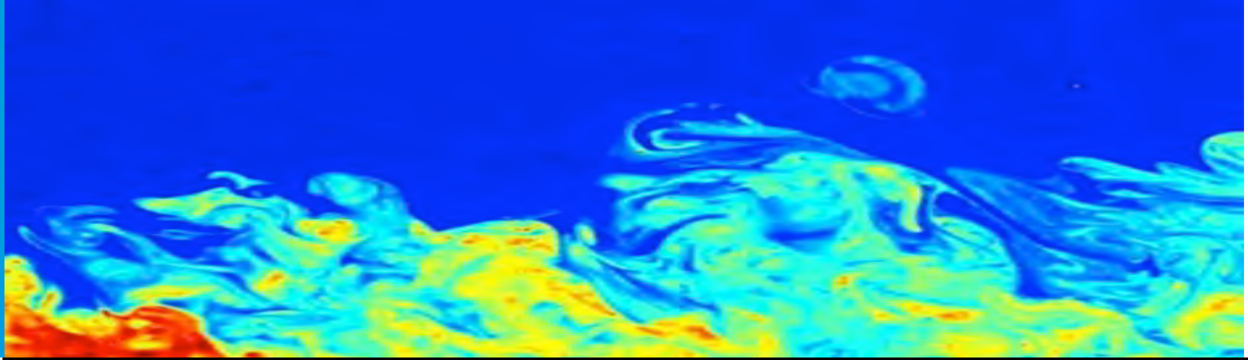

Quantifying Turbulence Model Inadequacy with Bayesian Scenario Averaging

London Validation Workshop

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Overview

1. Reynolds Averaged Navier-Stokes (RANS) closure models
2. Statistical modelling of simulation error
    - Approach #1: Kennedy + O'Hagan
    - Approach #2: Closure model coefficients
3. A *predictive* capability with Bayesian Scenario Averaging

Framework: Flat-plate boundary-layers (with BL-code)

Navier-Stokes equations

- Incompressible Navier-Stokes equations:

$$\nabla \cdot \mathbf{u} = 0$$

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} = -\frac{1}{\rho} \nabla p + \frac{1}{\rho} \nabla \left(\mu \nabla \mathbf{u} \right)$$

- Reynolds averaged:

$$\mathbf{u} = \bar{\mathbf{u}} + \mathbf{u}'$$

$$\nabla \cdot \mathbf{u} = 0$$

$$\frac{\partial \bar{\mathbf{u}}}{\partial t} + \bar{\mathbf{u}} \cdot \nabla \bar{\mathbf{u}} = -\frac{1}{\rho} \nabla \bar{p} + \frac{1}{\rho} \nabla \left(\mu \nabla \bar{\mathbf{u}} - \rho \overline{\mathbf{u}'\mathbf{u}'} \right)$$

Closure models for: $-\rho\overline{\mathbf{u}'\mathbf{u}'}$

- k-eps models:

$$\nu_T = C_\mu f_\mu \frac{k^2}{\tilde{\varepsilon}},$$

$$\frac{\partial k}{\partial t} + \bar{u}\frac{\partial k}{\partial x_1} + \bar{v}\frac{\partial k}{\partial x_2} = \nu_T\left(\frac{\partial \bar{u}}{\partial x_2}\right)^2 - \varepsilon + \frac{\partial}{\partial x_2}\left[\left(\nu + \frac{\nu_T}{\sigma_k}\right)\frac{\partial k}{\partial x_2}\right],$$

$$\frac{\partial \tilde{\varepsilon}}{\partial t} + \bar{u}\frac{\partial \tilde{\varepsilon}}{\partial x_1} + \bar{v}\frac{\partial \tilde{\varepsilon}}{\partial x_2} = C_{\varepsilon 1} f_1 \frac{\tilde{\varepsilon}}{k}\nu_T\left(\frac{\partial \bar{u}}{\partial x_2}\right)^2 - C_{\varepsilon 2} f_2 \frac{\tilde{\varepsilon}^2}{k} + E + \frac{\partial}{\partial x_2}\left[\left(\nu + \frac{\nu_T}{\sigma_\varepsilon}\right)\frac{\partial \tilde{\varepsilon}}{\partial x_2}\right],$$

- Launder-Sharma:

$$C_\mu = 0.09, \quad C_{\varepsilon 1} = 1.44, \quad C_{\varepsilon 2} = 1.92, \quad \sigma_k = 1.0, \quad \sigma_\varepsilon = 1.3.$$

=> θ

- Jones-Launder:

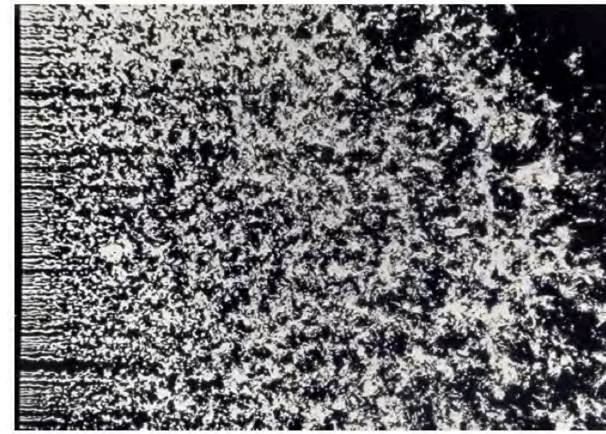
$$C_\mu = 0.09, \quad C_{\varepsilon 1} = 1.55, \quad C_{\varepsilon 2} = 2.0, \quad \sigma_k = 1.0, \quad \sigma_\varepsilon = 1.3.$$

Model coefficients are not sacred!

