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Rigorous LES Assessment for Predictive Simulations

Myra Blaylock, Cosmin Safta, Jeremy Templeton

Goal:

Validated predictive model with quantified uncertainty in their parameters

Model Calibration requires:
- Experimental and/or high-fidelity simulation data
- Model/sub-model evaluations
- Statistical tools for
  - model calibration
  - evaluating model predictive fitness

Using Bayesian methods to calibrate and check predictive quality of LES models

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}

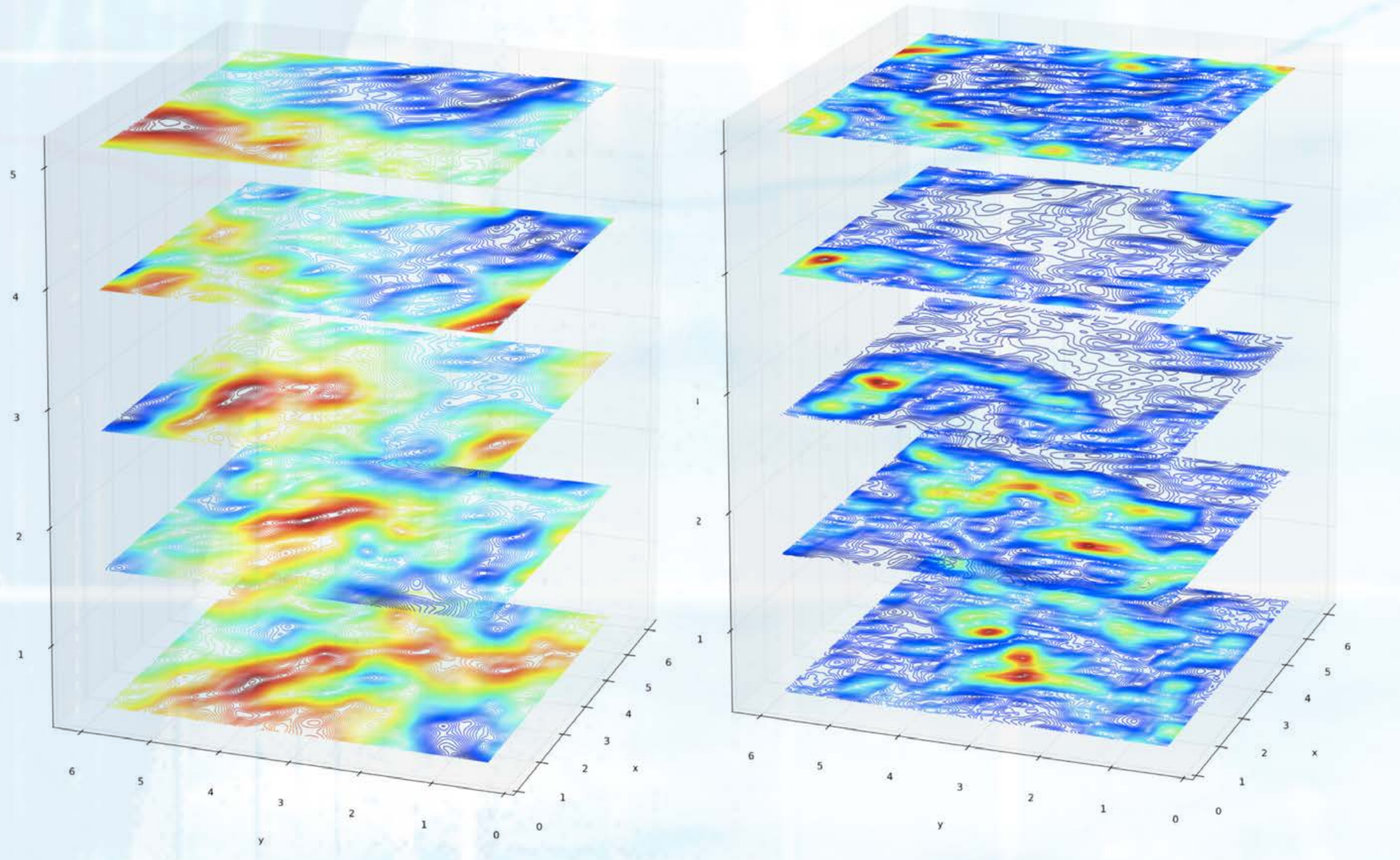
Dataset for k^{sgs} Model Calibration

DNS Dataset
- Forced Isotropic Turbulence obtained from the Johns Hopkins Turbulence Database (JHTDB) at http://turbulence.pha.jhu.edu
- Grid resolution 1024^3
- Taylor-scale Reynolds number fluctuates around $Re_\lambda \approx 433$

