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# Uncertainty Quantification with model Error

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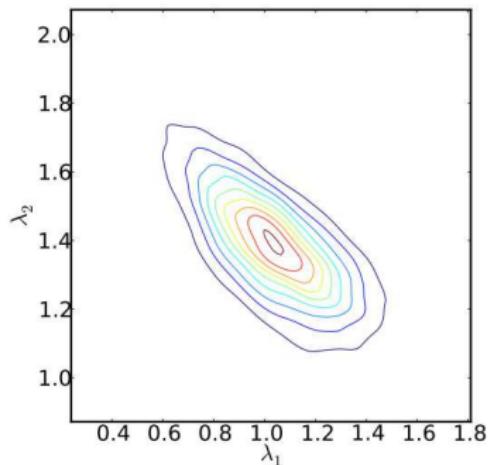
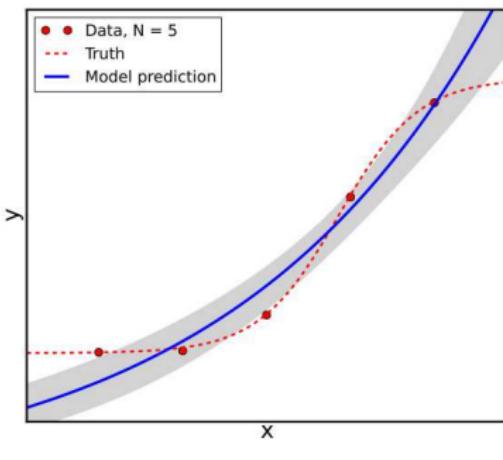
# Outline

- 1 Model Error
- 2 Introduction
- 3 Proposed Approach
- 4 Model-to-model Calibration – no data noise
- 5 Chemistry model calibration
- 6 Model calibration with noisy data
- 7 LES with model error
- 8 Closure

# Motivation

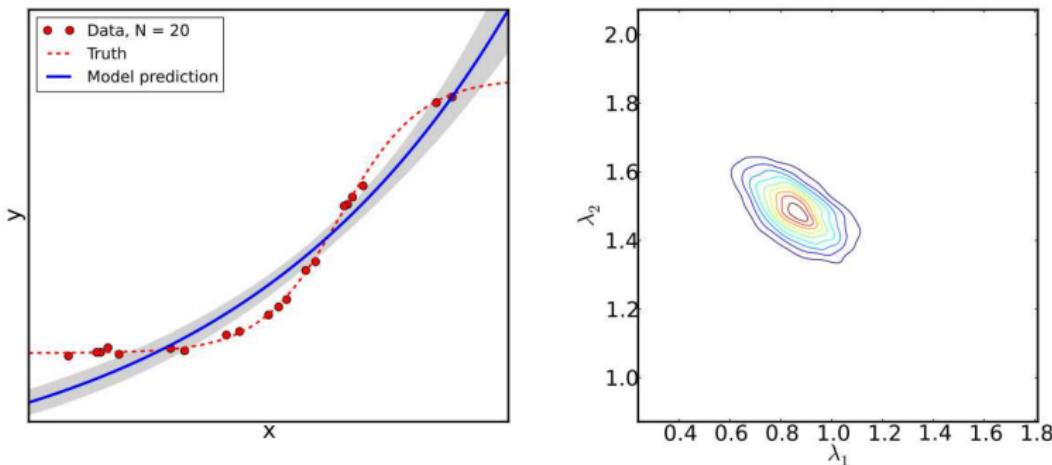
- All models are wrong in principle
- Models of physical systems rely on
  - Presumed theoretical framework
  - Mathematical formulation
- Practical models of complex physical systems rely on
  - Simplifying assumptions
  - Numerical discretization of governing equations
  - Computational software & hardware
- model error is frequently non-negligible
- Estimating model error is useful for
  - model comparison & validation
  - model improvement & scientific discovery
  - reliable computational predictions

