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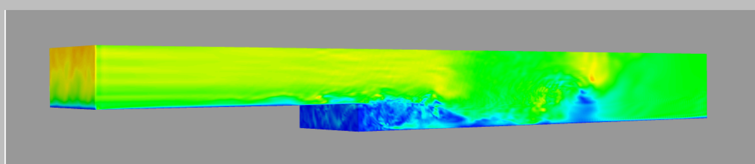

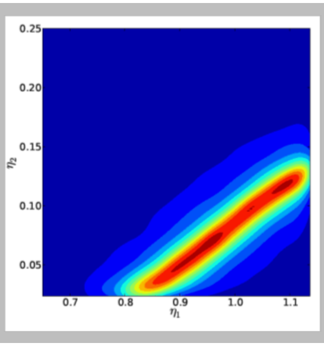

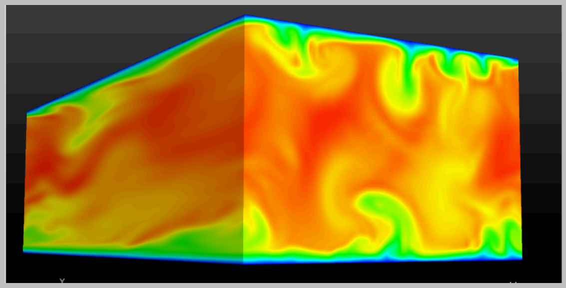

A Novel Approach to Wall Model Treatment for Large Eddy Simulations

Myra Blaylock

U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

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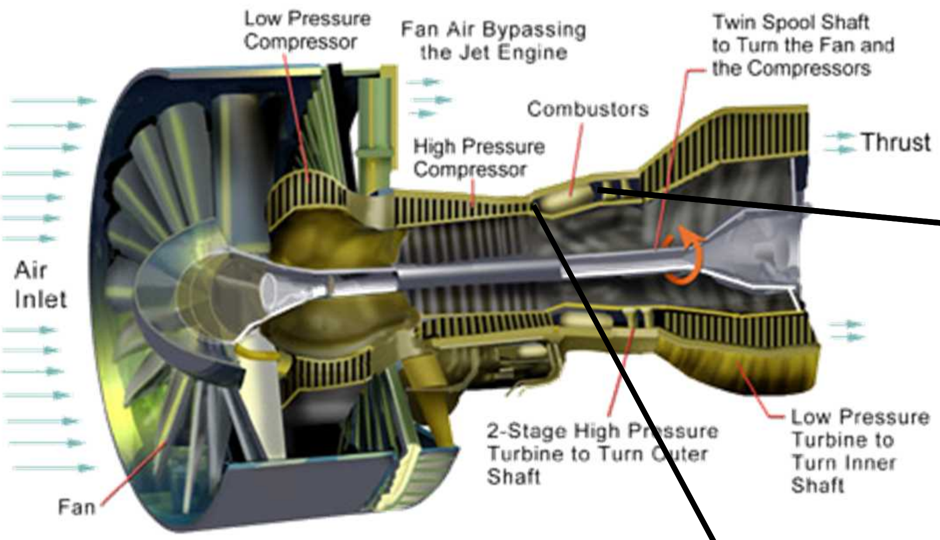
Group Effort

- Myra Blaylock
- Cosmin Safta
- Jeremy Templeton
- Stefan Domino
- John Hewson
- Julia Ling
- Raj Kumar

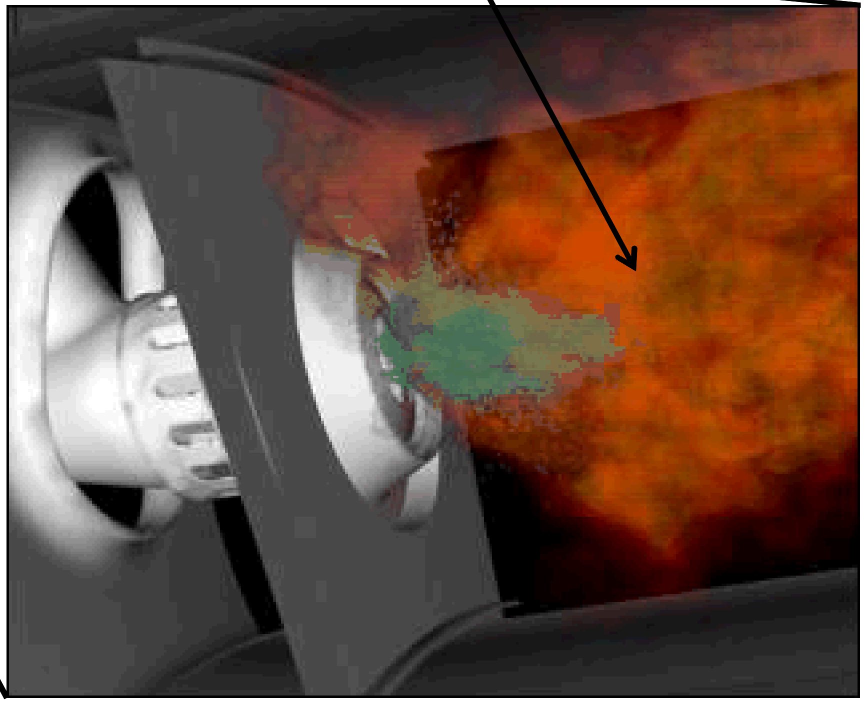
Gas Turbine Challenges

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



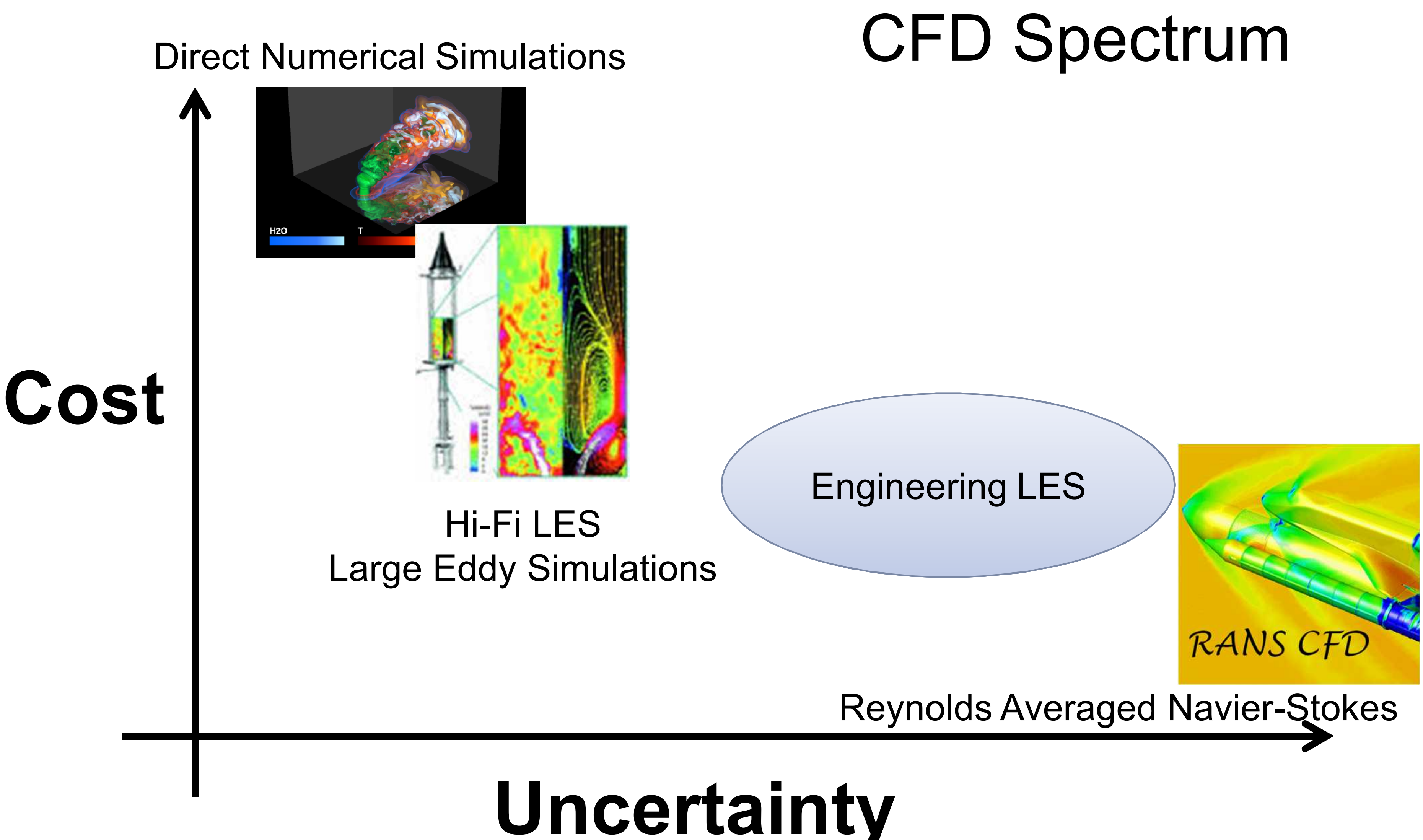
Gas Turbine Engine

Complex flow physics coupled with chemistry drives efficiency and pollutant emissions