- E.g. Isotropic decaying turbulence
- Equations reduce to

$$\frac{dk}{dt} = -\varepsilon,$$

$$\frac{d\varepsilon}{dt} = -C_{\varepsilon 2}\frac{\varepsilon^2}{k}.$$



- With exact solution

$$k(t) = k_0 \left(\frac{t}{t_0}\right)^{-n}$$

$$n = 1/(C_{\varepsilon 2} - 1)$$

- Values for $C_{\varepsilon 2}$ vary a lot:
  - Commonly used 1.92
  - RNG k-eps 1.68
  - k-tau 1.83
  - Best fit to data (n=1.3) 1.77

Approach #1: Bayesian calibration of coefficients *(a la Kennedy+O'Hagan)*

1. Find a flow of interest *(scenario S)*
2. Preparation stage
    - Collect experimental data on the flow (*z*)
    - Calibrate closure model (*M*) given *z* => coefficients (θ^*)
3. Prediction stage
    - Apply *M* using θ^* to a new flow (no exp. data available)

* Kennedy and O'Hagan (2001). *Bayesian Calibration of Computer Models*. Journal of the Royal Society B. 63(3).

Statistical model

Relate *z* to $\boldsymbol{\theta}$:

$$z = \eta(y^+;\boldsymbol{\gamma}) \cdot M(y^+;\boldsymbol{\theta}) + \epsilon$$

$$\epsilon \sim \mathcal{N}(0, \sigma_z^2)$$

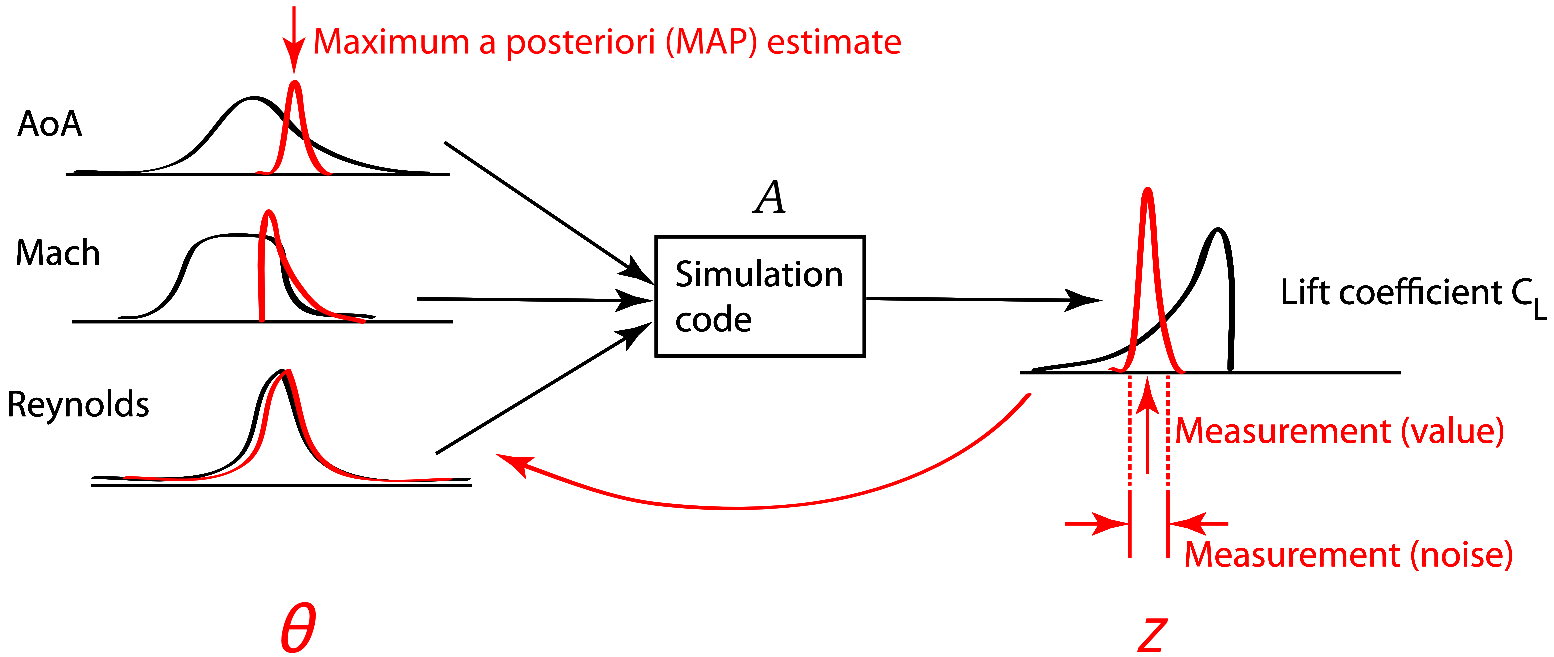
$$\eta \sim \mathcal{GP}(1, \Sigma_\eta(\boldsymbol{\gamma}))$$