# Challenges with Model Calibration due to Model Error



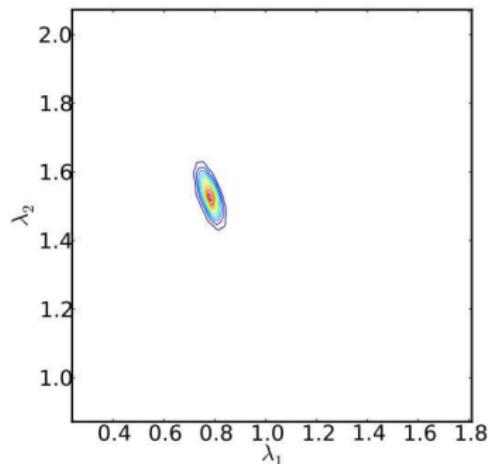
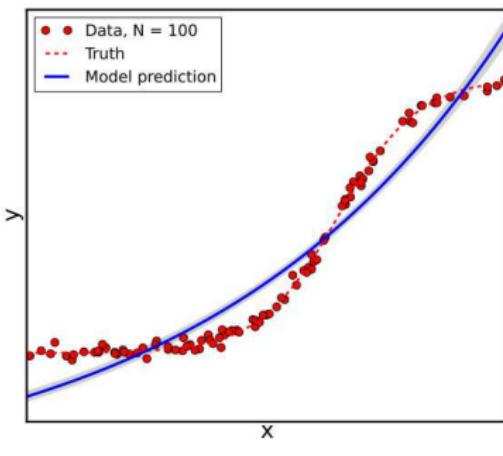
- Conventional parameter estimation context:  $y_{\text{data}} = f(x, \lambda) + \epsilon_d$
- Additional data results in reduced parameteric posterior uncertainty
- One gets more confident about predictions with the wrong model
- Predictive uncertainty in calibrated model has no utility for prediction
- Ignoring model error leads to irrelevant predictive errors

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# Statistical modeling of model error

## Error framework:

Measurements:  $y_{\text{data}} = y_{\text{truth}} + \epsilon_d$

Model predictions:  $y_{\text{truth}} = y_{\text{model}} + \epsilon_m$

Thus:  $y_{\text{data}} = y_{\text{model}} + \epsilon_m + \epsilon_d$

## Error modeling – example

Model:  $y_{\text{model}} = f(x, \lambda)$

Data Error:  $\epsilon_d \sim \mathbf{N}(0, \sigma^2)$

Model Error:  $\epsilon_m \sim \mathbf{GP}(\mu(x), C(x, x'))$

## Model calibration:

Estimate model parameters  $\lambda$  along with those of  $\epsilon_m, \epsilon_d$

Kennedy & O'Hagan 2001; Bayarri et al. 2002

# Challenges - Physical Models

- Arbitrary choice of statistical model (e.g. GP) spatial structure does not take the physical model into acct
  - Potential violation of implicit constraints in physical models
  - e.g. incompressible flow:  $\nabla \cdot v = 0$
- Difficulty in disambiguation of model & data error
- Calibration of model error on measured observable does not impact quality of other model predictions

# Key idea - Targeted model error embedding

- Embed model error in specific submodel phenomenology
  - a modified transport or constitutive law
  - a modified formulation for a material property
- Pros:
  - Allows placement of model error term in locations where key modeling assumptions and approximations are made
    - as a correction or high-order term
    - as a possible alternate phenomenology
  - explore if it can explain discrepancy on observable
  - naturally preserves model structure and associated constraints
- Cons:
  - complex likelihood  $p(y|\lambda)$  for general nonlinear  $f(x, \lambda, \epsilon_m)$

# Consider a simple no-data-noise setting

- Calibration of a (simple) model against a complex model
- Let the complex model be presumed to represent the truth
- In this context, the data has no noise
- Discrepancy between model and data is all due to model error

$$y_{\text{data}} = y_{\text{truth}} = y_{\text{complex\_model}} = y_{\text{model}} + \epsilon_m$$