Gas Turbine Combustor Flow
Stanford ASCI Alliance Center

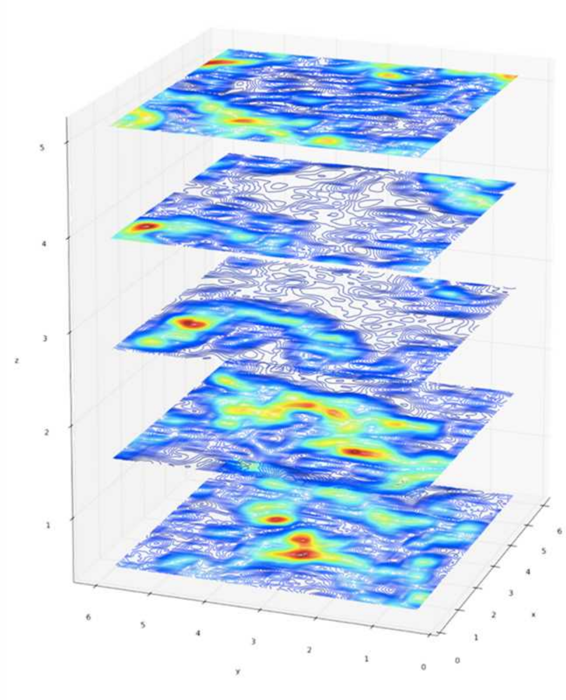
What is Engineering LES?



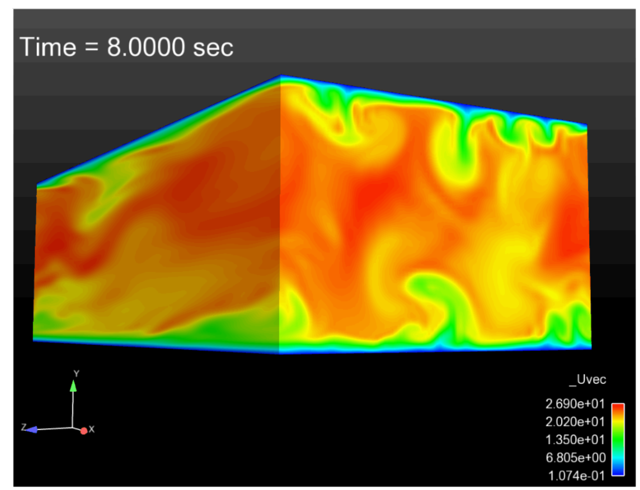
Starting simple…

- Calibrated parameters for Isotropic Turbulence
- Forward Uncertainty Quantification for 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:

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

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

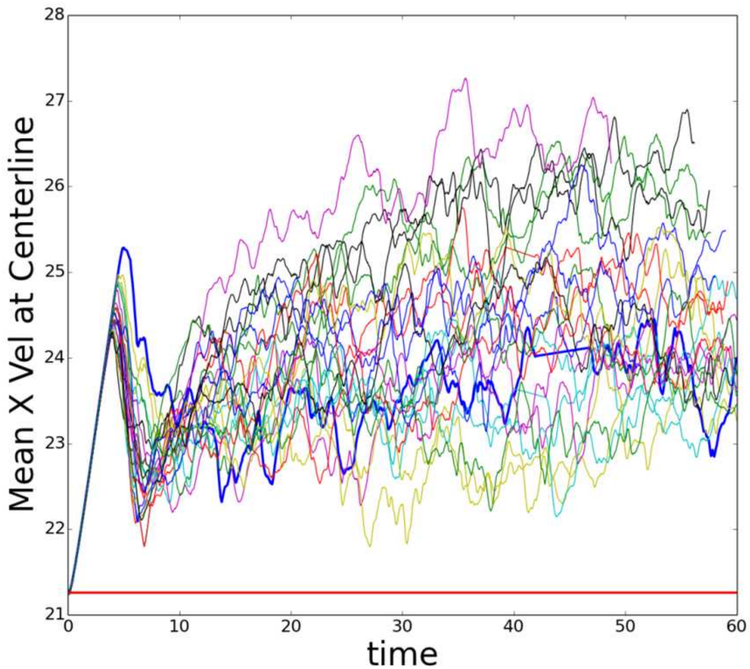
$$\mu_t = C_{\mu_\epsilon} \Delta \sqrt{k^{sgs}}$$

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

Calibrate: C_ϵ and C_{μ_ϵ}

"Parameter Uncertainty in LES of Channel Flow" by Safta, et al.

- See paper for skipped steps
- 25 Engineering LES Channel Flow Cases with different C_ϵ and C_{μ_ϵ}
- Not as predictive as we would have hoped…