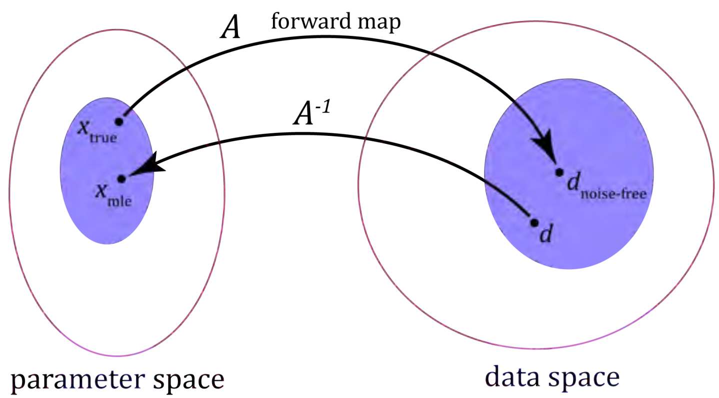
For specified $\boldsymbol{\theta}$ we can calculate the probability of any z.

I.e. $\rho(z|\boldsymbol{\theta})$ at a cost of one evaluation of $M(y^+;\boldsymbol{\theta})$

Use Markov-Chain Monte-Carlo to sample distribution of $\rho(\boldsymbol{\theta}|z)$

Bayesian calibration step





Bayesian calibration

Bayes theorem: $\rho(\boldsymbol{\theta}|z) \propto \rho(z|\boldsymbol{\theta}) \cdot \rho_0(\boldsymbol{\theta})$

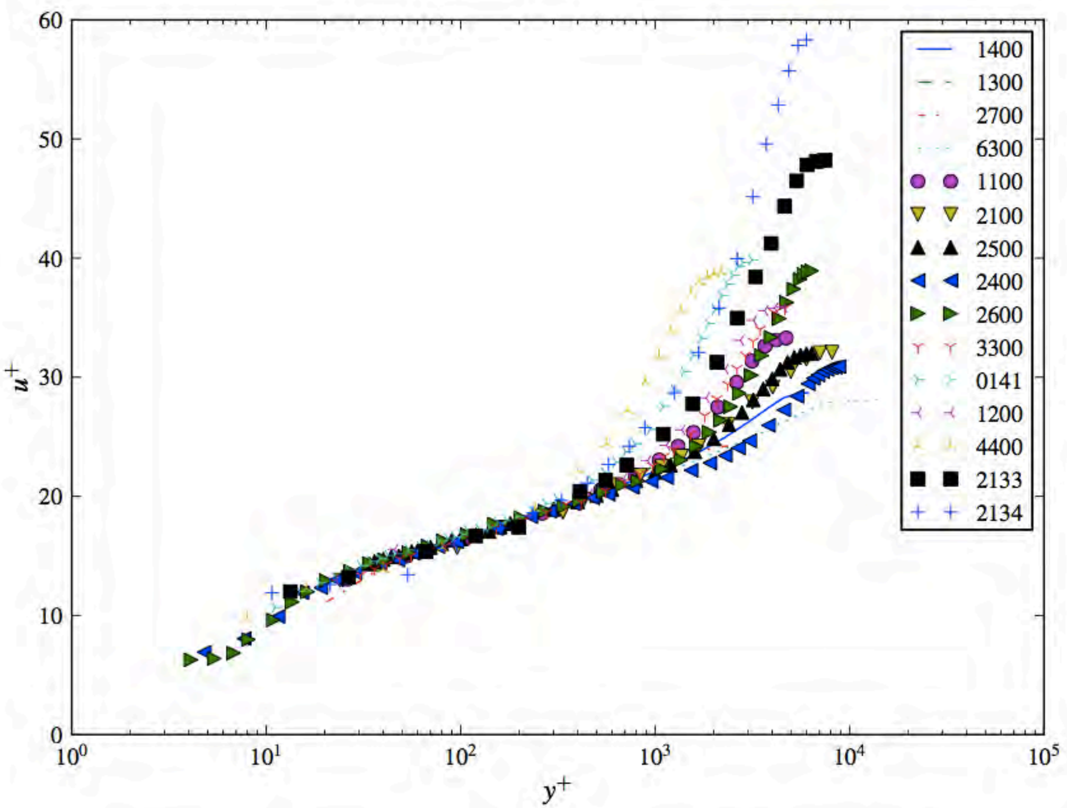
Need to specify two probability distributions:

Prior $\rho_0(\boldsymbol{\theta})$ - existing knowledge of θ (possibly non-informative)

Likelihood $\rho(z|\boldsymbol{\theta})$ - chance of observing z given θ need statistical model

