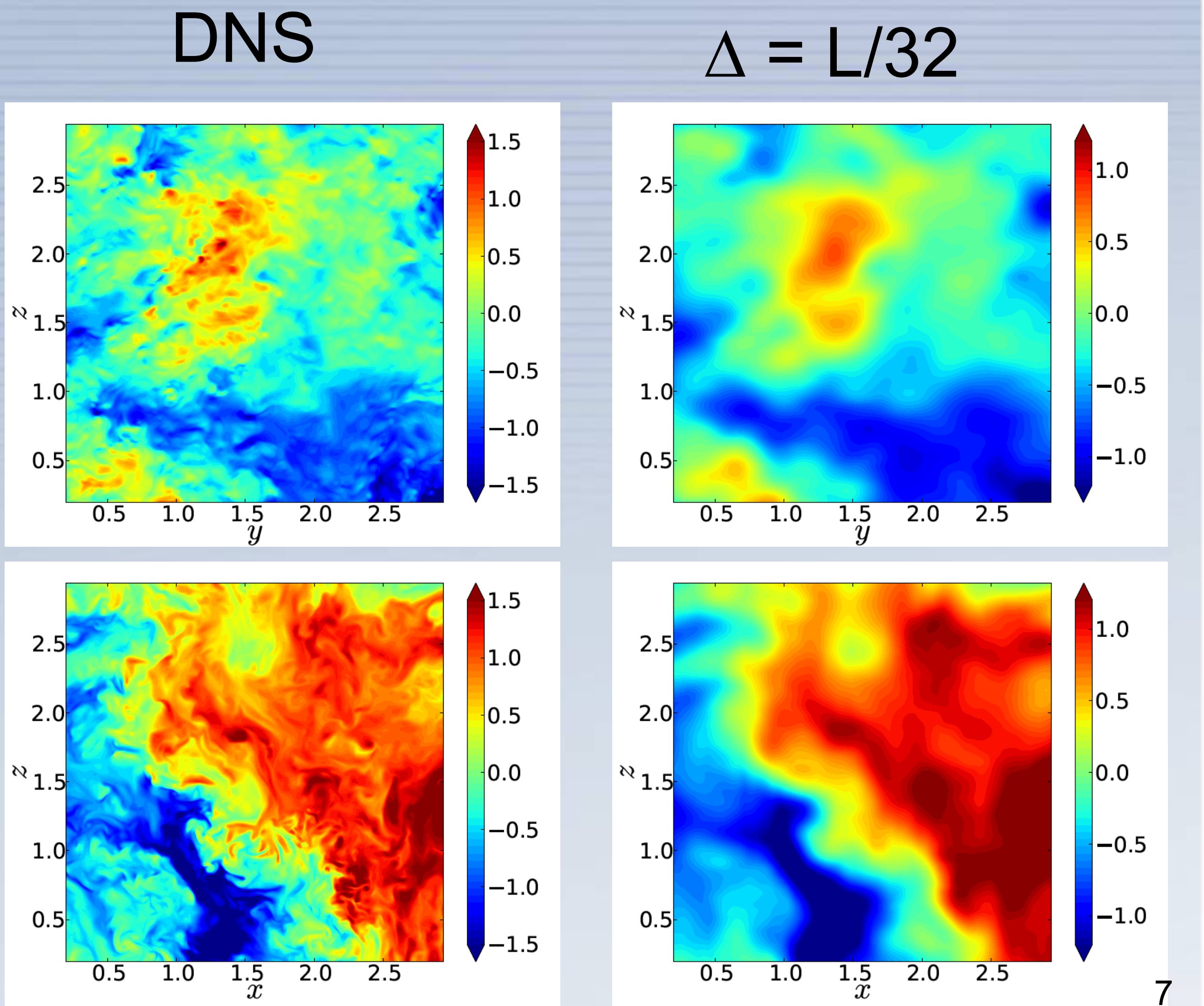
- Data *D* based on DNS of Isotropic Turbulence
- Model parameters θ are the k^{sgs} model constants: C_ϵ & $C_{\mu\epsilon}$
- The likelihood $P(D|\theta)$ is the likeliness of observing D given θ. If C_ϵ & $C_{\mu\epsilon}$ values are right, what are the chances of seeing D.
- The prior distribution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

Data is Filtered DNS to LES scale

3 Filter sizes:

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



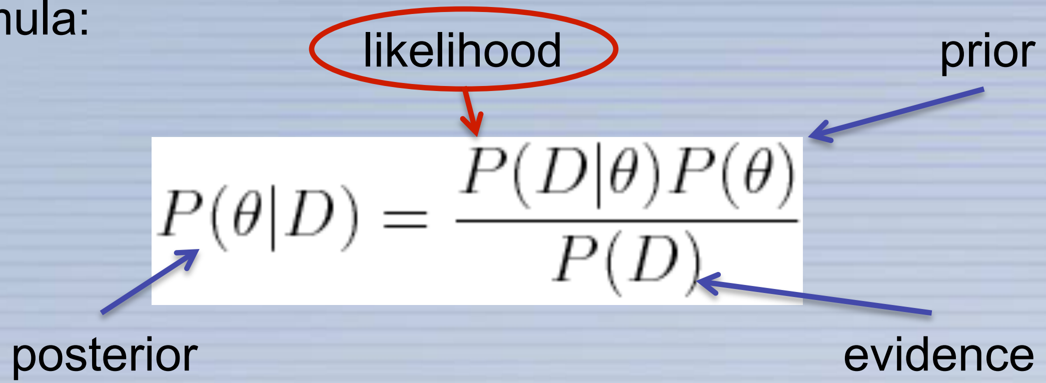


DNS

$\Delta = L/32$

Bayesian Calibration: Likelihood

Bayes formula:



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

- 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 likeliness 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. MVN with diagonal covariance, 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.

PEM Likelihood Function

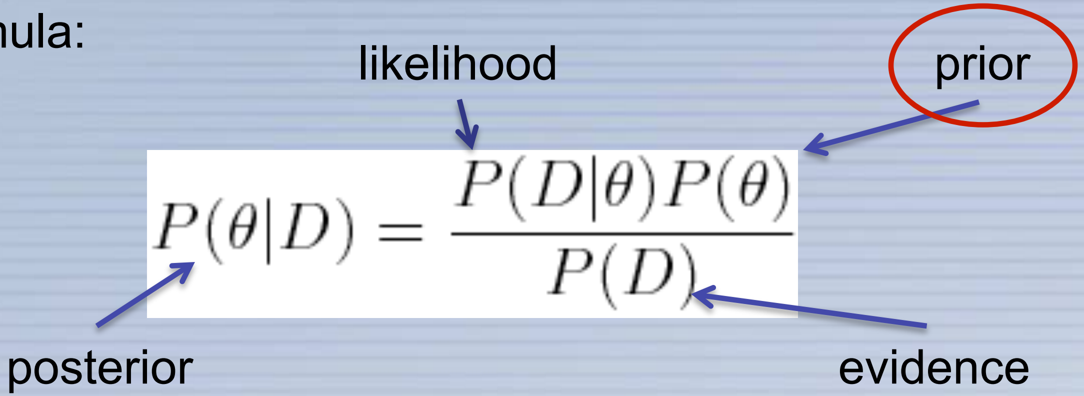
- **Presumed Error (Classical) Model (PEM)**

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

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

Bayesian Calibration: Prior

Bayes formula:



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

- 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 likeliness 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. MVN with diagonal covariance, 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.