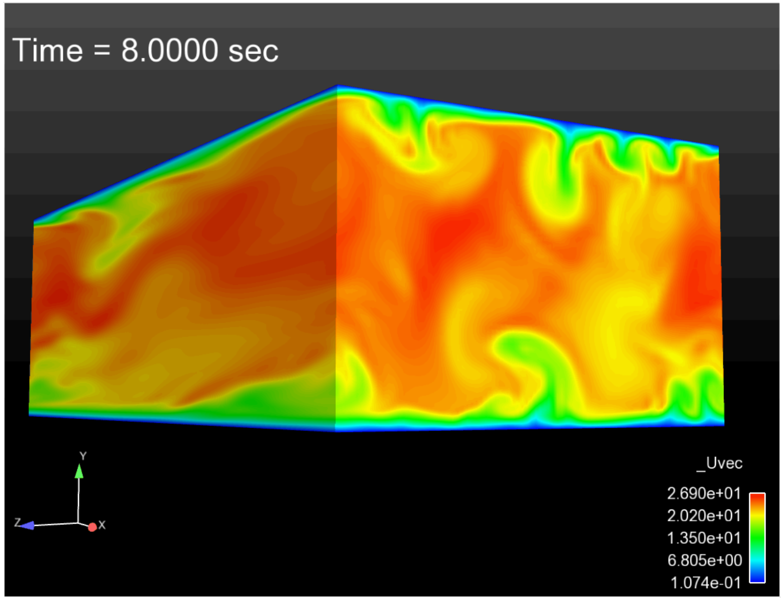
DNS = 21.26

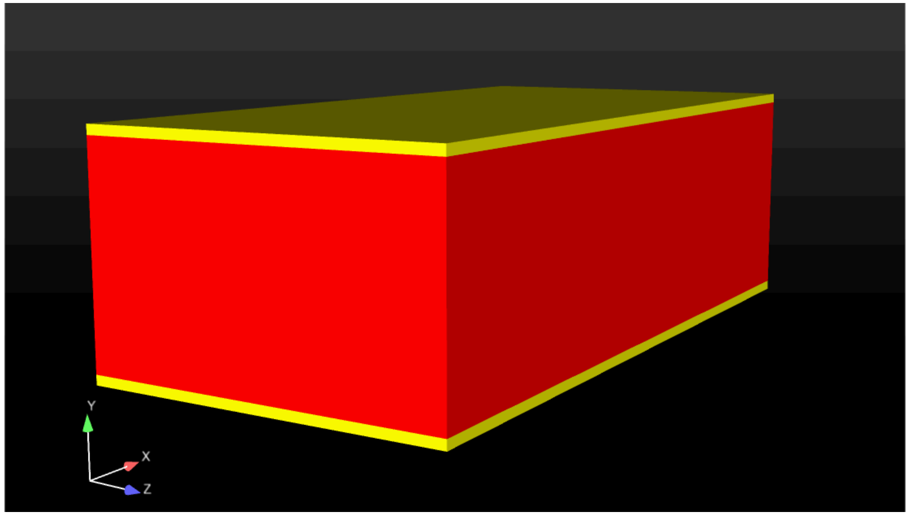
DNS: Moser, Kim, Mansour 1999

Calibration of Channel Flow

Engineering LES for Channel Flow

Adding "Wall Model": calibrating wall and center regions separately

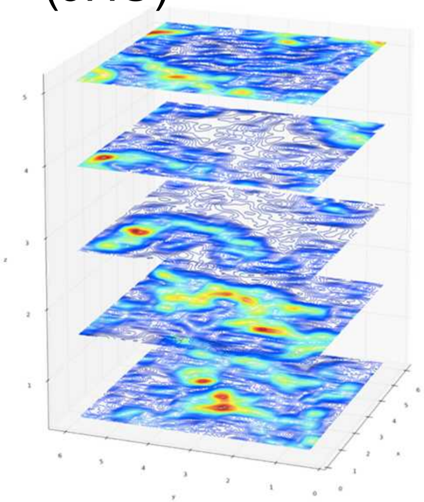


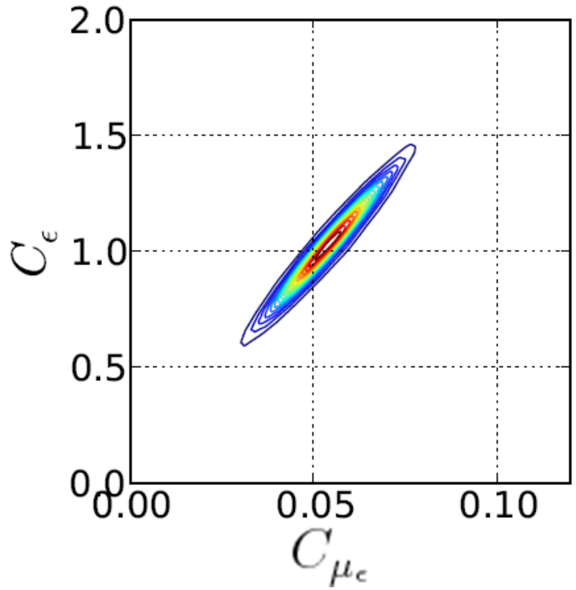


Principal Component Analysis

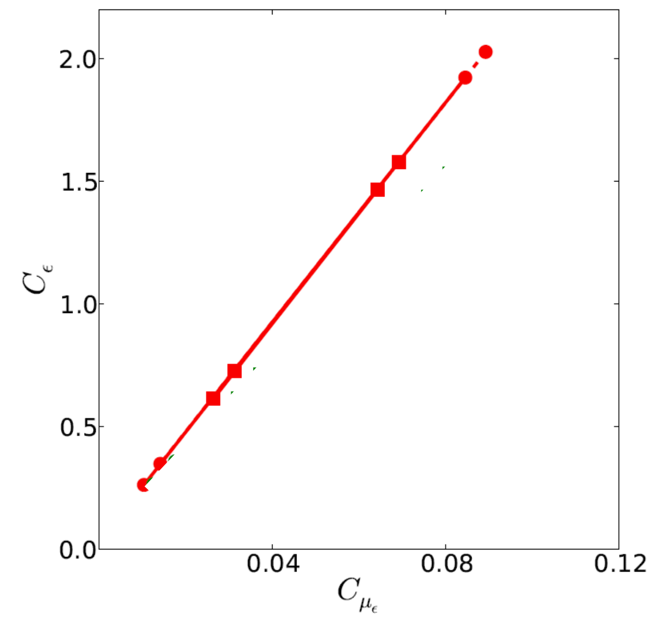
- Previous study found the ratio of $C_{\mu\epsilon}$ and C_ϵ is a constant
- Reduces number of variables

DNS of Isotropic Turbulence (JHU)