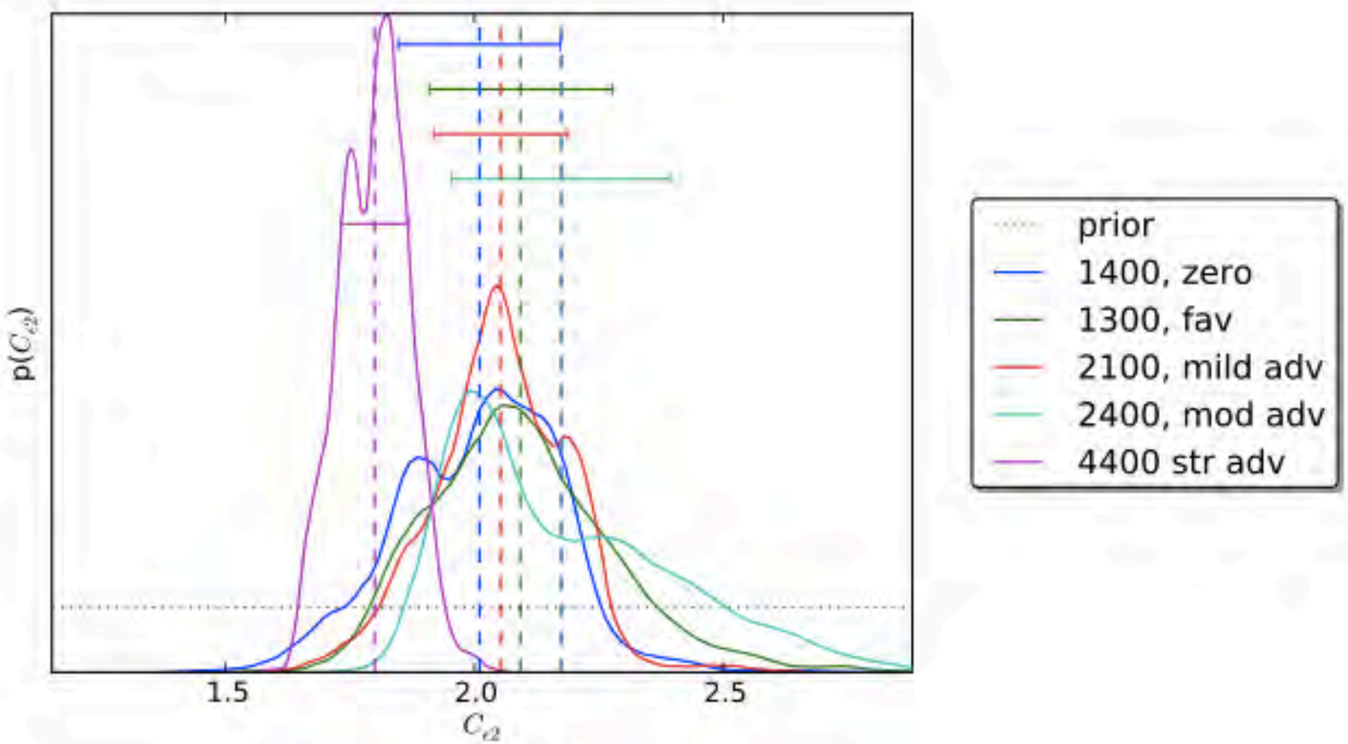
Framework: Flat-plate BLs

- Class of flows: flat-plate boundary-layers
- Data: 1968 AFOSR-IFP-Stanford conference
- Solver: Wilcox EDDYBL, multiple turb. models (1 solve ~5 sec)



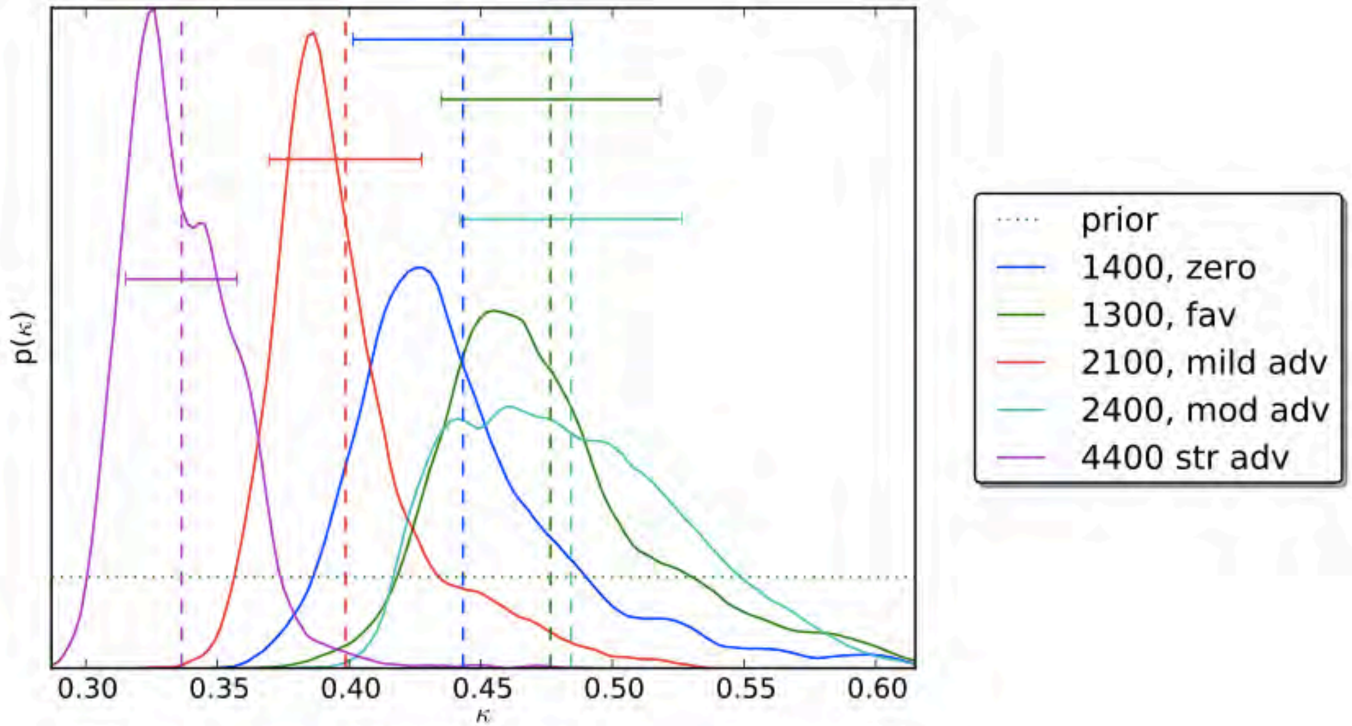
Calibration Results - k-ε

- Posterior distributions for $C_{\varepsilon 2}$ for a favorable, zero, mild, moderate and strongly adverse $d\bar{p}/dx$.