Data Processing:
- Tophat filter; several filter sizes were employed, Δ=16,32,64 grid cells
- Time derivatives for total subgrid-scale kinetic energy computed using time-adjacent solutions
- Volume integrals computed on a sub-domain covering 512^3 grid cells

Sample Processed Data

Sample $\tilde{u}$ Sample k^{sgs}



Bayesian Calibration

Bayes formula:

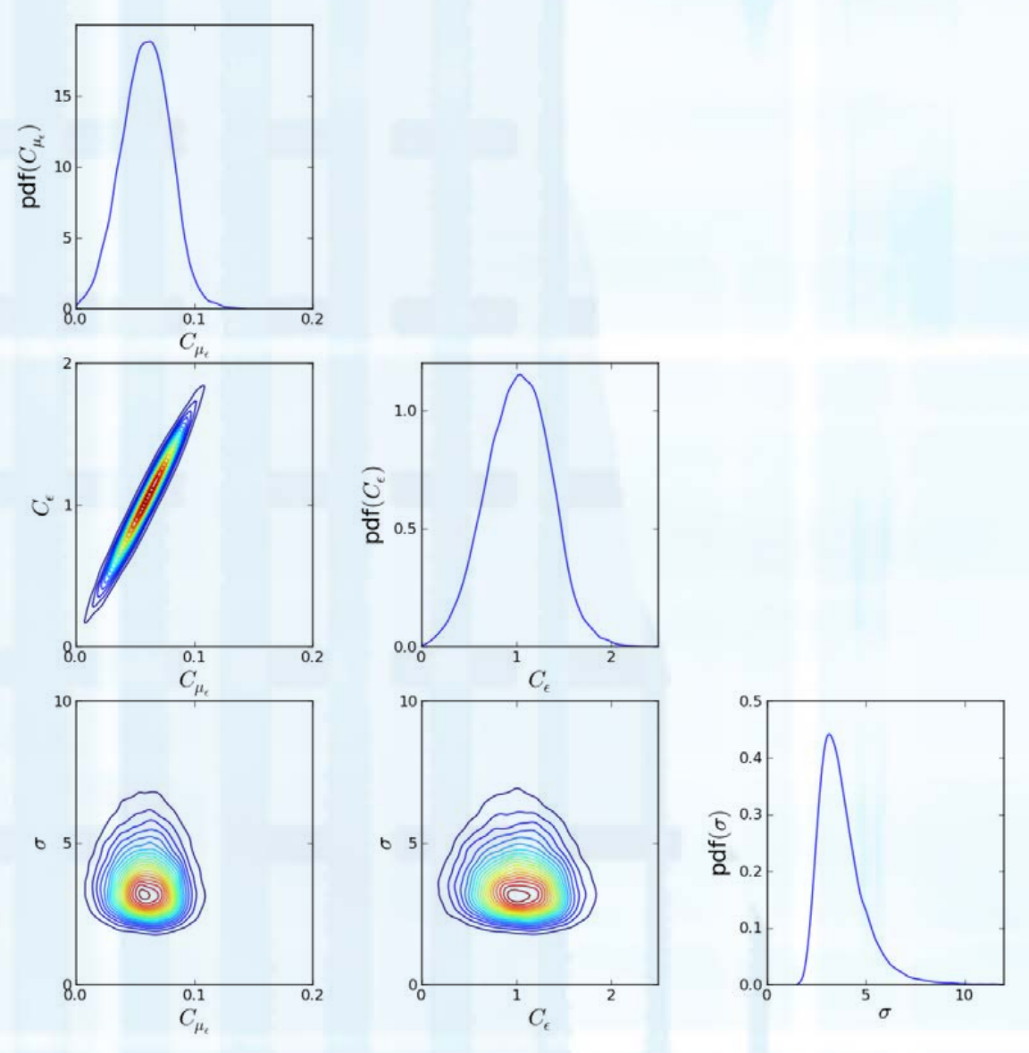
likelihood prior

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

posterior evidence

- Data *D* based on DNS of Isotropic Turbulence
- Model parameters *θ* are the k^{sgs} model constants
- The prior distribution *P(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

Sample Posterior Distributions



Model parameters are highly correlated while the model discrepancy shows little correlation with the model parameters