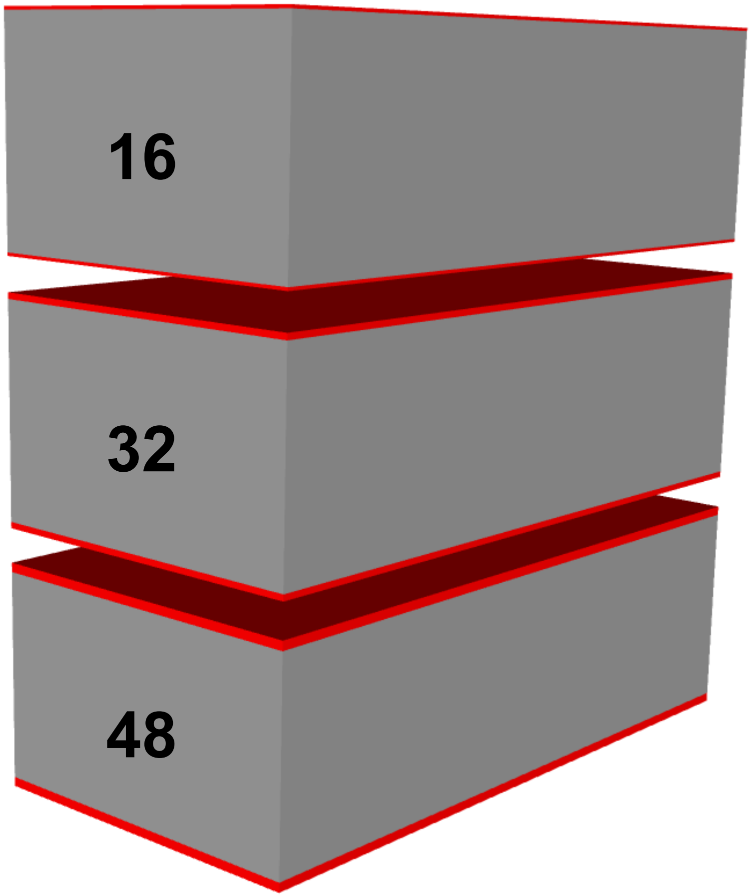


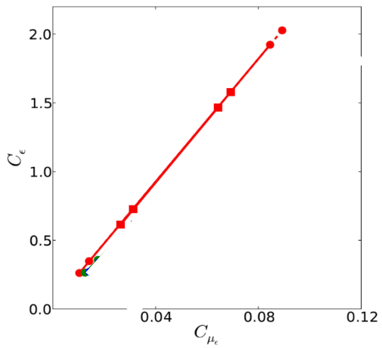
1st Principal Component
1%-99%



Wall Regions

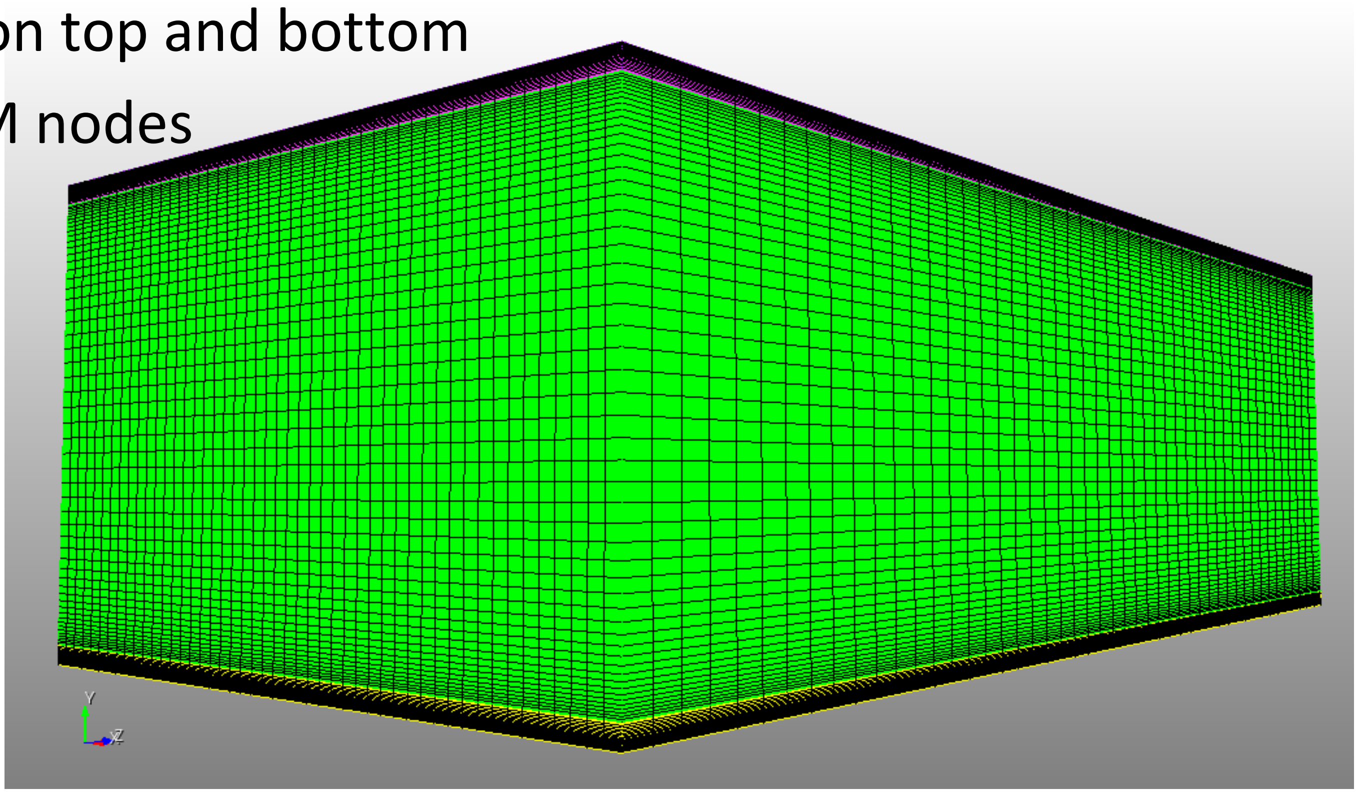
- 3 heights for wall region: y^+ = 16, 32, and 48
- Changing the parameters for the wall region and the center region separately
- 5 parameter pairs for both regions = 25 cases for each height





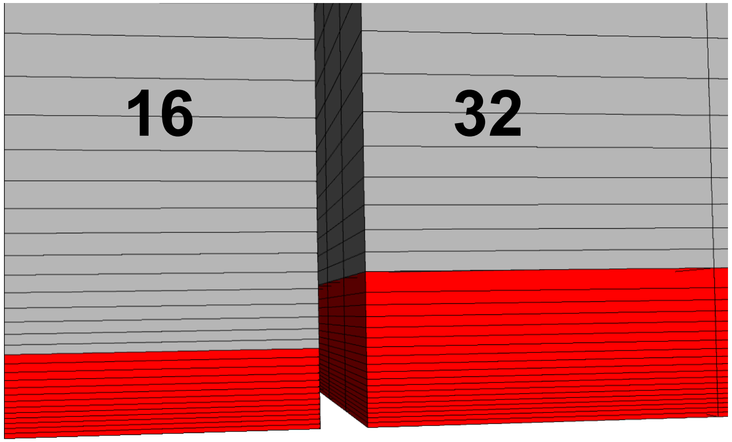
Meshing and Boundary Conditions

- $2\pi h \times 2h \times \pi h$ in the streamwise, wall-normal, and spanwise directions (like Moser, et al.)
- Streamwise and spanwise: periodic BC and 49 nodes in both directions
- No slip walls on top and bottom
- Moser: ~ 37 M nodes
- 250k nodes



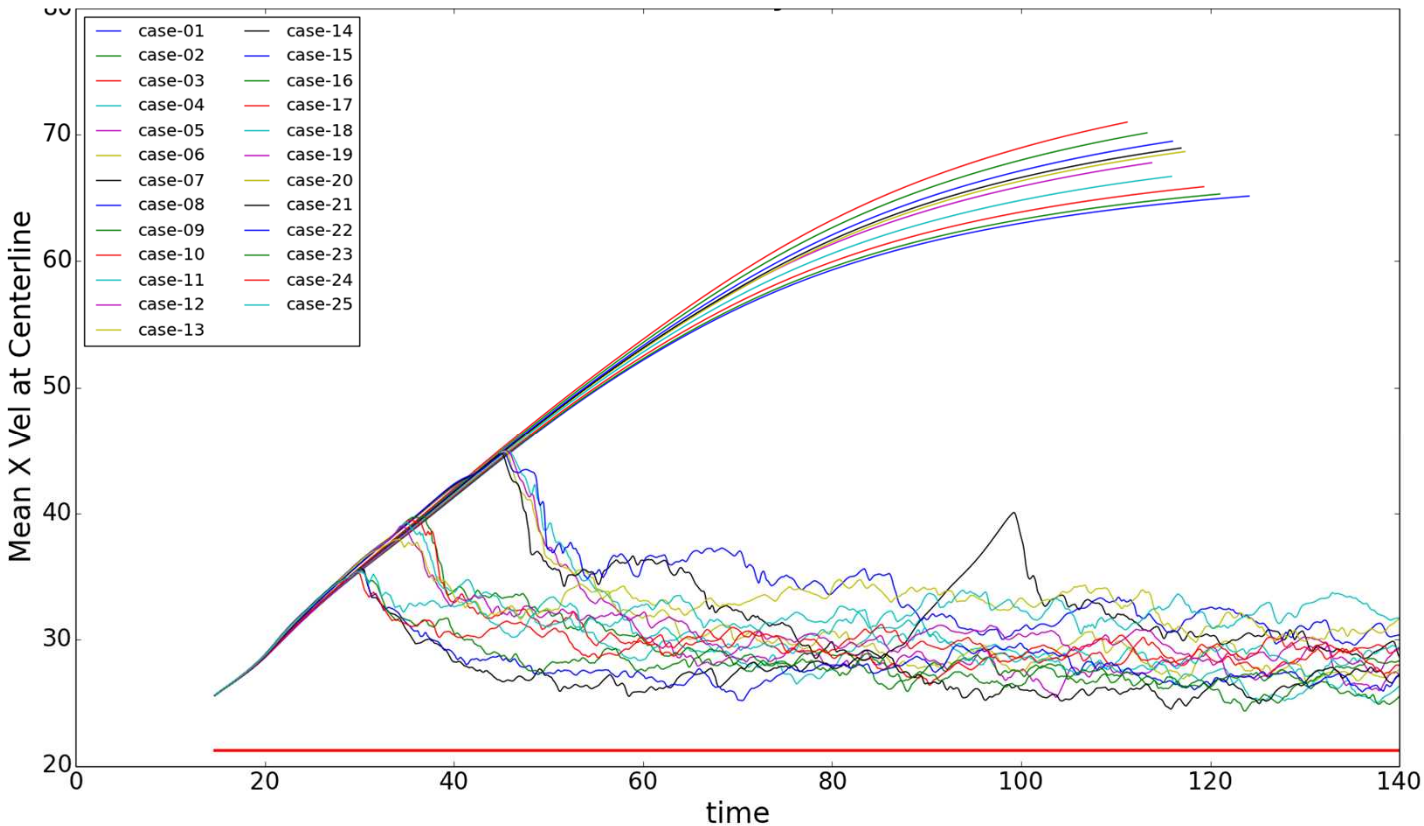
Meshing – Wall Normal Direction

- Wall region is "resolved"
  - $y^+ \approx 1$ for first 4 nodes
  - Height of $y^+ = 16$ has 12 nodes,
    32 has 18 nodes,
    48 has 23 nodes
- 97 total nodes in y direction for all three cases
- Spacing at centerline matches spacing in spanwise direction



Not all cases turbulent…

- Wall Region $y^+ = 16$
- Mean Centerline Velocity



DNS = 21.26

Not all cases turbulent…

- Mean Centerline Velocity
  - DNS value = 21.26 (Moser, et al.)