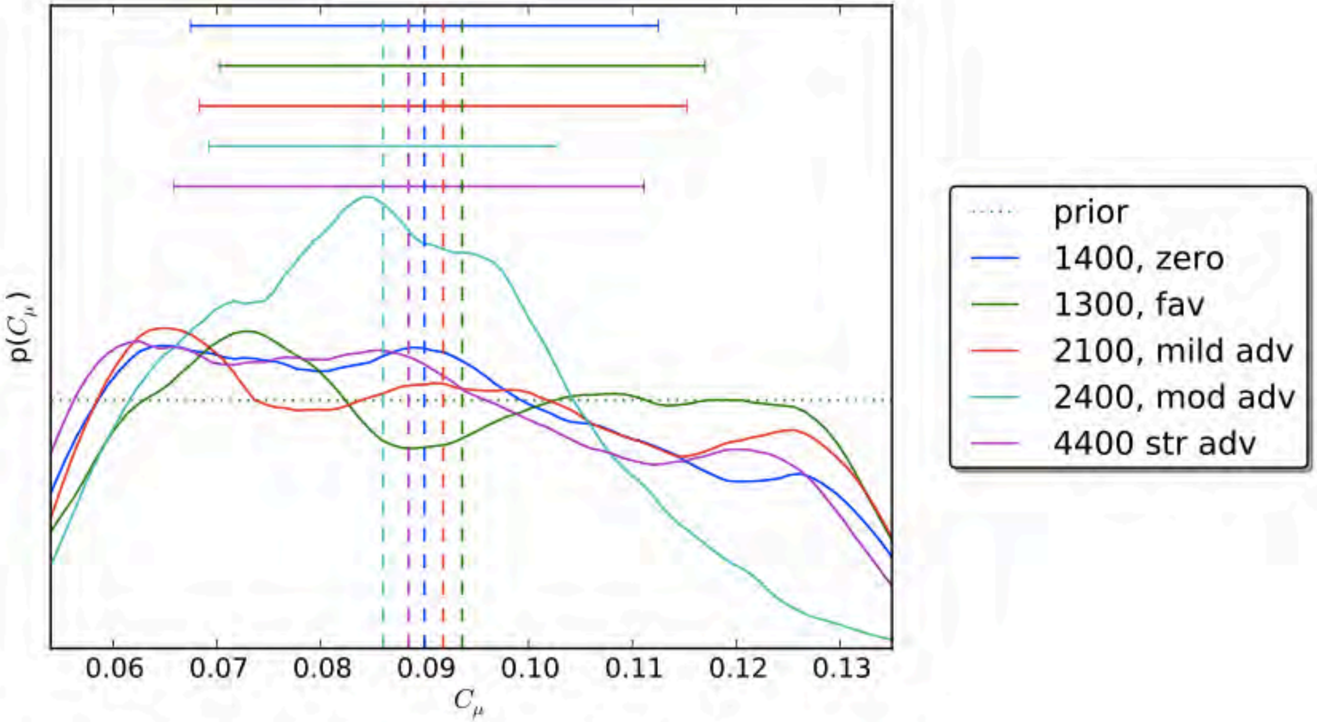
Calibration Results - k-ε

- Posterior distributions for κ for a favorable, zero, mild, moderate and strongly adverse $d\bar{p}/dx$.