Forward UQ – Predictive Assessment

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

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

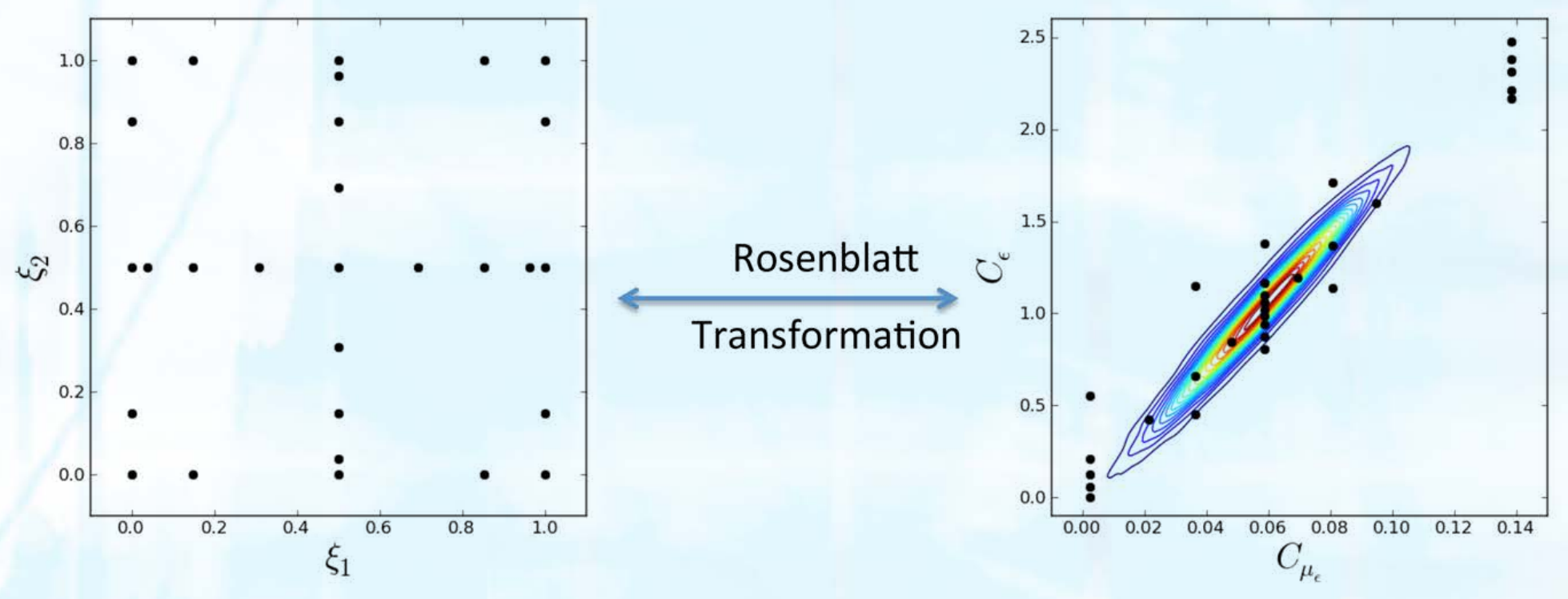
$$C_\epsilon = C_\epsilon\left(\xi_1, \xi_2\right), \; C_{\mu_\epsilon} = C_{\mu_\epsilon}\left(\xi_1, \xi_2\right)$$

Employ quadrature to compute PC coefficients

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

The PC Expansion is cheap to evaluate for forward UQ and parameter calibration.