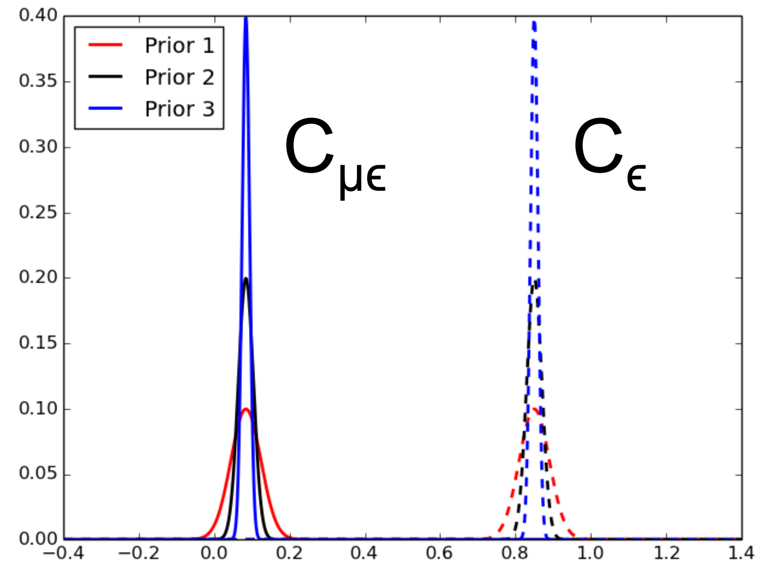
Priors Chosen From Literature

- **Centered at values from the literature ($C_{\mu\epsilon}$, C_{ϵ})**
  (0.0845,0.85) **(0.07,1.05)**

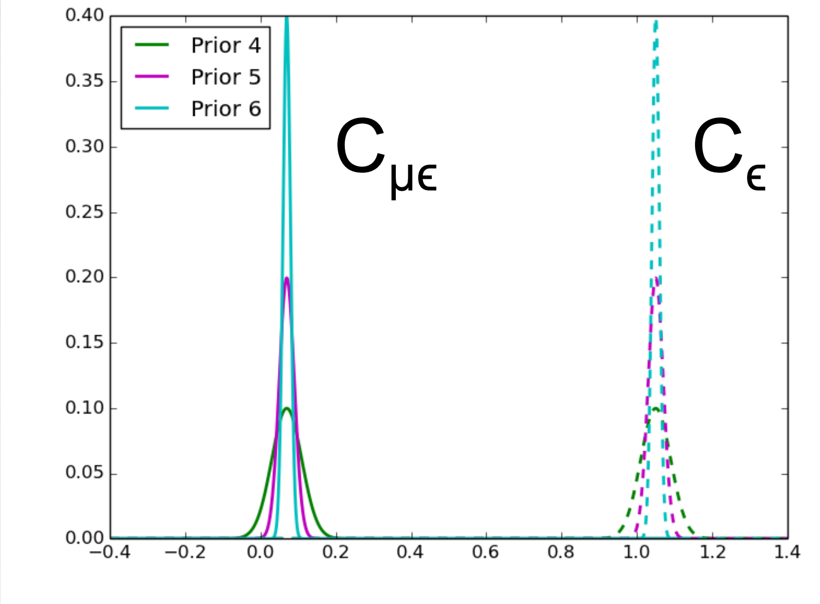
- **Range of Marginal Standard Deviations**

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

(0.0845,0.85)



(0.07,1.05)



Bayesian Calibration: Posterior

Bayes formula:

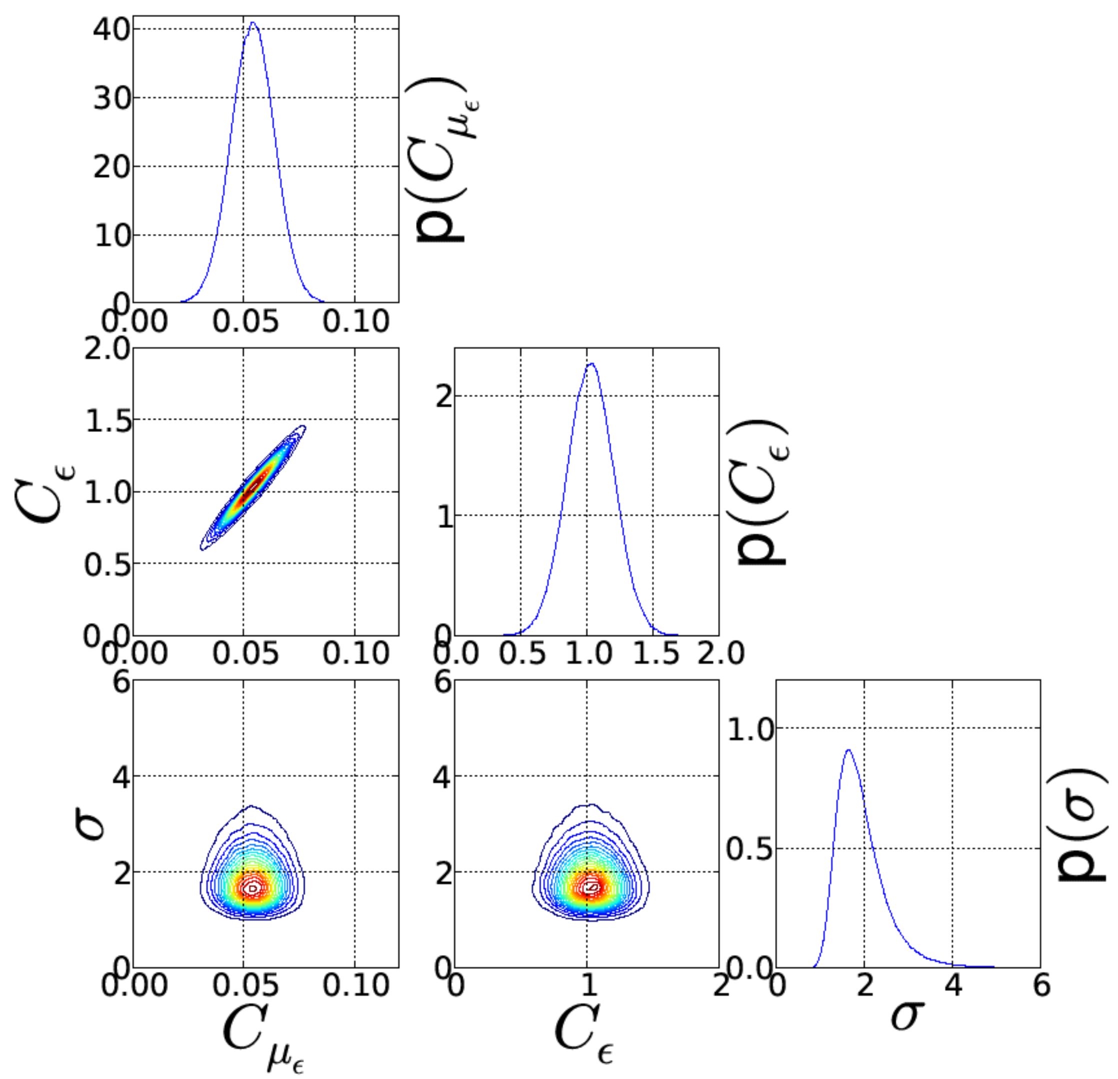
likelihood prior

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

posterior evidence

- Data *D* based on DNS of Isotropic Turbulence
- Model parameters *θ* are the k^{sgs} model constants: C_ϵ & $C_{\mu\epsilon}$
- The likelihood *P(D|θ)* is the likeliness 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. MVN with diagonal covariance, 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.