Laminar	Turbulent

$y^+ = 16$

Wall Region C's \ Center C's	1	2	3	4	5
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

$y^+ = 32$

Wall Region C's \ Center C's	1	2	3	4	5
1	64.02				21.4
2					22.4
3					24.01
4					27.95
5				65.1	33.9

$y^+ = 48$

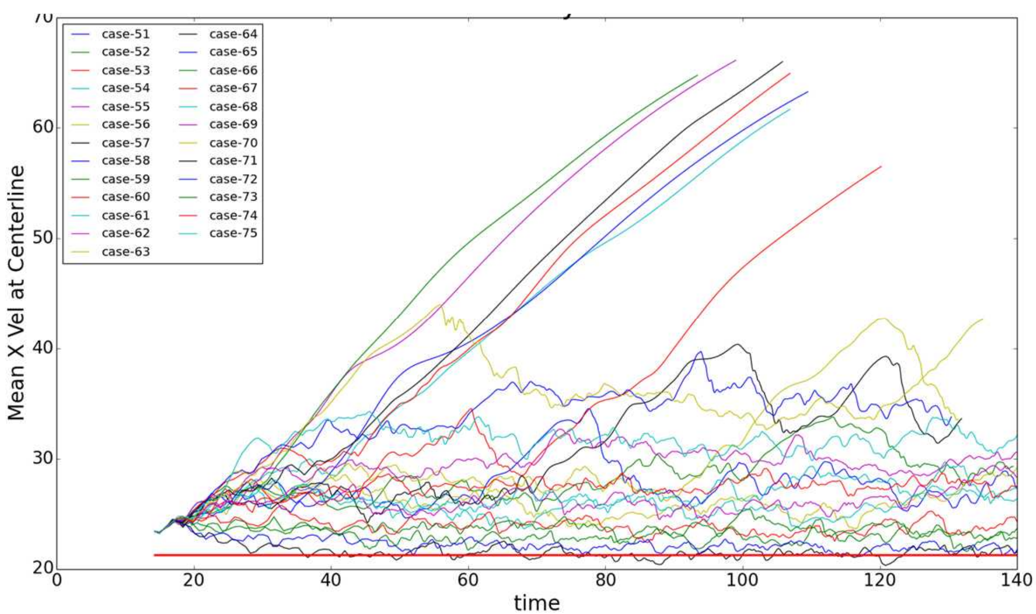
\ Center C's	1	2	3	4	5
1	27.5	26.2	26.1	22.9	21.5
2	30.7	35.9	26.7	23.6	21.9
3	46.6	54	36.3	27.5	23.6
4	52	56	56.3	29.7	27.7
5	57	55	35.7	35.6	31.6

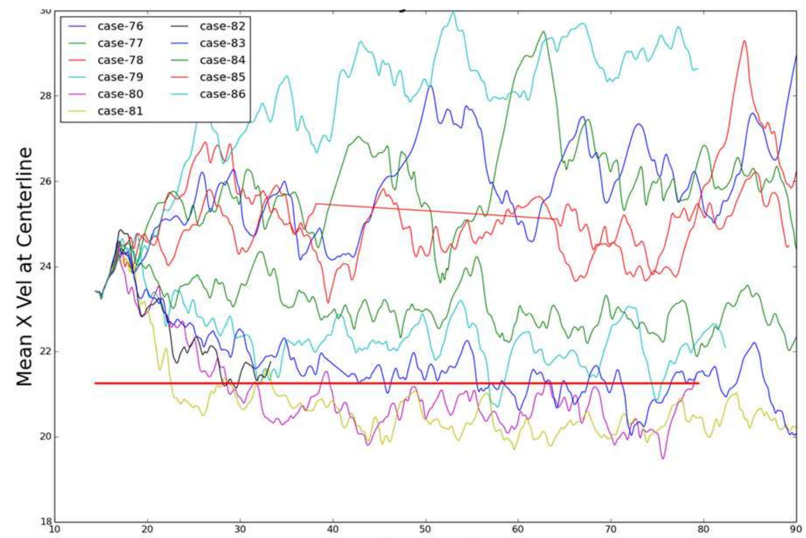
More cases for largest Wall Region

$y^+ = 48$

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





DNS = 21.26

Bayesian Calibration

Bayes formula:

likelihood

prior

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

posterior

evidence

- The posterior distribution *P(θ|D)* is the probability that θ is correct after taking into account D.
- The prior distribution *P(θ)* is the belief of what θ should be: uniform prior
- Data *D* from DNS of Channel Flow (Moser, et al.)
- Model parameters *θ* are the pairs of k^{sgs} model constants:

$$\theta = \{\eta_{wall}(C_{\epsilon}, C_{\mu\epsilon}), \eta_{center}(C_{\epsilon}, C_{\mu\epsilon})\}$$

- The likelihood *P(D|θ)* is the probability of observing D given θ. If parameter values are right, what are the chances of seeing D.

Bayesian Calibration - Likelihood

- $\theta = \{\eta_{wall}, \eta_{center}\}$
  - $\eta_{wall} = (C_{\epsilon}, C_{\mu\epsilon}), \eta_{center} = (C_{\epsilon}, C_{\mu\epsilon})$

- Likelihood assumes normal discrepancy between data and model

- $P(D|\theta) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp(-\frac{(\overline{u_{DNS}} - f(\eta_{wall}, \eta_{center}))^2}{2\sigma^2})$

- Model: Multiquadric Radial Basis Function:
  - $f(\theta) \approx \sum_{i=1}^{N} \omega_i \sqrt{1 + (\varepsilon \|\theta - \theta_i\|)^2}$

Construct a Response Surface

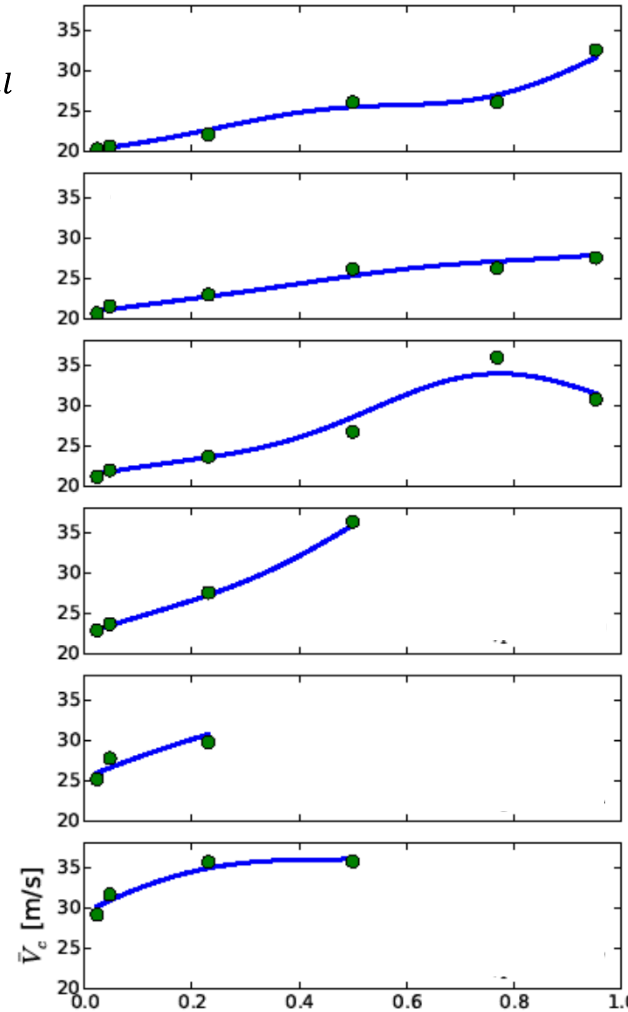
- Radial Basis Functions (RBF) to construct a surrogate model (f)