Sparse Quadrature to Construct PC Expansion for Model Output

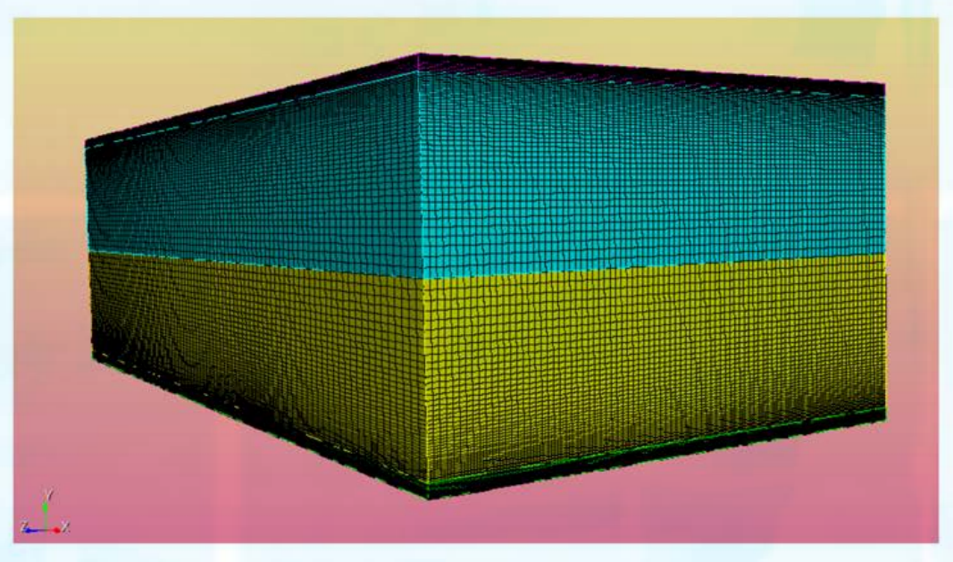


Fuego LES Simulations with Calibrated Parameters

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

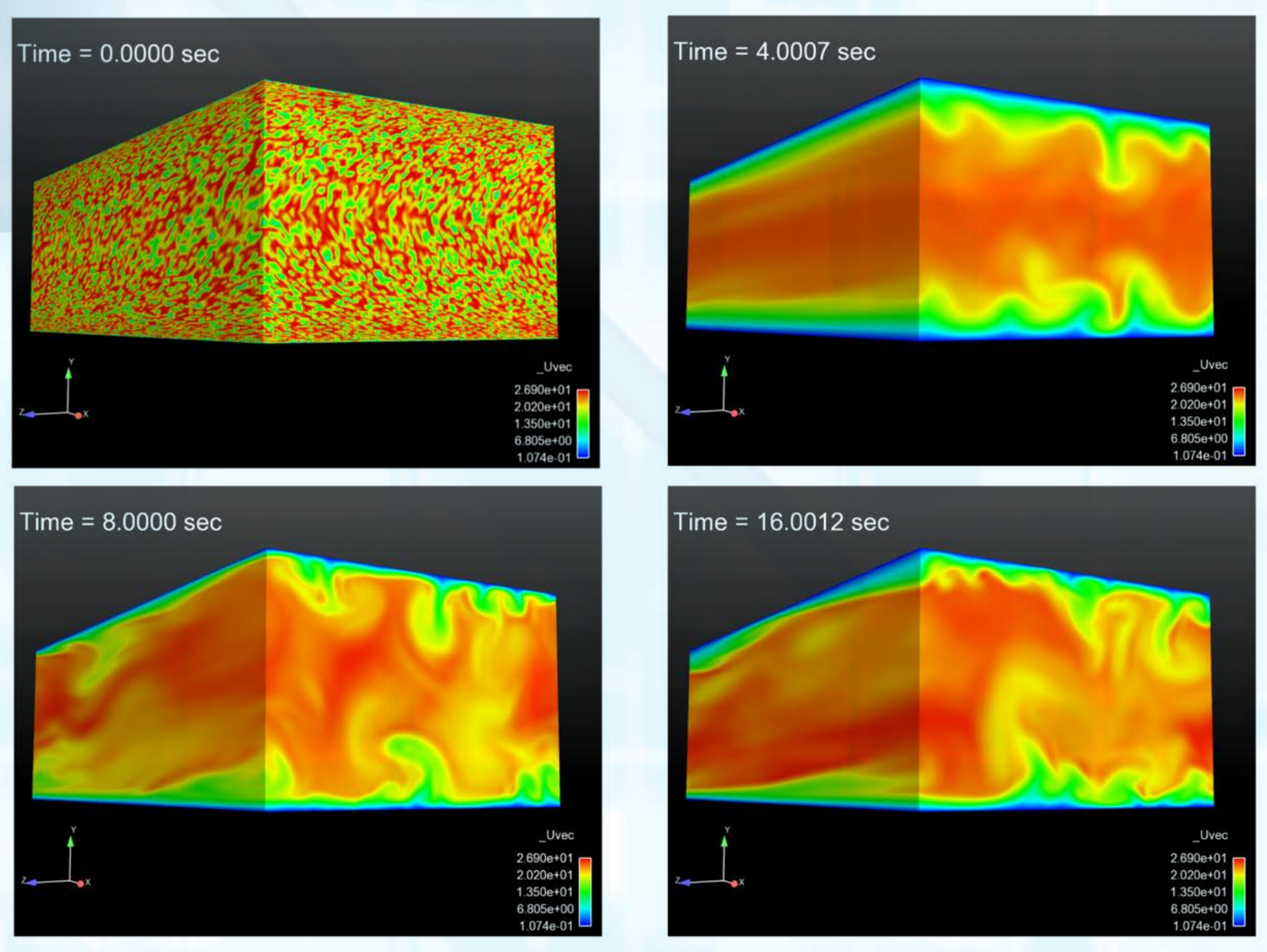
Mesh

- Dimensions:
  - Flow direction: x = 2π (periodic)
  - Wall normal direction: y = 2
  - Cross flow direction: z = π (periodic)
- Grid size:
  90 × 116 × 90 =
  931500 points
- y^+ ≈ 1.15 at walls