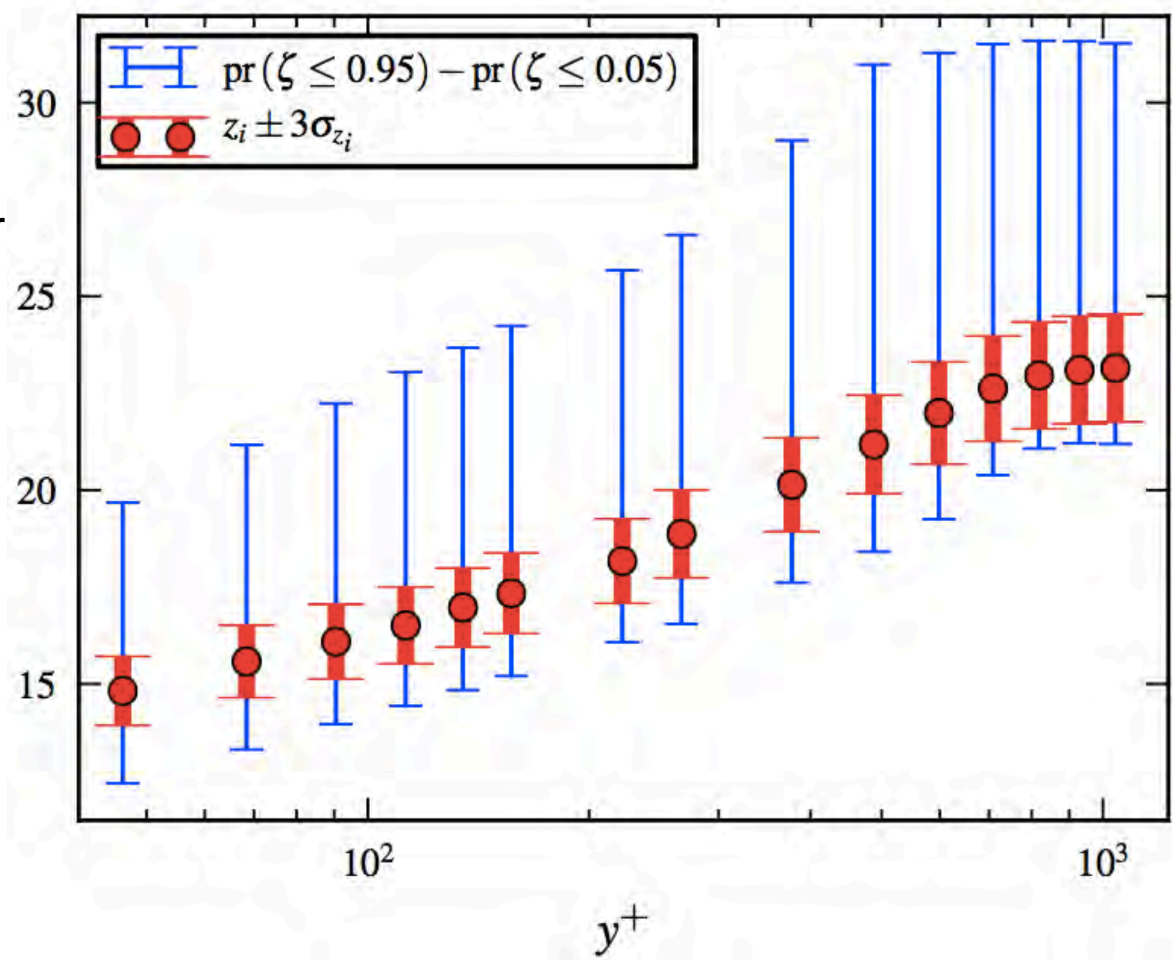
Calibration Results - k-eps

- Posterior distributions for C_μ for a favorable, zero, mild, moderate and strongly adverse $d\bar{p}/dx$.



Prediction – *Kennedy + O'Hagan* – k-ε

- New BL flow outside of set of scenarios *S*
- Measurements used for validation only
- 90% credible intervals based on posterior coefficient pdfs



Approach #2: Inadequacy captured by closure coefficients

- Define a class of flows of interest (flat-plate BLs, varying pressure-grads)
- Preparation stage
  - Collect data ($z_k \in \mathcal{Z}$) for some scenarios ($S_k \in \mathcal{S}$) in class (1968 AFOSR-IFP-Stanford conference)
  - Calibrate multiple closure models ($M_i \in \mathcal{M}$) for each scenario to get coefficient posteriors ($\theta^\star_{i,k}$) (k-w, k-eps, SA, BL)
- Prediction stage
  - Build posterior predictive distribution for QoI Δ in a new scenario, conditioned on all data via all models and scenarios.

Bayesian model averaging - prediction

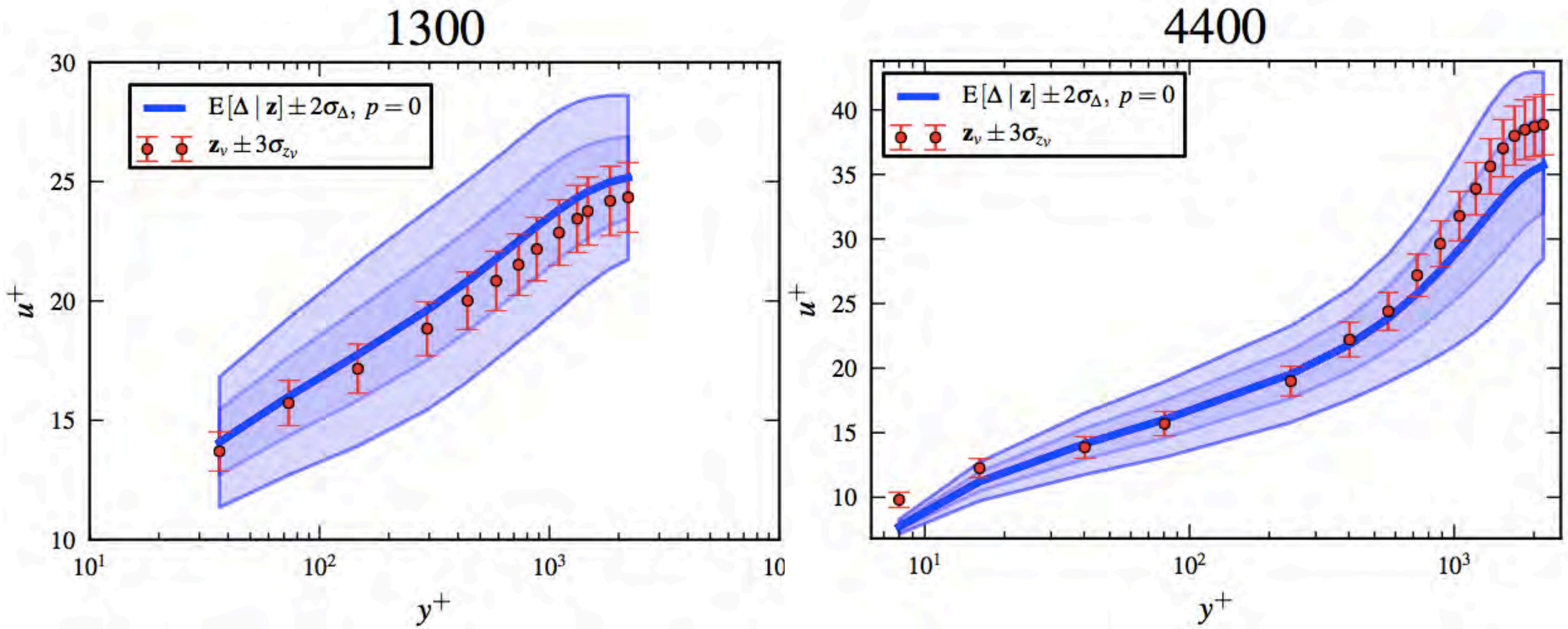
- Let M_i be a turbulence model in set $\mathcal{M}$, S_k a $d\bar{p}/dx$ scenario in set $\mathcal{S}$ and $\mathcal{Z}$ be the set of all experimental calibration data.
- The BMA prediction of a QoI Δ is then [2]:

$$\mathrm{E}(\Delta \mid \mathcal{Z}) = \sum_{i=1}^{I} \sum_{k=1}^{K} \mathrm{E}(\Delta \mid M_i, S_k, \mathbf{z}_k)\, \mathrm{pr}(M_i \mid S_k, \mathbf{z}_k)\, \mathrm{pr}(S_k) \tag{4}$$

- The scenario of Δ does not have to be in the set $\mathcal{S}$.
- Each individual expectation in (4) is weighted by
  - The posterior model probability $\mathrm{pr}(M_i \mid S_k, \mathbf{z}_k)$.
  - The prior scenario probability $\mathrm{pr}(S_k)$.

Bayesian scenario averaging – Posterior predictive distribution

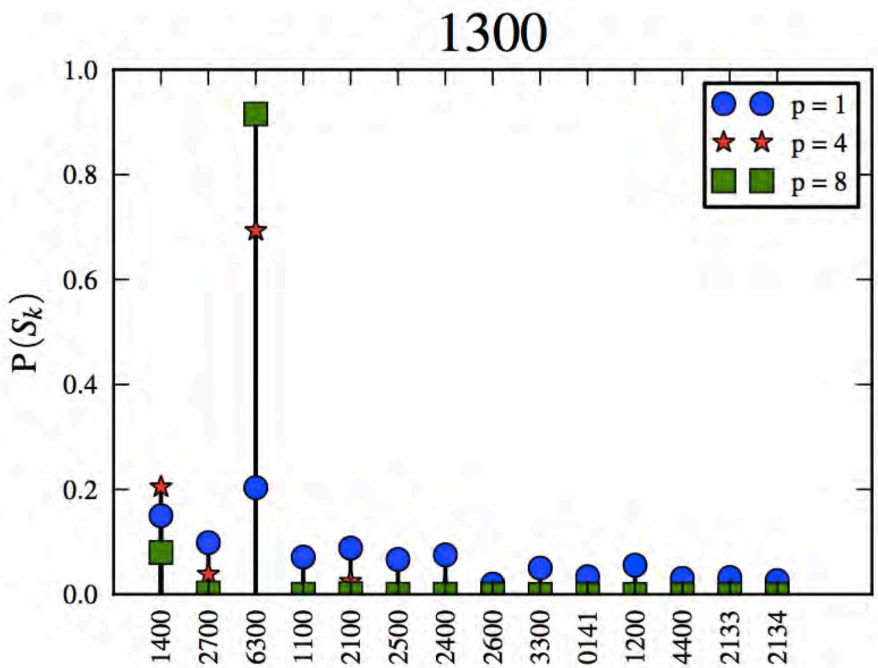
$$p(\Delta|\mathbf{z}, \mathcal{M}, \mathcal{S}) = \ldots$$