Wall Region C's

η_{wall}							
	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

η_{center}

η_{wall}

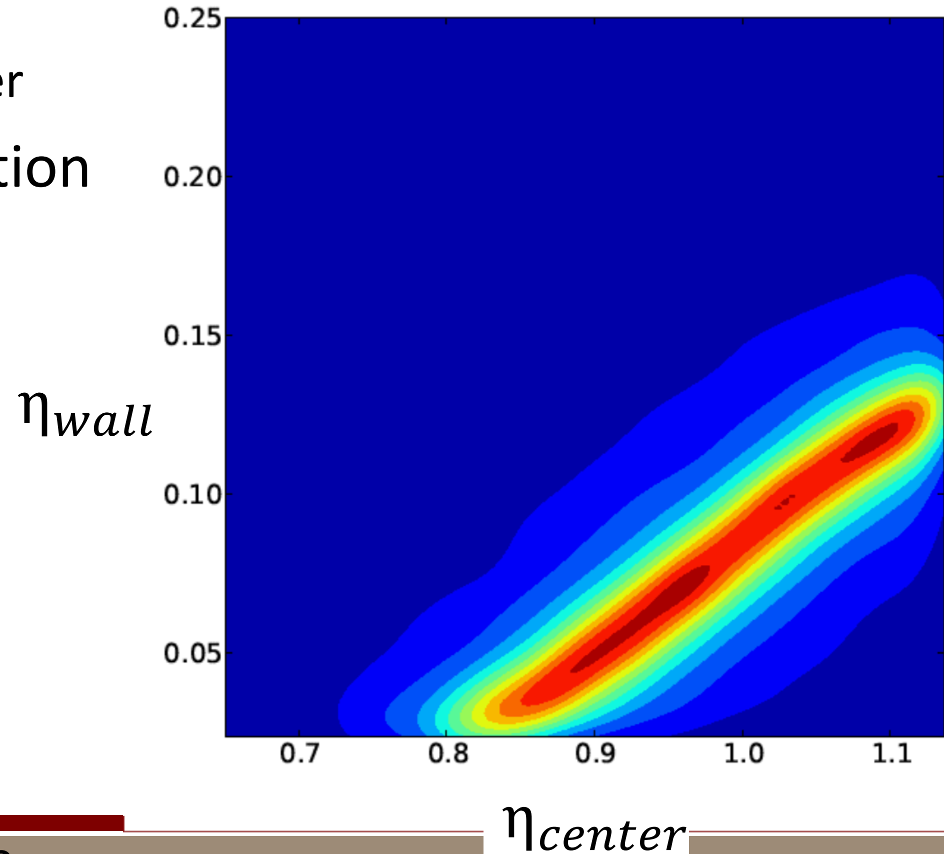


η_{center}

DNS = 21.26

Posterior - Joint PDF

- Values from literature:
  - $(C_{\mu\epsilon}, C_{\epsilon})=(0.0845,0.85)$[1] – isotropic turbulence
  - $(C_{\mu\epsilon}, C_{\epsilon})=(0.07,1.05)$[2] – shear flow
- Best values:
  - $(C_{\mu\epsilon}, C_{\epsilon})=(0.0975, 1.841)$-wall
    $(C_{\mu\epsilon}, C_{\epsilon})=(0.0195, 0.4108)$-center
- More production and dissipation in wall region



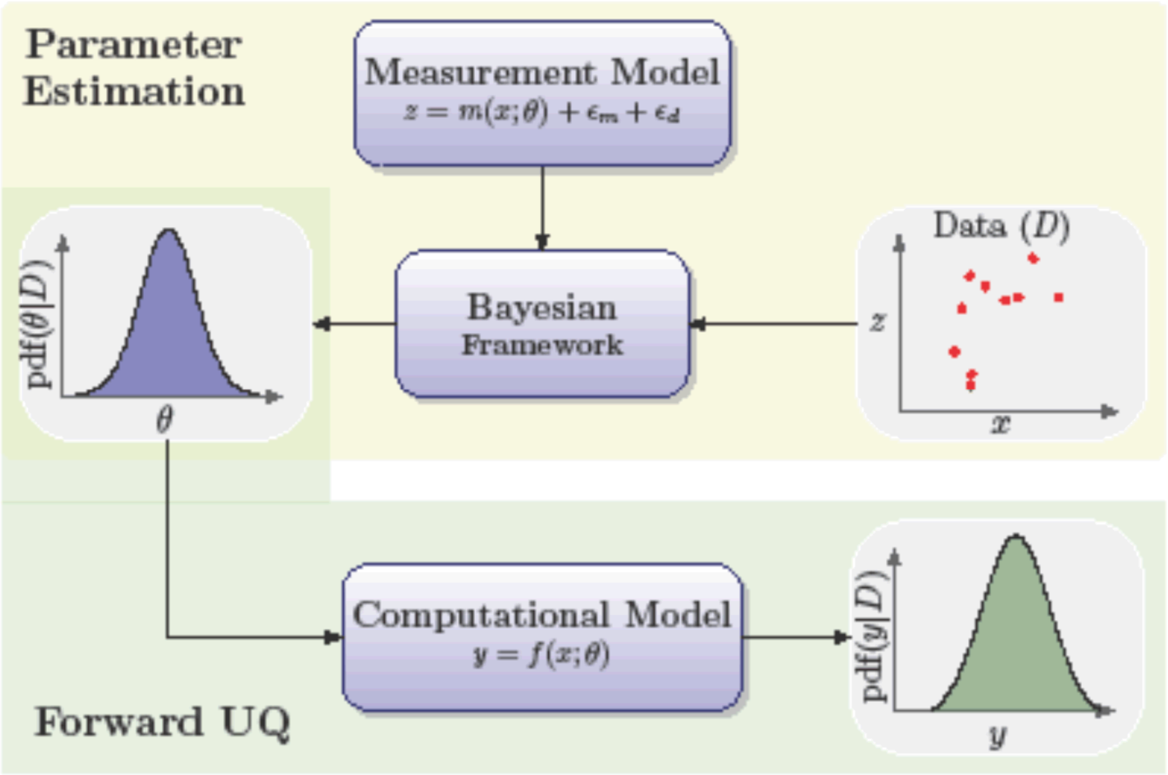
1. Shumann, 1991 2. Yoshizawa, 1986

Forward UQ for Parameter Values

- Use RBF response surface for Quantity of Interest (QoI)
  - Velocity at centerline
- Sample to get PDF's for QoI (y)

LES Channel

θ : wall and center region parameters



y : Velocity

Forward UQ

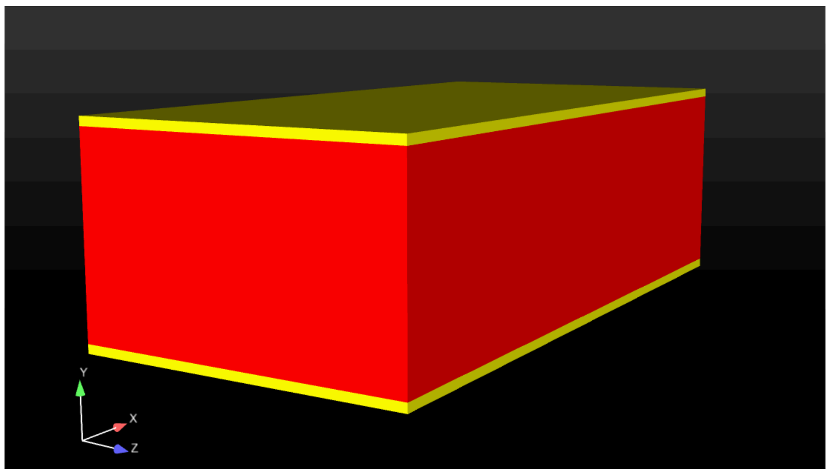
- Error bars on our values

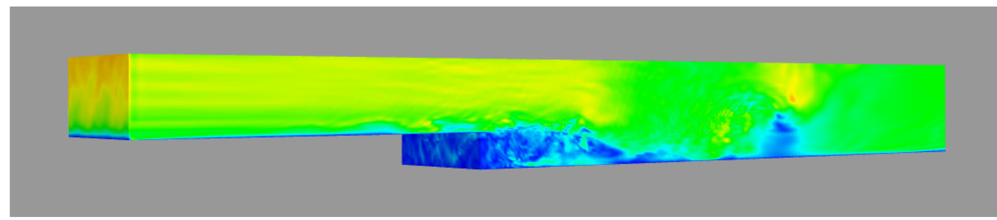
Conclusions

- Engineering LES can achieve correct quantities of interest for channel flow IF the turbulence model parameters are tuned correctly.
- This can be achieved easier if wall region and center region are tuned separately.
- Height of the wall region matters.
- Bayesian Calibration and surrogate models allow us to explore the region of parameter space that leads to the correct QoI values with uncertainties
- Compared to values in literature, center region has lower parameter values and wall region higher (for this channel flow case)