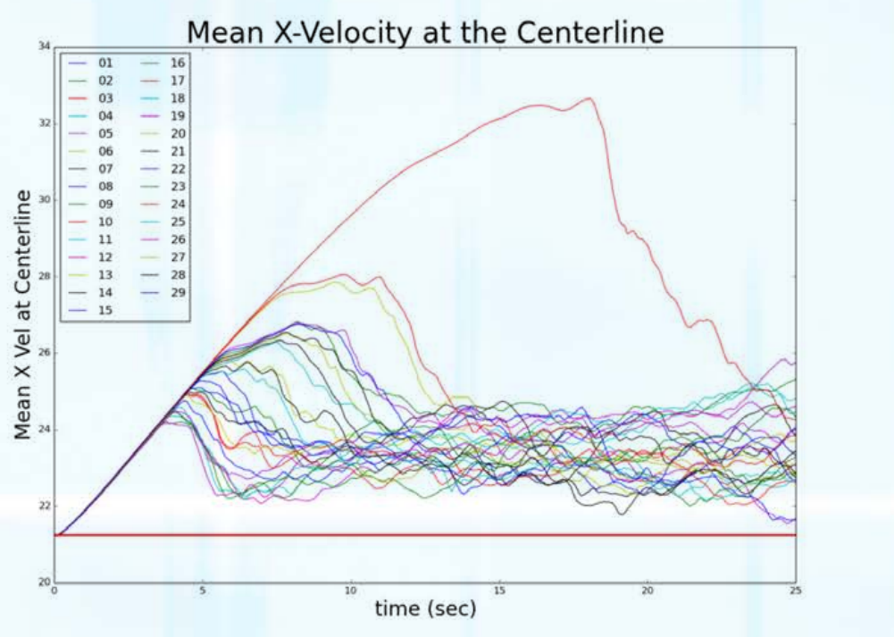
Simulation Results

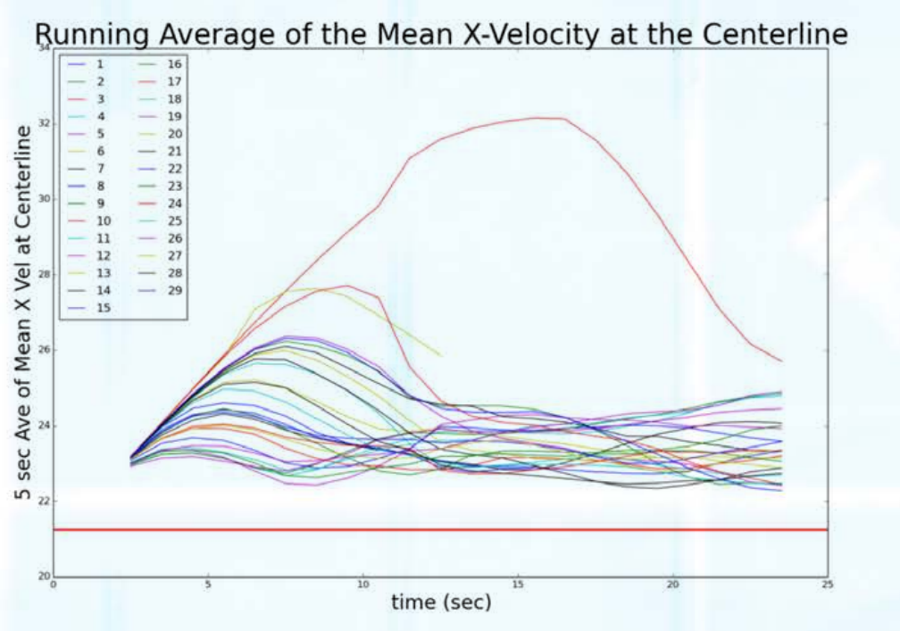
- Starts with turbulent input
  - Mean and standard deviation same as Moser, et al.
  - Helps turbulence develop



Generate QoIs at Quadrature Points

- Moser et al.'s DNS Results:
  - Mean X-velocity at Centerline: 21.26 +/- 0.78
- k^{sgs} Results:
  - Mean X-Velocity at every time step
  - Running 5 sec average
- Compute PC expansions for centerline velocities





PREDICTIVE ENGINEERING SCIENCE PANEL

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