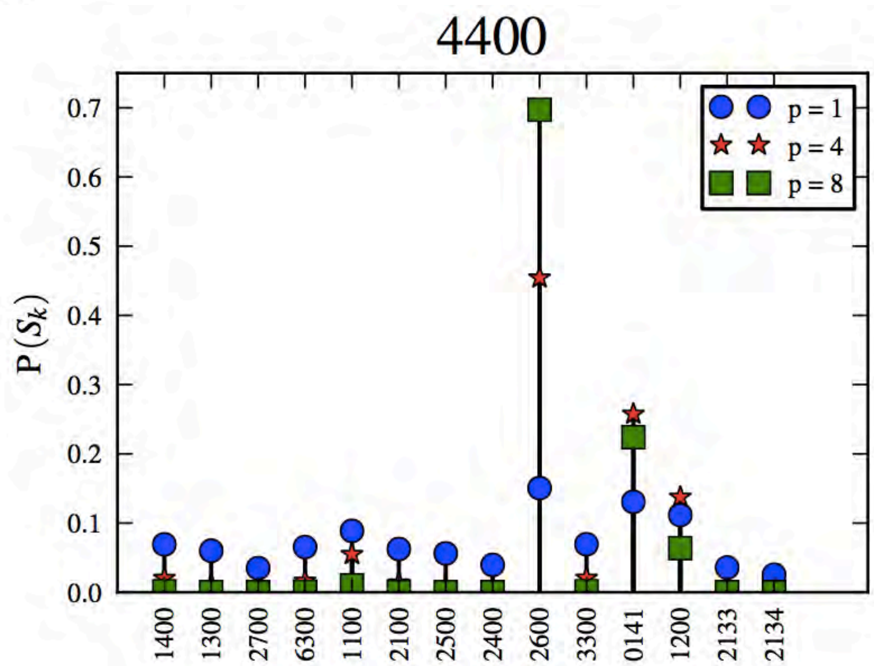


Bayesian scenario averaging – Smart scenario weighting

$$\mathcal{E}_k = \sum_{i=1}^{I} \left(\mathbb{E}[\hat{\Delta}_{i,k}] - \mathbb{E}\left[\Delta \mid \mathbf{S}_k, \mathbf{z}_k\right] \right)^2$$

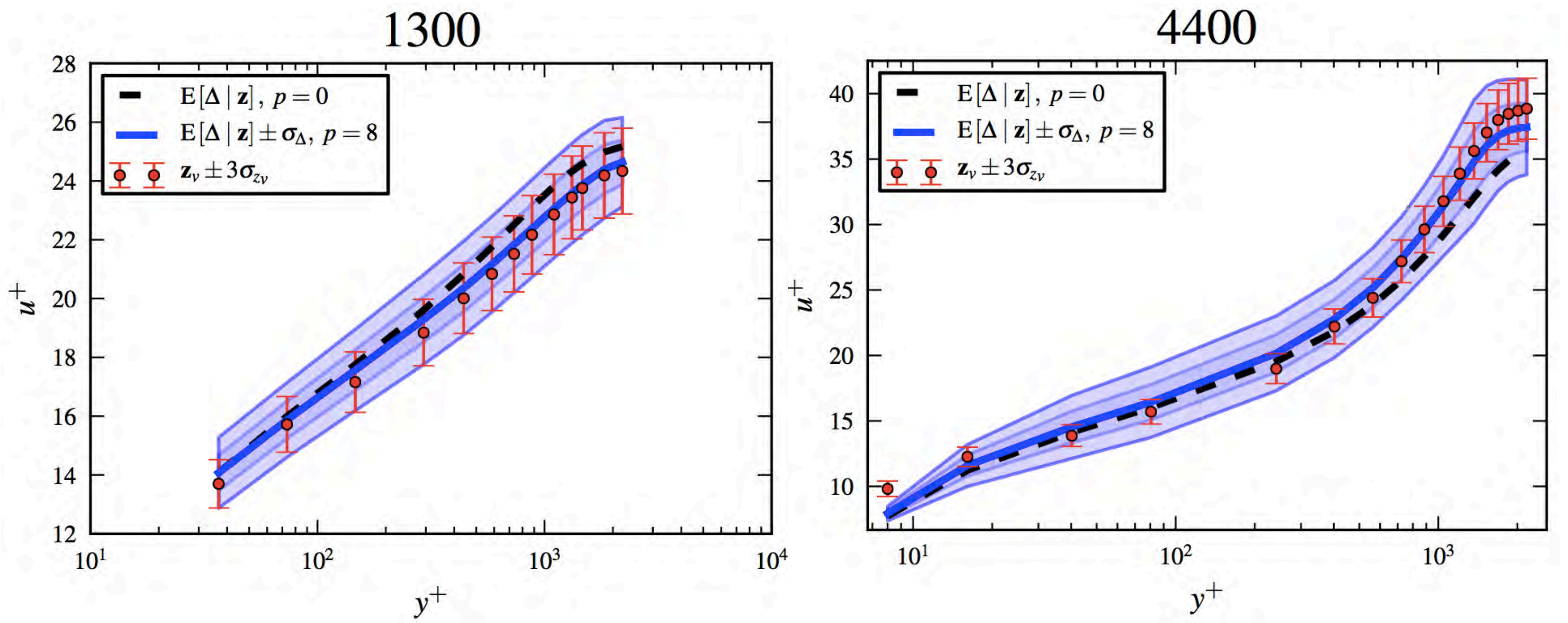
$$\mathbb{P}\left(\mathbf{S}_k\right) = \frac{\mathcal{E}_k^{-p}}{\sum_{k=1}^{K} \mathcal{E}_k^{-p}}, \quad \forall \mathbf{S}_k \in \mathcal{S}.$$





Bayesian scenario averaging – Posterior predictive distribution

$$p(\Delta|\mathbf{z}, \mathcal{M}, \mathcal{S}) = \dots$$



Conclusions

1. Capturing model inadequacy with K+O'Hagan-like terms lead to much too large prediction variance.
2. Large variability of closure coefficients seen.
3. No single coefficient values reproduce truth even for very limited classes of flow (and for any model!)
4. Capturing inadequacy within model makes more sense.
5. RANS-model error estimate proposed.

* Edeling, Cinnella, Dwight (2013). *Bayesian Estimates of Parameter Variability in the k-epsilon turbulence model*. Journal of Computational Physics. (online)

Thank you for your attention!