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



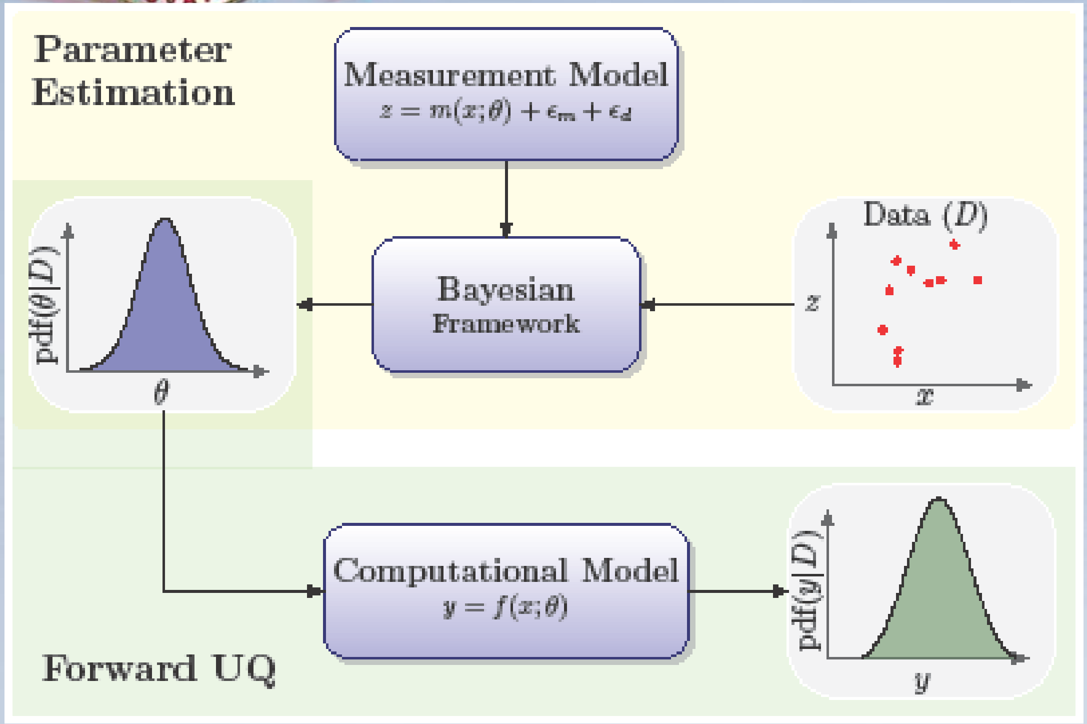
Filter:

- Δ = L/16

Prior:

- $(0.0845, 0.85)$
- $\sigma = (0.01, 0.1)$

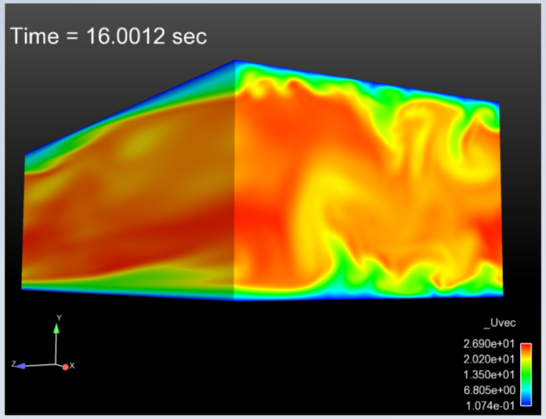
Forward UQ Uses PC Expansion



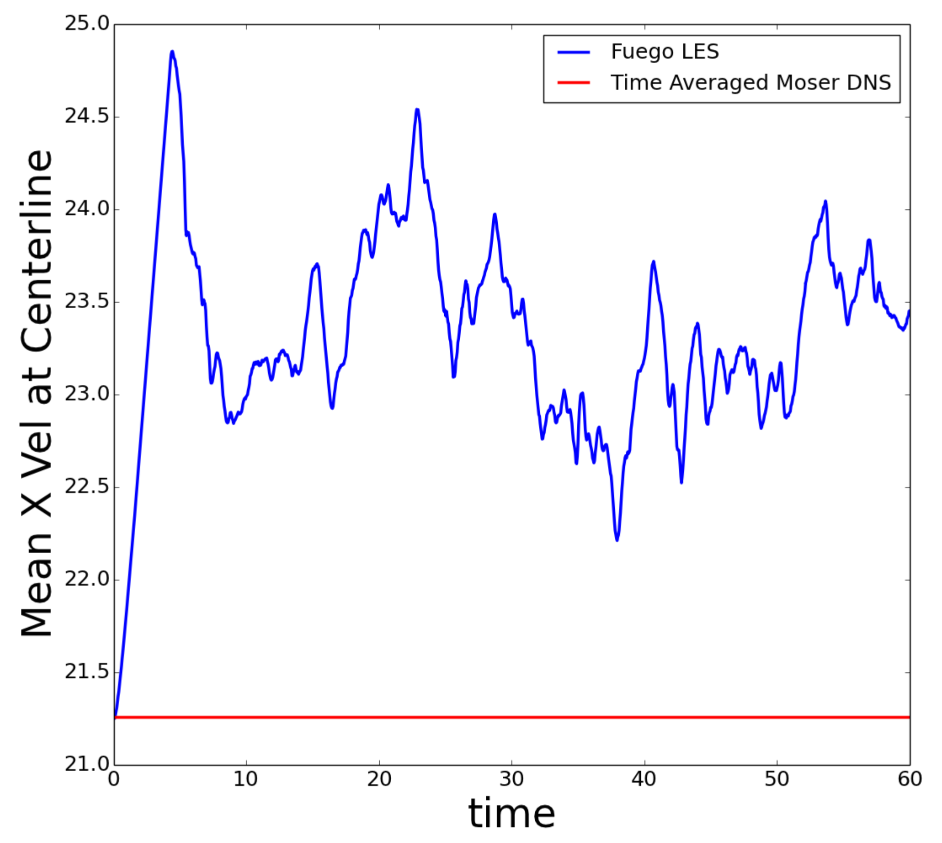
$$y(\theta(\boldsymbol{\xi})) \approx \sum_{k=0}^{N_t} c_k \Psi_k(\xi_1, \xi_2, \ldots, \xi_n)$$

$$c_k = \frac{\langle y \Psi_k \rangle}{\langle \Psi_k^2 \rangle}$$

- y – quantity of interest: mean x velocity, rms, m
- Modeled by Polynomial Chaos Expansion