Yet to come…
Forward UQ for Backward Facing Step

Engineering LES for Channel Flow → Engineering LES for Backward Facing Step

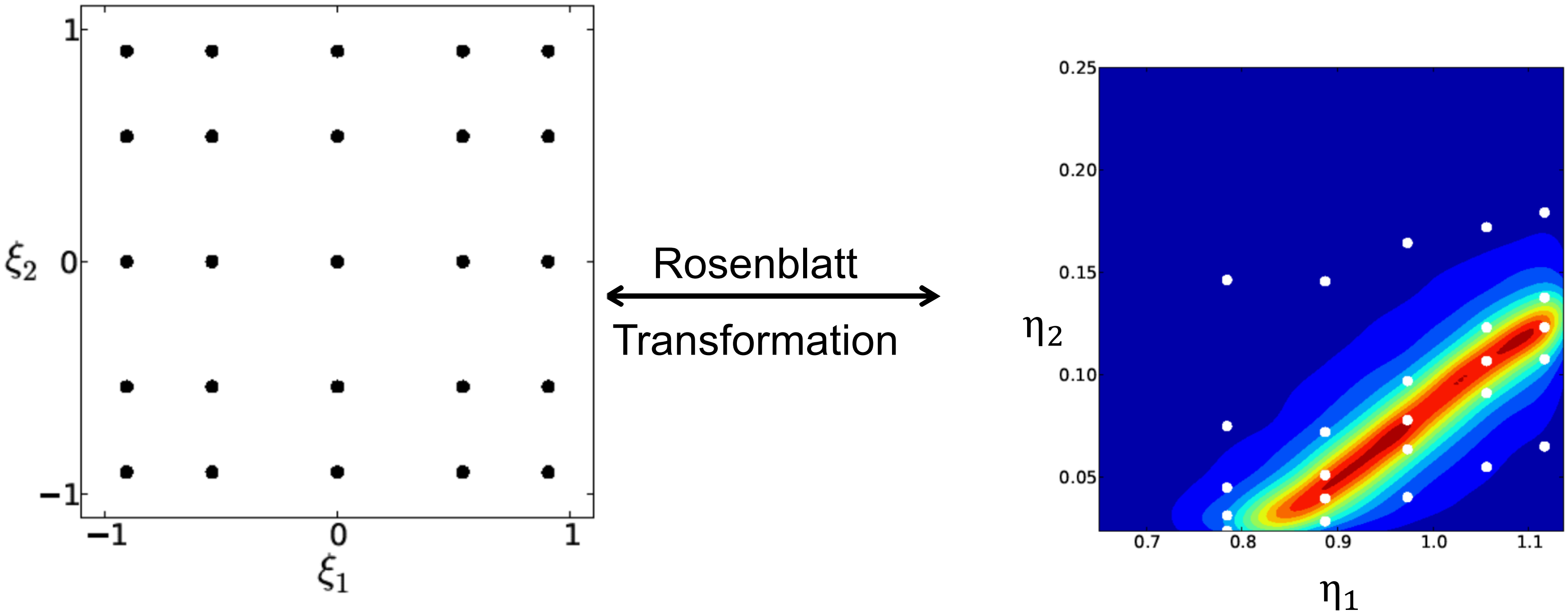




Thank you!

Quadrature to Construct PC Expansion for Model Output

$$\eta_1 = \eta_1(\xi_1, \xi_2),\ \eta_2 = \eta_2(\xi_1, \xi_2)$$



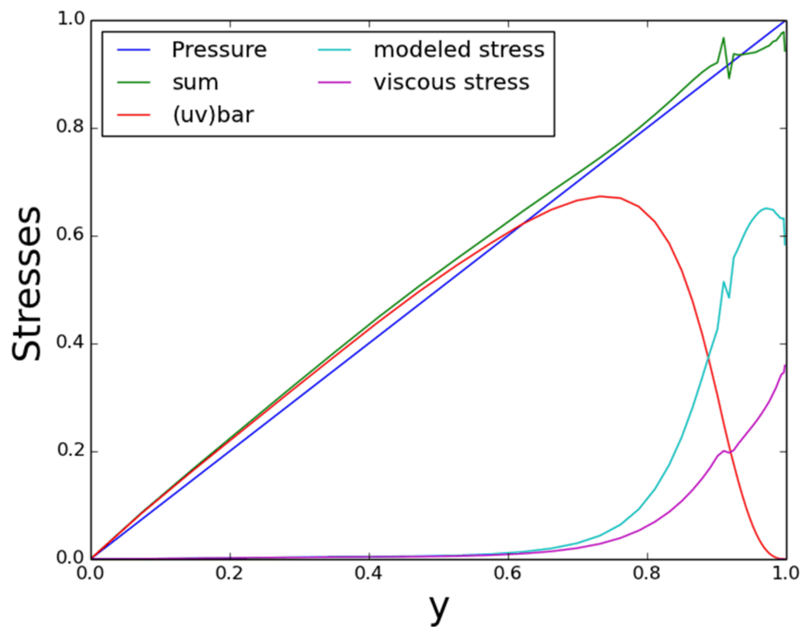
Stress Budget

Viscous

$$\overline{uv} = -\frac{dP}{dx}y + \left(\frac{1}{Re} + \nu_y\right)\frac{d\bar{u}}{dy}$$

Convective

Modeled

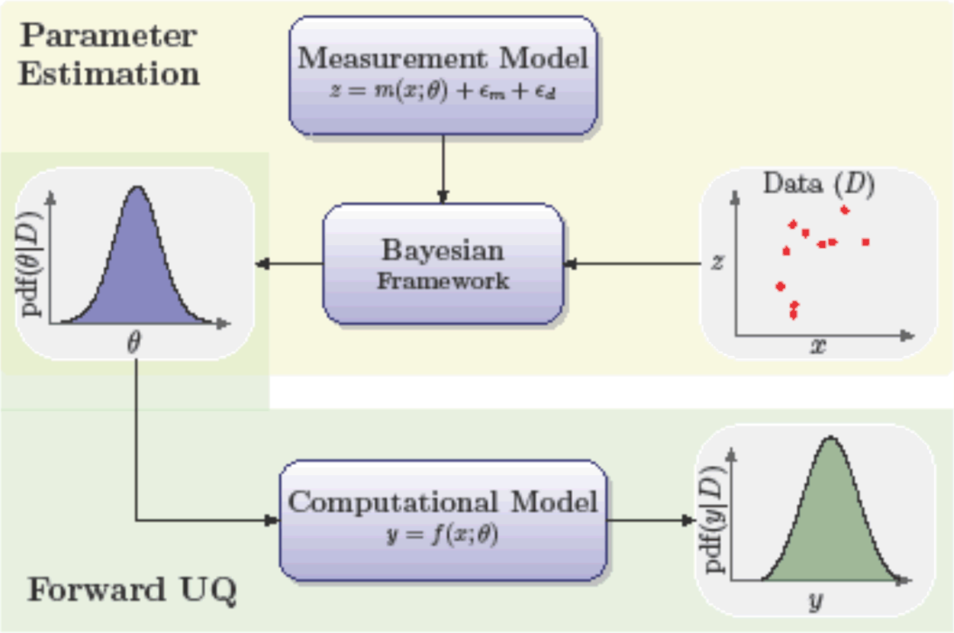


Forward UQ for Backward Facing Step

- Run 25 BFS cases at ξ quadrature points
- Create PCE response surface for Quantity of Interest (QoI)
  - Re-attachment point
- Sample to get PDF's for QoI (y)

LES Channel

θ : wall and center region parameters



y : BFS re-attachment

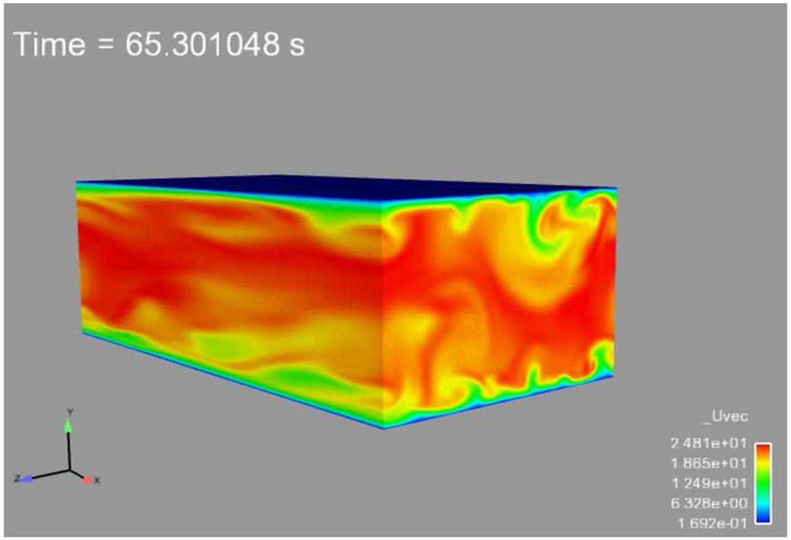
What does it mean?