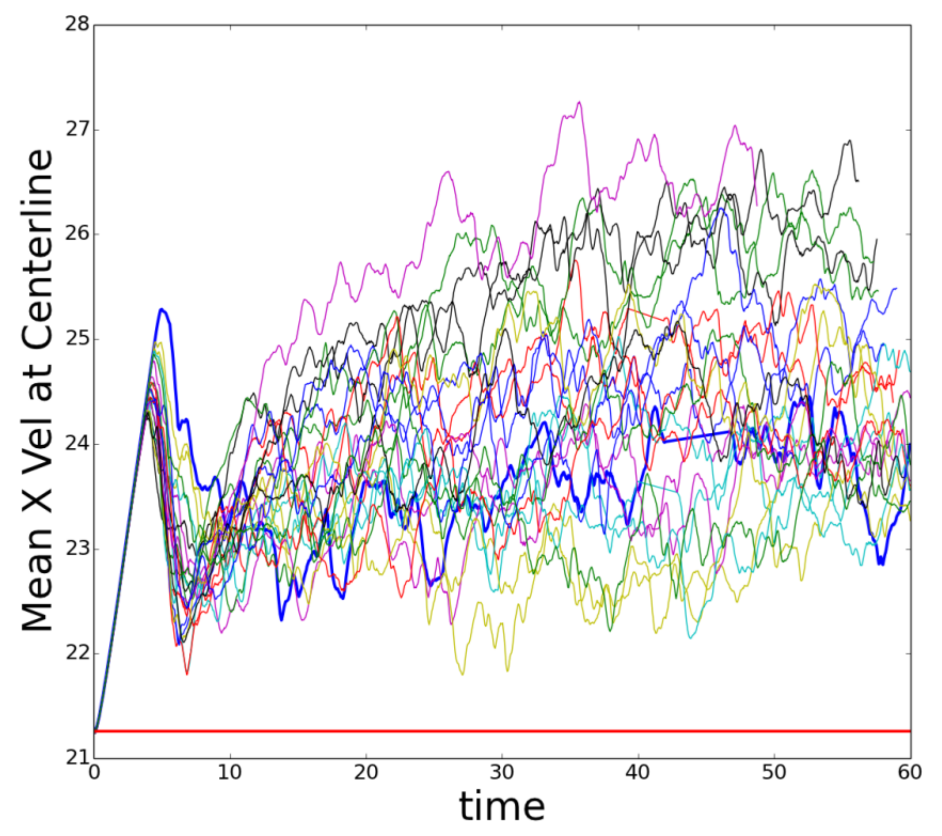
Average Velocity at the Centerline



Moser DNS time averaged value: 21.26

- 15% off

Average Velocity at the Centerline



Moser DNS time averaged value: 21.26

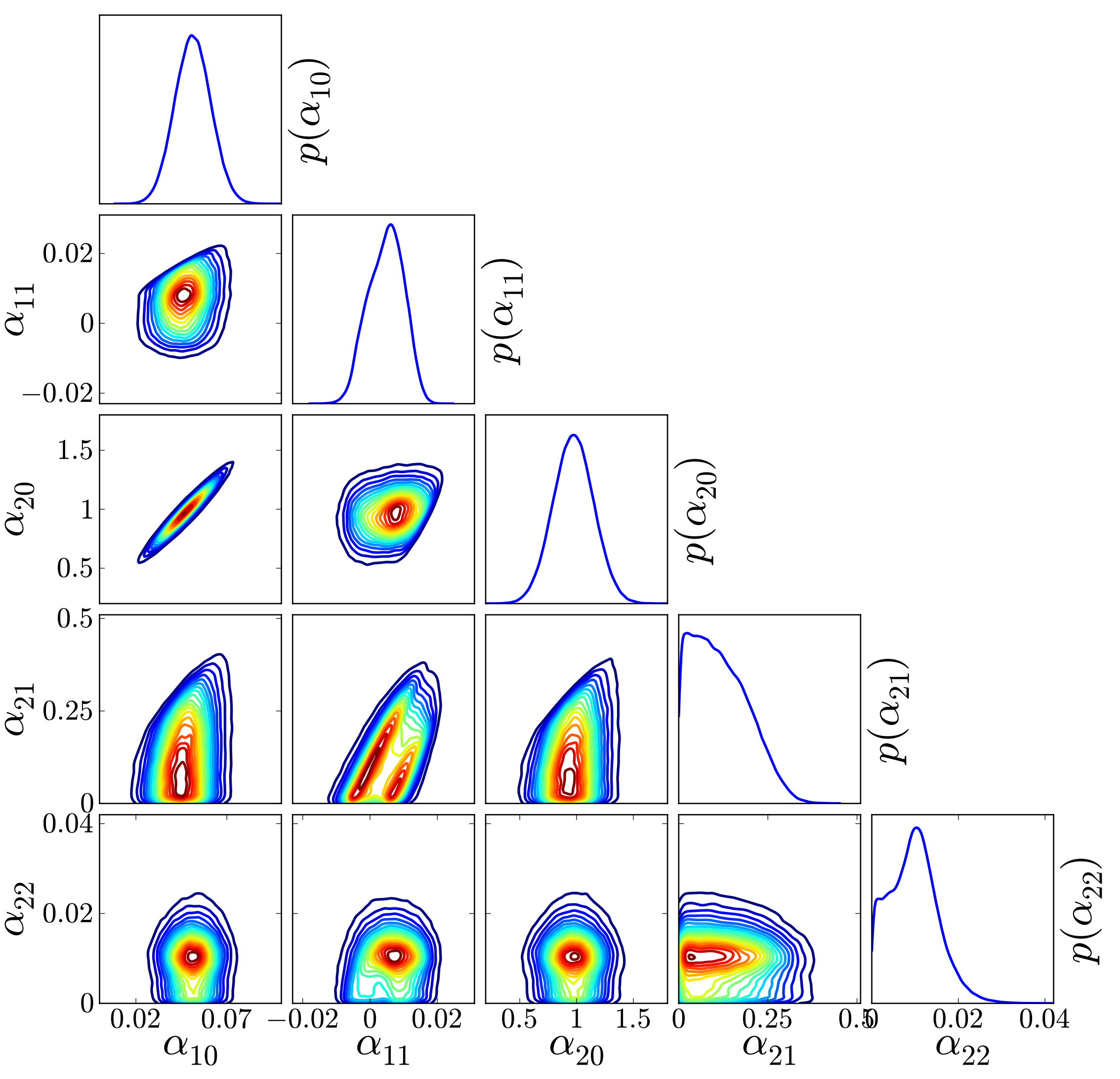
- 15% off

EEM Likelihood Function

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

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

EEM Still Recovers Production to Dissipation Ratio

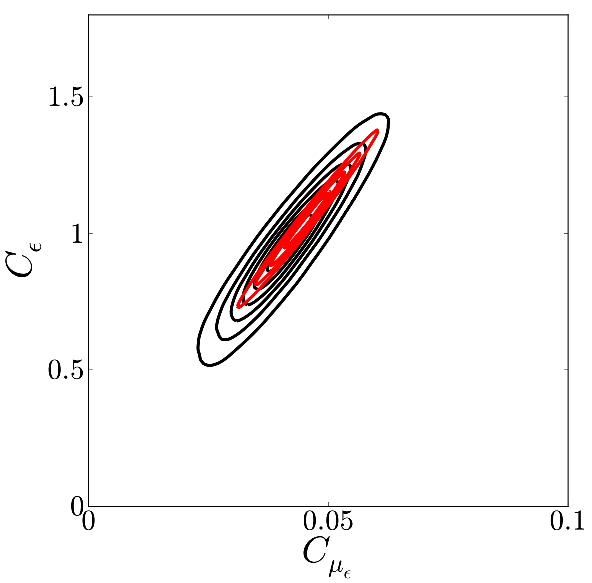


Filter:
- Δ = L/16

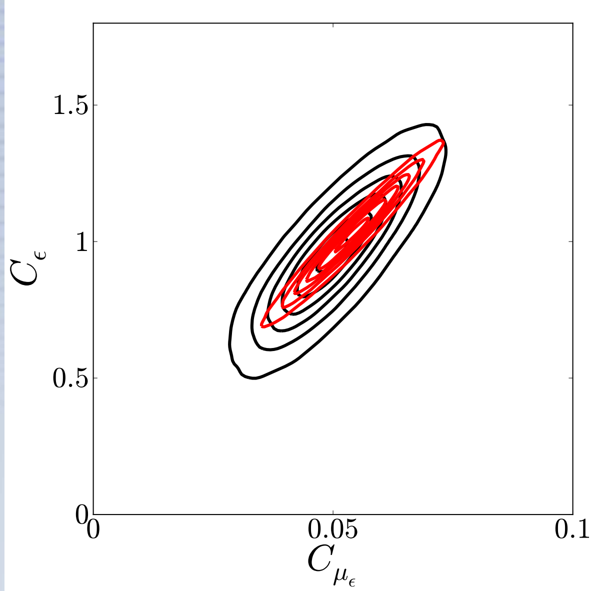
Prior:
- $(0.0845, 0.85)$
- σ = (0.01, 0.1)

EEM Approach Results in Greater Model Uncertainty

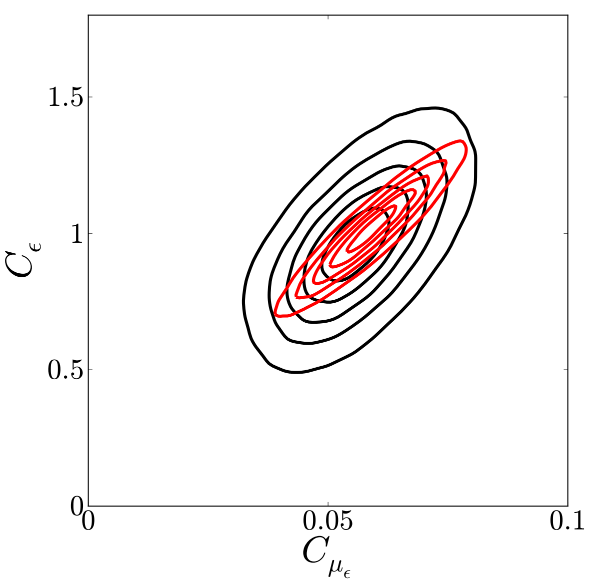
Small Prior Uncertainty



Medium Prior Uncertainty

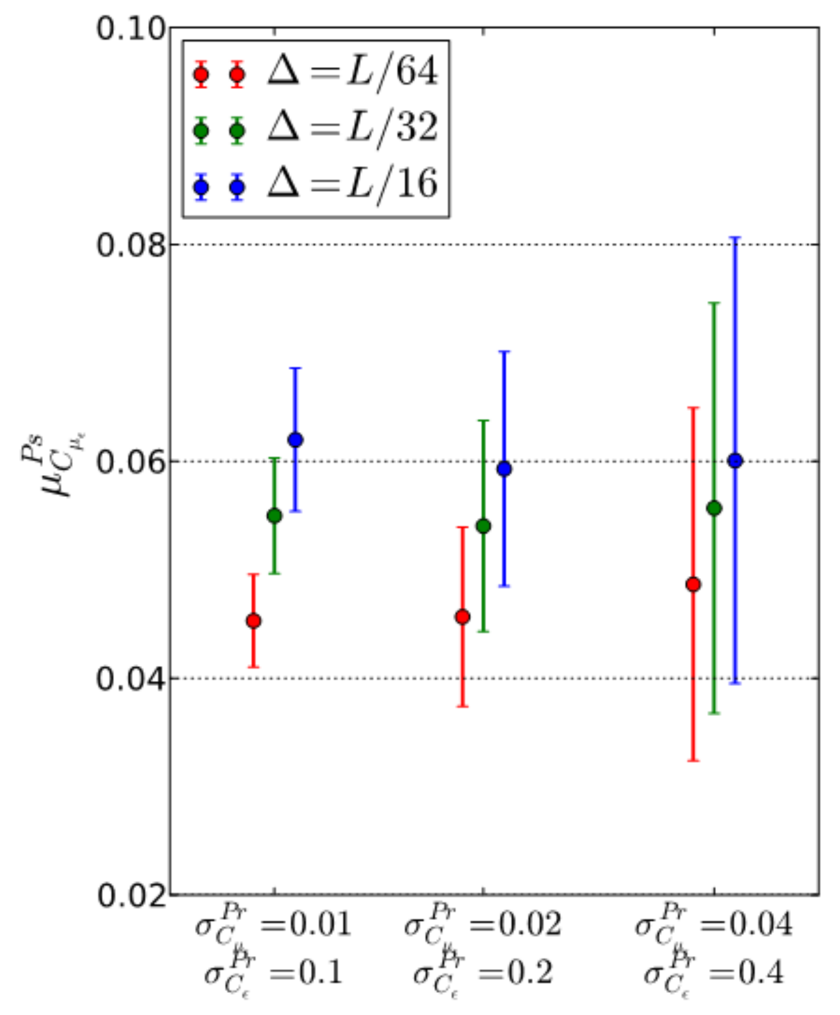


High Prior Uncertainty

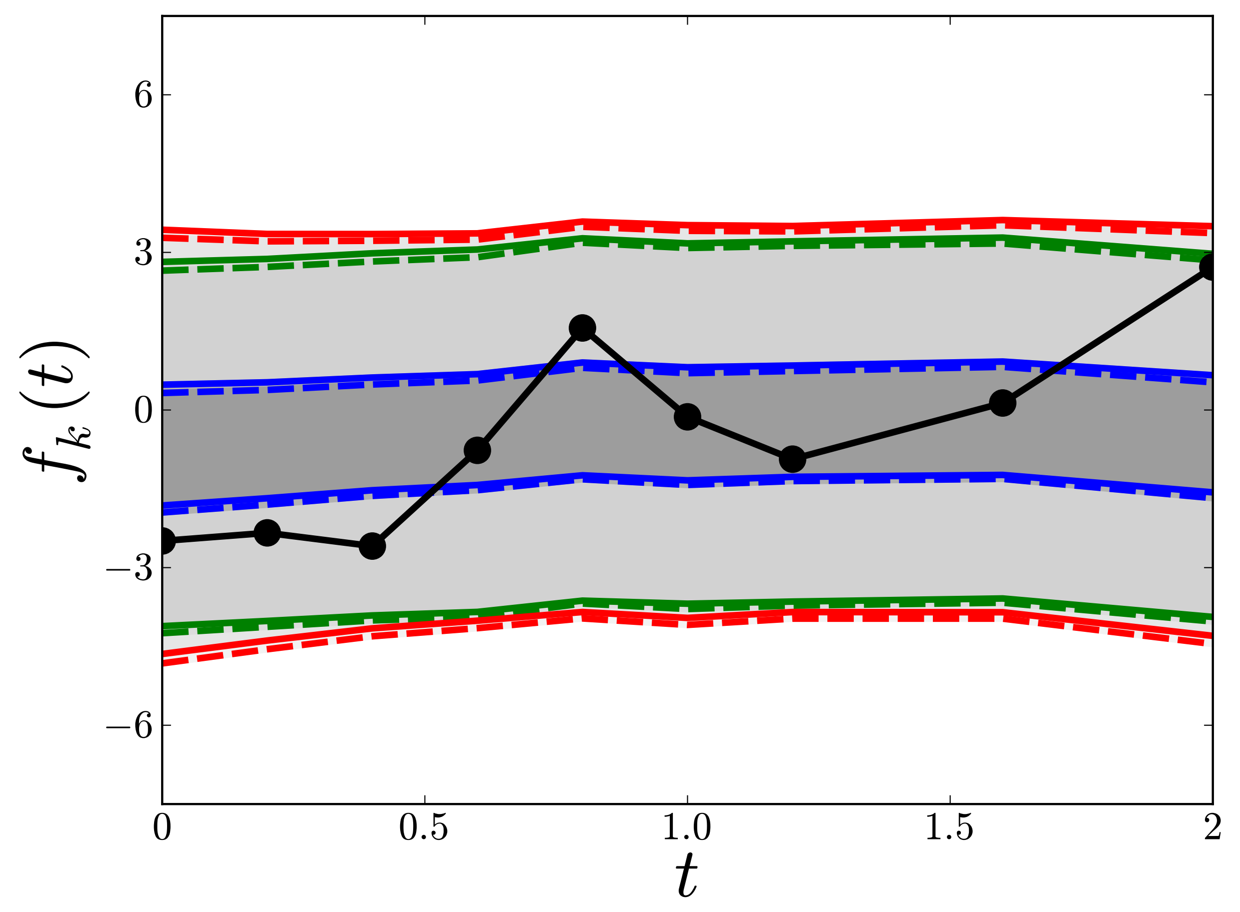


Results are Insensitive to Prior Uncertainty

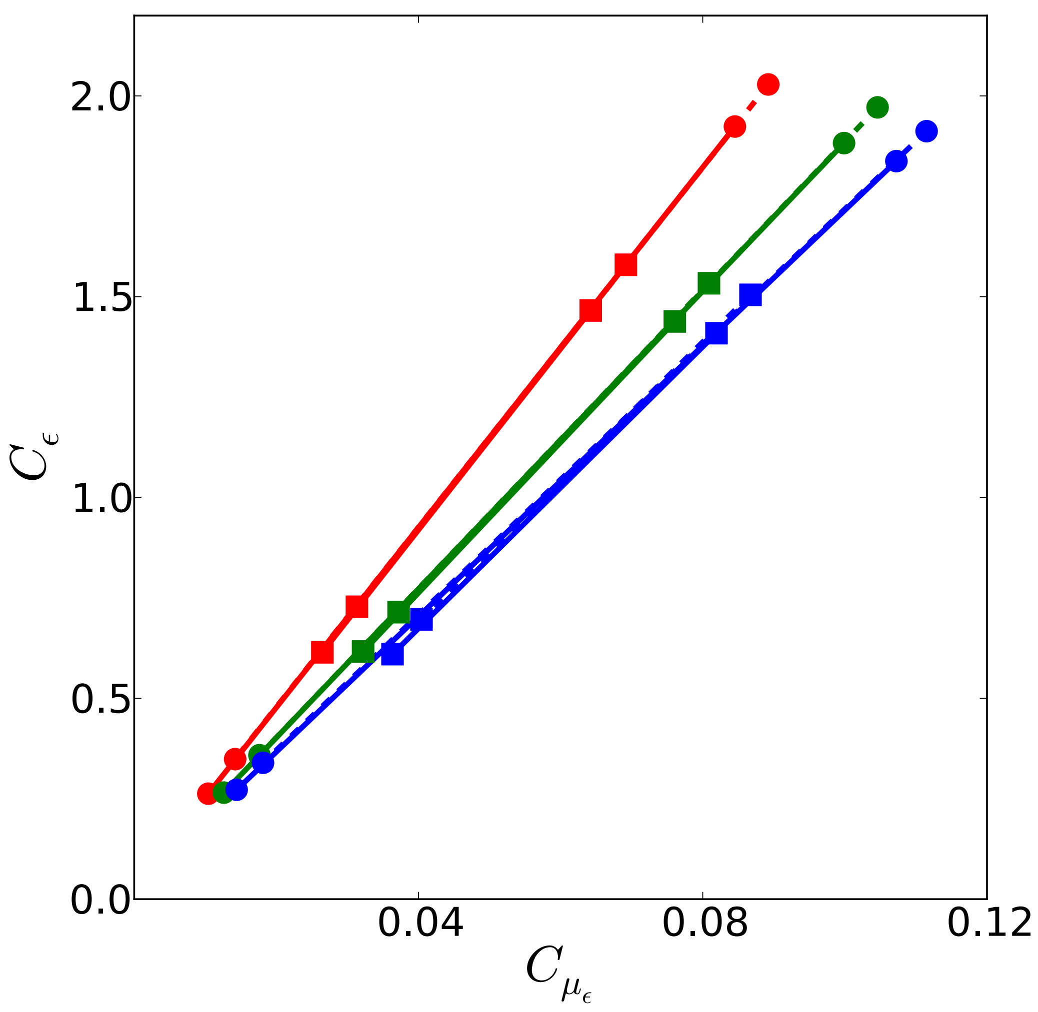