- Values from literature: $(C_{\mu\epsilon}, C_{\epsilon})=(0.0845, 0.85)$[1], $(0.07, 1.05)$[2]
- Ratio is the same, numbers change

	C-mu-epsilon	C-epsilon
0	0.1118	2.1039
1	0.0958	1.8066
2	0.0797	1.5093
3	0.0563	1.0739
4	0.0328	0.6385
5	0.0167	0.3411
6	0.0087	0.1925

1. Shumann, 1991   2. Yshizawa, 1986

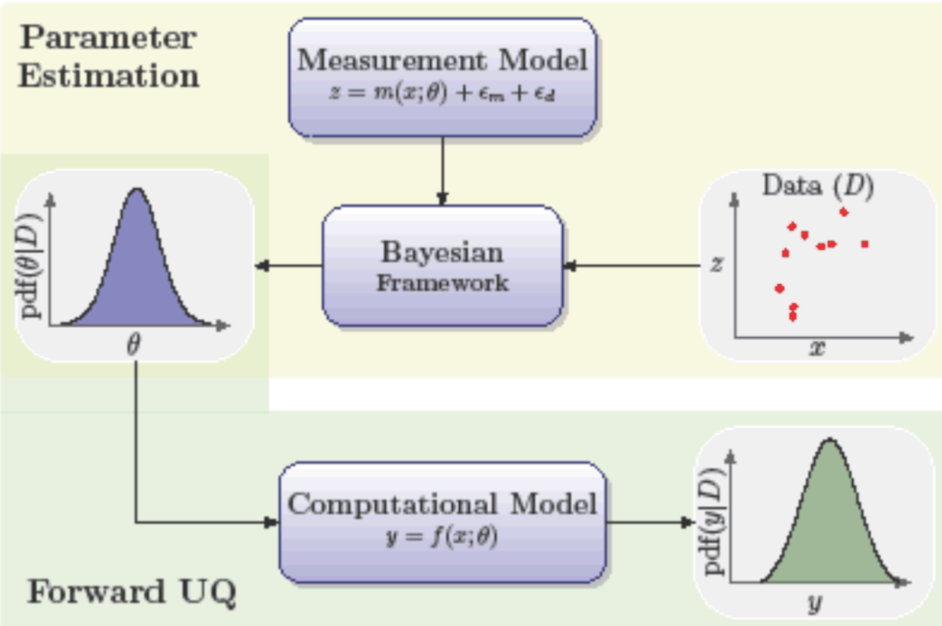
Fuego LES Simulations with Calibrated Parameters



- **250k nodes**
  - ***y*$^+$ ≈ 1.15 at walls**
  - **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)

Forward UQ – Predictive Assessment

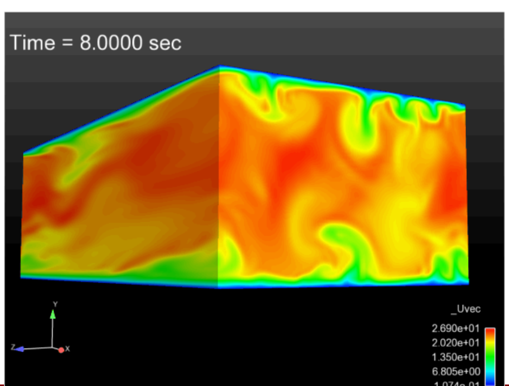


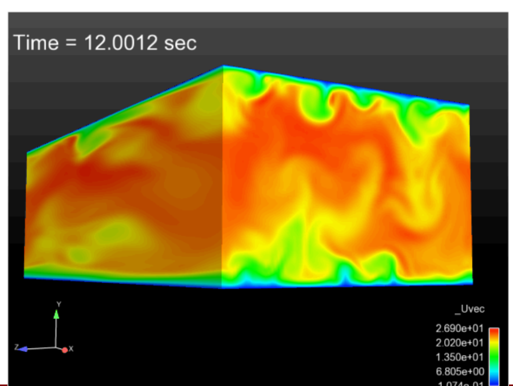
- y – quantity of interest: mean x velocity, rms, $\dot{m}$
- Modeled by Polynomial Chaos Expansion

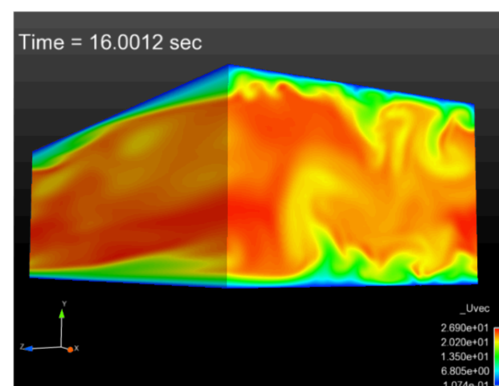
$$y(C_\epsilon, C_{\mu\epsilon}) = \Sigma\, c_k \Psi_k(\xi_1, \xi_2)$$

- Galerkin projection:

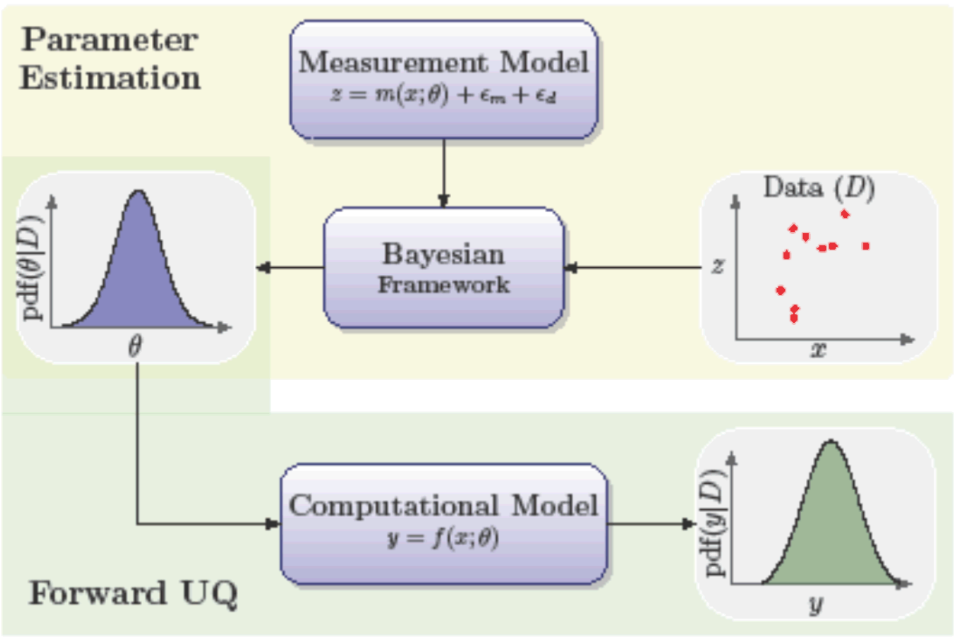
$$c_k = \frac{\langle y(C_\epsilon, C_{\mu\epsilon}) \Psi_k(\xi_1, \xi_2) \rangle}{\langle \Psi_k{}^2(\xi_1, \xi_2) \rangle}$$







Forward UQ – Predictive Assessment



- y – quantity of interest: re-attachment point
- Modeled by Polynomial Chaos Expansion

$$\boldsymbol{y}(\eta_w,\eta_c) = \Sigma\, \boldsymbol{c_k}\, \Psi_k(\xi_1,\xi_2)$$

- Galerkin projection:

$$\boldsymbol{c_k} = \frac{\langle \boldsymbol{y}(\eta_{\mathbf{w}}, \eta_{\boldsymbol{\mu\epsilon}})\boldsymbol{\Psi}_{\boldsymbol{k}}(\xi_1,\xi_2)\rangle}{\langle \boldsymbol{\Psi}_{\boldsymbol{k}}{}^2(\xi_1,\xi_2)\rangle}$$