Posterior for $C_{\mu\epsilon}$



A Posteriori Test Shows EEM Recovers Data Uncertainty



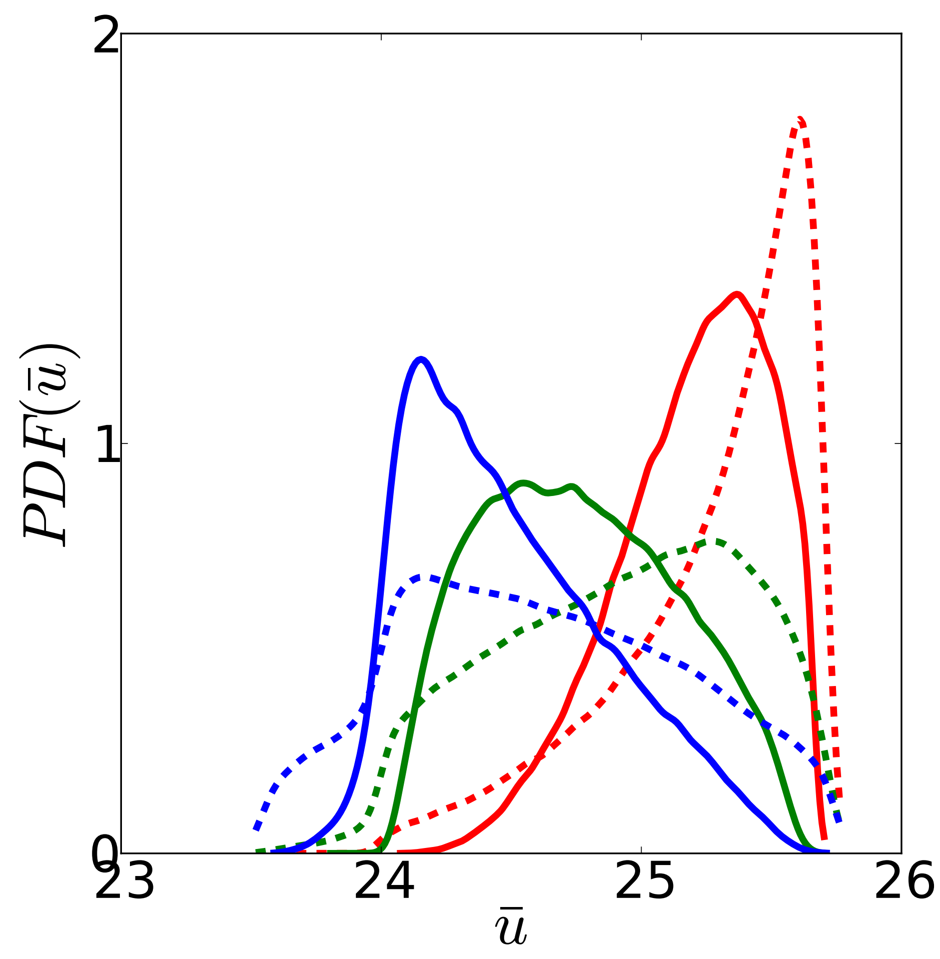
Results are Sensitive to Filter Width



Filter Size:

L/16
L/32
L/64

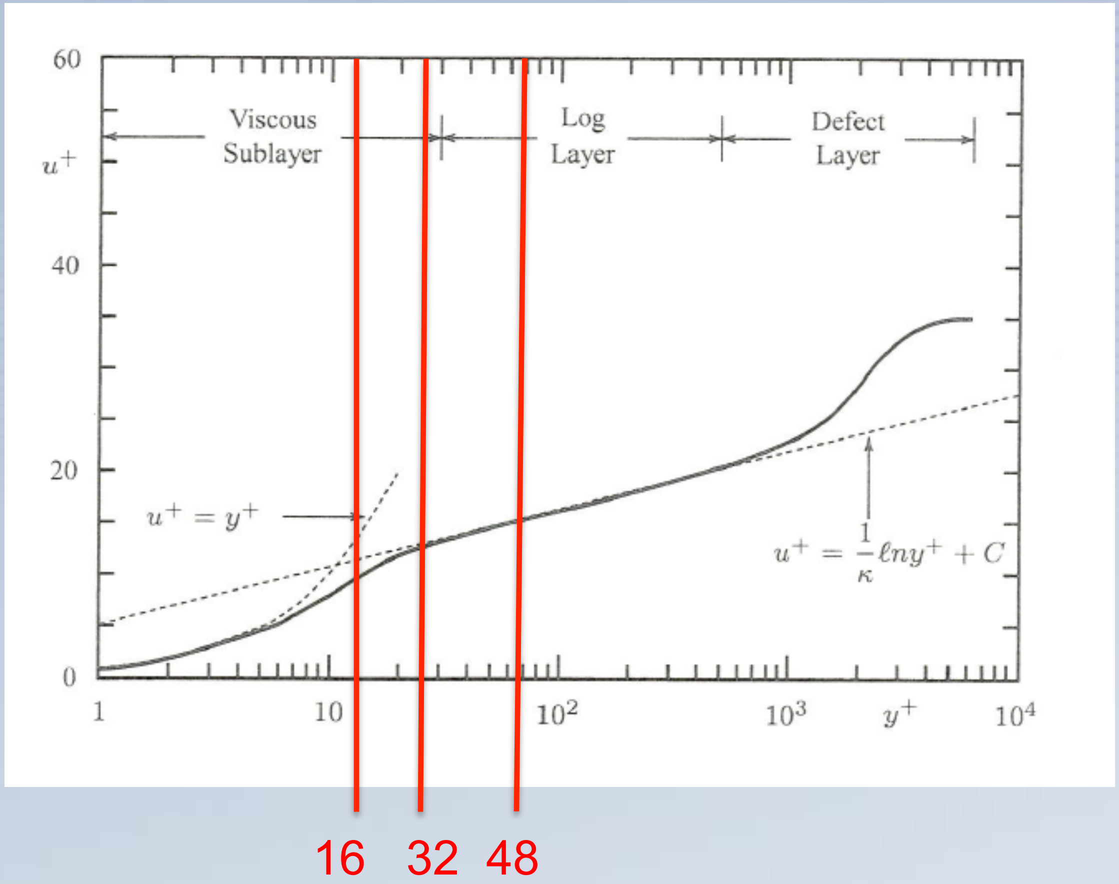
EEM PDFs Do Not Encapsulate Uncertainty



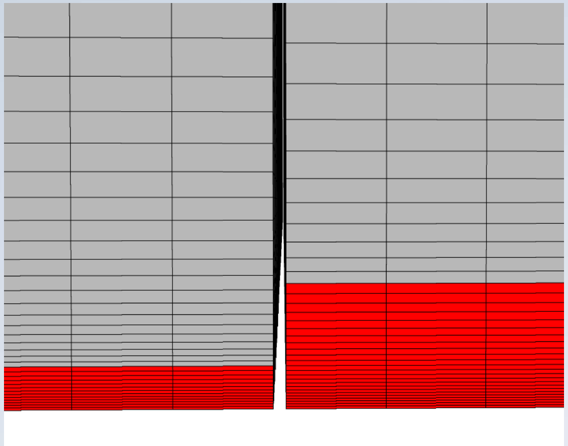
Filter Size:

L/16
L/32
L/64

Direct Calibration Incorporating Physical Knowledge



Use 97 nodes in wall-normal direction, Alter allocation between wall and bulk regions



Only The Log Layer Configuration is Robust

🟥 Laminar 🟩 Turbulent

Dimensionality reduction by using PCA to construct parameter groups of ($C\mu\varepsilon$, C_ε)

y^+ = 16: viscous sublayer

Wall Region C's

1	🟥 63	🟥	🟩 27.1	🟩 26.25	🟩 26.19
2	🟥	🟥	🟩 27.55	🟩 28.6	🟩 27.19
3	🟥	🟥	🟩 28.2	🟩 28.3	🟩 27.2
4	🟥	🟥	🟩 30.7	🟩 29.25	🟩 29.09
5	🟥	🟥 66	🟩 31.5	🟩 31.7	🟩 32.1
Center C's	1	2	3	4	5

y^+ = 32: buffer layer

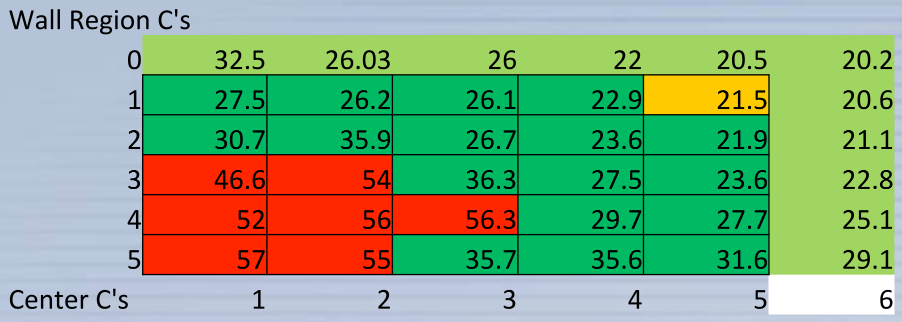
Wall Region C's

1	🟥 64.02	🟥	🟥	🟥	🟨 21.4
2	🟥	🟥	🟥	🟥	🟩 22.4
3	🟥	🟥	🟥	🟥	🟩 24.01
4	🟥	🟥	🟥	🟥	🟩 27.95
5	🟥	🟥	🟥	🟥 65.1	🟩 33.9
Center C's	1	2	3	4	5

y^+ = 48: log layer

1	🟩 27.5	🟩 26.2	🟩 26.1	🟩 22.9	🟨 21.5
2	🟩 30.7	🟩 35.9	🟩 26.7	🟩 23.6	🟩 21.9
3	🟥 46.6	🟥 54	🟩 36.3	🟩 27.5	🟩 23.6
4	🟥 52	🟥 56	🟥 56.3	🟩 29.7	🟩 27.7
5	🟥 57	🟥 55	🟩 35.7	🟩 35.6	🟩 31.6
Center C's	1	2	3	4	5

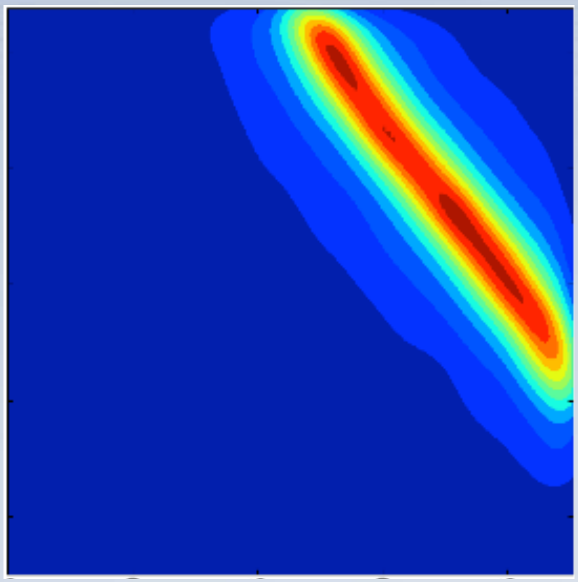
Radial Basis Function Provides Good Approximation



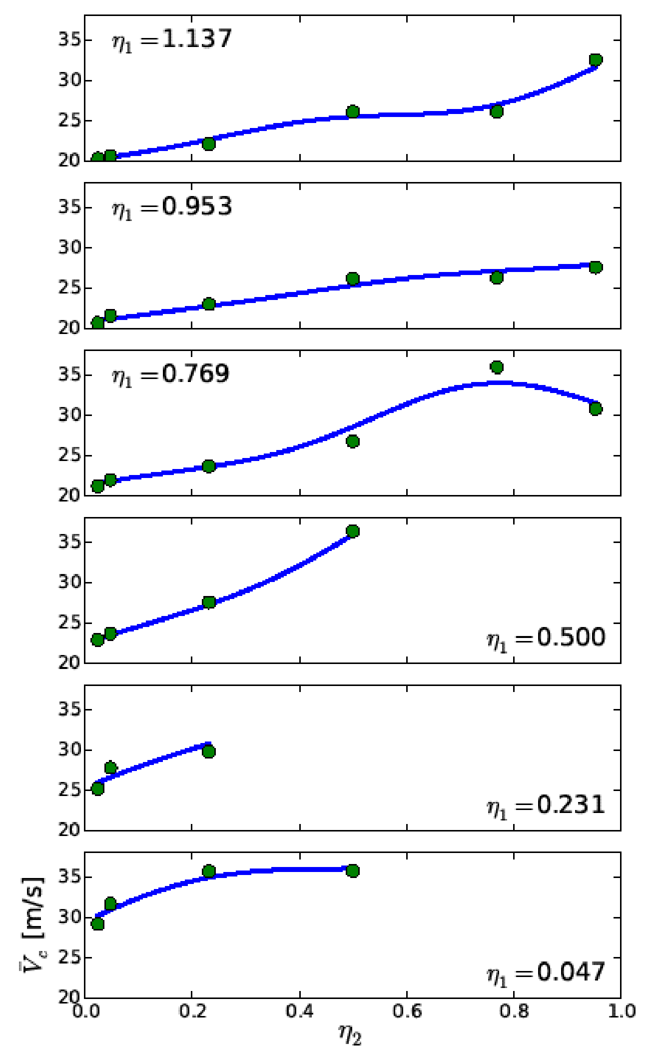
Wall Region C's

0	32.5	26.03	26	22	20.5	20.2
1	27.5	26.2	26.1	22.9	21.5	20.6
2	30.7	35.9	26.7	23.6	21.9	21.1
3	46.6	54	36.3	27.5	23.6	22.8
4	52	56	56.3	29.7	27.7	25.1
5	57	55	35.7	35.6	31.6	29.1
Center C's	1	2	3	4	5	6

Wall Region C’s

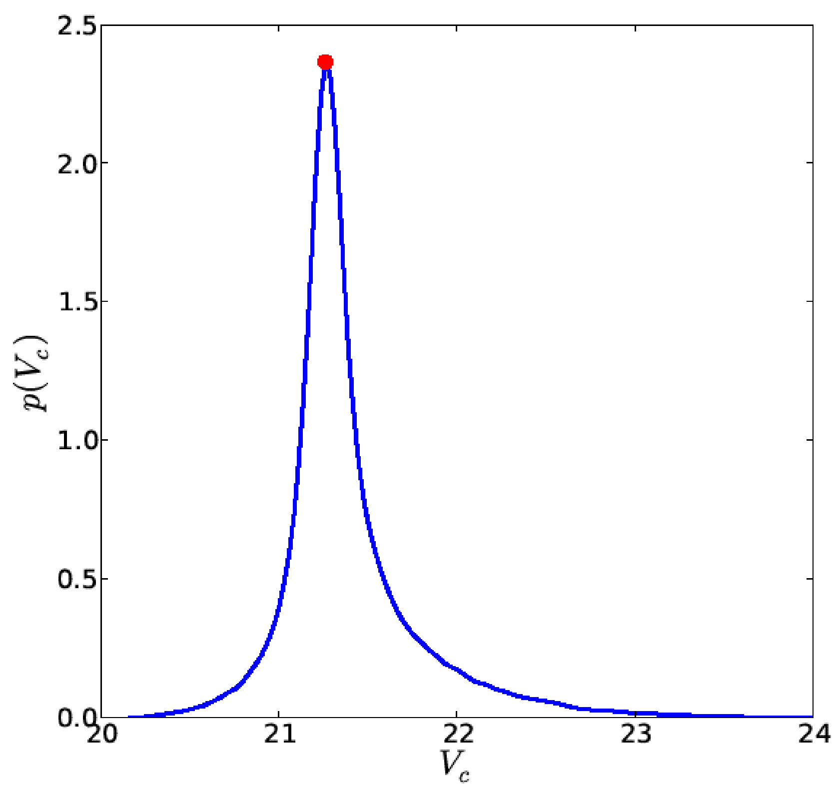


Center C’s

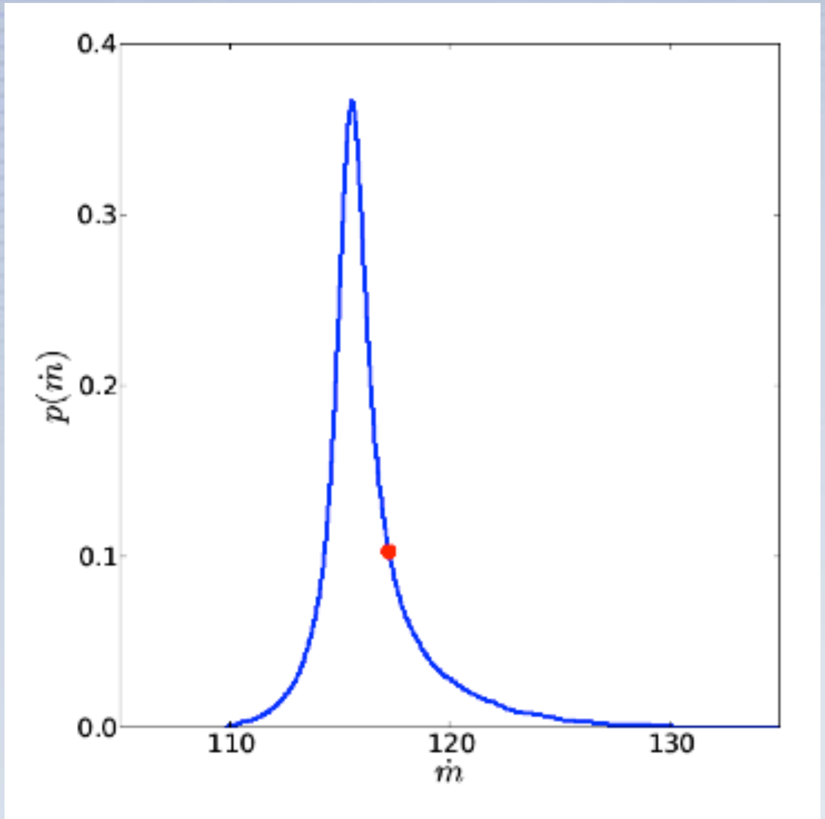


Calibrated Model Recovers Centerline Mean and Mass Flux

Center Velocity PDF



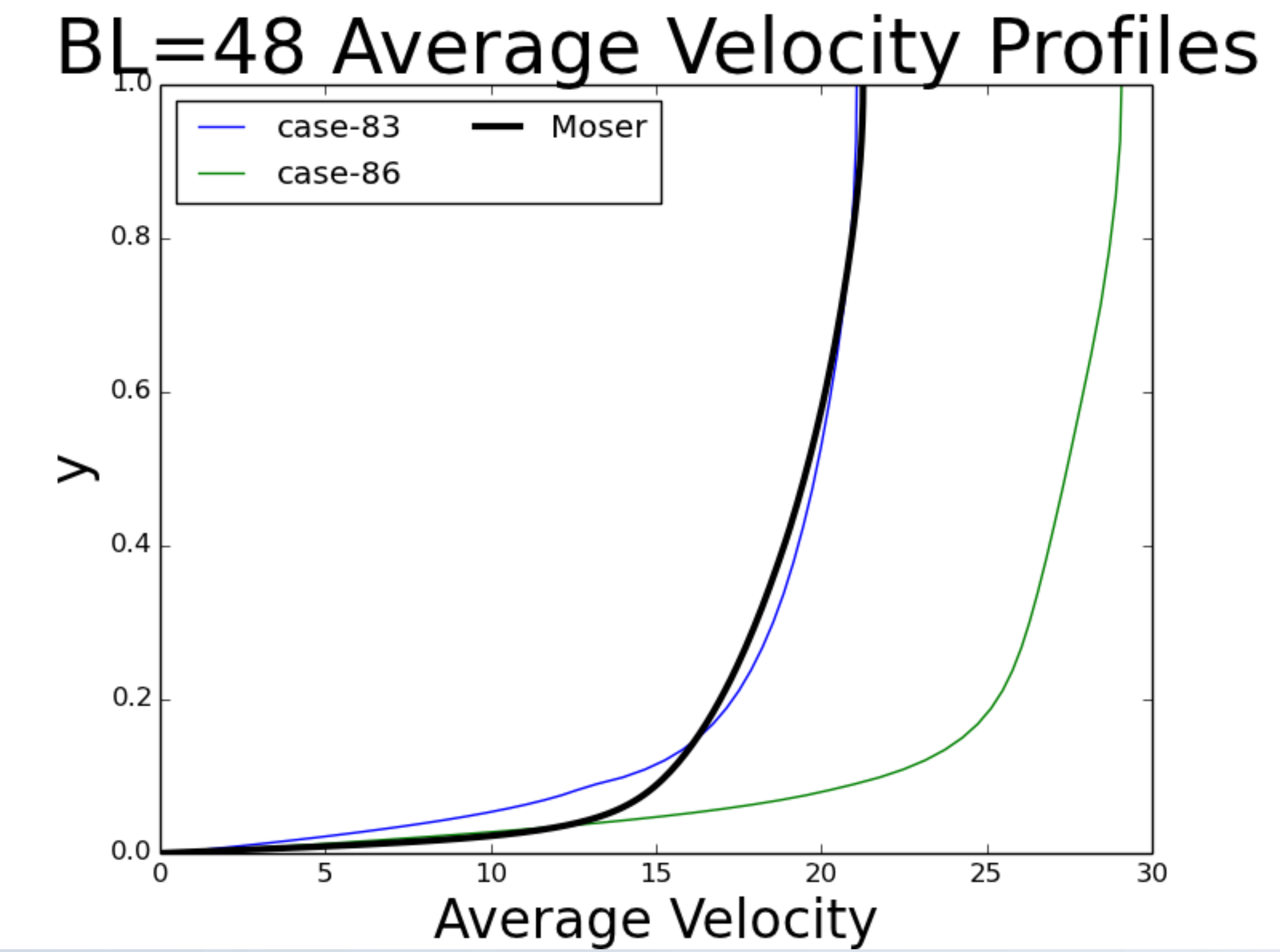
Mass Flux PDF



Model = 21.4 ± 0.4, DNS = 21.3

Model = 116 ± 2.5, DNS = 117

Trade-offs are necessary in the calibration process



Conclusions

- **First principles calibration insufficient for engineering LES**
- **Direct calibration of engineering LES improves predictions**
  - Requires knowledge of physics and mesh
- **High-fidelity data can reduce dimensionality of parameter space and associated cost**
- **Model-form error likely the cause of trade-offs in the calibration process**