- $\epsilon_m = y_{\text{data}} - y_{\text{model}}$  is a deterministic quantity
- The only information as to the quality of the calibrated uncertain model, e.g. via a posterior predictive check, is in a unique  $\epsilon_m$  for any  $x$

# model-to-model calibration

Model:  $y = f(x, \lambda, \phi(\epsilon_m))$

- Random variable  $\phi$  in augmented model components carries model error

Data:  $D = \{(x_i, y_{\text{data},i}), i = 1, \dots, N\}$

- Goal:
  - Establish  $\lambda, p(\phi)$  such that the likelihood of the data is high, based on the posterior predictive  $p(y|D)$
- This puts us in a density estimation framework for  $\phi$ :
  - The utility of additional data is to improve the specification of  $\lambda$ , and  $p(\phi)$

# Present Context

Embed  $\epsilon_m$  in  $\lambda$

- In other words:  $\lambda \leftarrow \lambda + \epsilon_m$
- Model:  $y = f(x, \lambda)$  with  $\lambda : \Omega \rightarrow \mathbb{R}^M$
- Density estimation problem for  $p(\lambda)$
- $\lambda$  : a random field  $\lambda(x, \omega)$ , or a random variable  $\lambda(\omega)$ 
  - focus on the latter
- Let the random variable  $\lambda$  be parameterized by  $\alpha$ 
  - For example, define  $\lambda$  as a polynomial chaos expansion

$$\lambda = \sum_{k=0}^P \alpha_k \Psi_k(\xi)$$

- Parameter estimation problem for  $\alpha = (\alpha_0, \dots, \alpha_P)$
- Bayesian setting
  - Prior  $\pi(\alpha)$
  - Likelihood  $L(\alpha) = p(D|\alpha)$

# Full Likelihood

$$L(\alpha) = p(D|\alpha) = \pi_f(y_{\text{data},1}, \dots, y_{\text{data},N}|\alpha)$$

where:

$\pi_f(\cdot|\alpha)$ :  **$N$ -variate density of the random variable  $(f_1, \dots, f_N)$**   
**with**  $f_i = f(x_i, \lambda(\xi; \alpha))$

**Problem:**  $\pi_f(\cdot)$  is degenerate in general when  $N > M$

- Consider a case with  $M = 1$ ,  $\lambda \sim N(\mu, \sigma^2)$ , and  $f = \lambda$
- Let  $N = 2$ , hence  $(f_1, f_2) = (\lambda, \lambda)$  for any  $\lambda$  sample
- With  $f_1 = f_2 = \lambda$ ,  $(f_1, f_2)$  are dependent and  $\pi_f(\cdot|\mu, \sigma)$  is non-zero only along the line  $f_2 = f_1$
- $\pi_f(y_{\text{data},1}, y_{\text{data},2}|\mu, \sigma)$  is non-zero only along the line  $y_{\text{data},2} = y_{\text{data},1}$   
 $\Rightarrow$  potentially can ameliorate singularity with a smoothing nugget

# Marginalized Likelihood

$$L(\alpha) = p(D|\alpha) = \prod_{i=1}^N \pi_{f_i}(y_{\text{data},i}|\alpha)$$

where

$\pi_{f_i}(\cdot, \alpha)$  is the univariate density of the RV  $f_i = f(x_i, \lambda(\alpha))$

Problem: the likelihood has multiple singularities corresponding to  $\alpha$  values leading to vanishing marginal variances at each  $x_i$

- Gaussian example: Let  $f_i \sim N(\mu_i(\alpha), \sigma_i(\alpha)^2)$ , then

$$L(\alpha) = \frac{1}{(2\pi)^{N/2}} \prod_{i=1}^N \frac{1}{\sigma_i(\alpha)} \exp\left(\frac{(\mu_i(\alpha) - y_{\text{data},i})^2}{2\sigma_i(\alpha)^2}\right)$$

- Multiple singularities,  $\sigma_i(\alpha) = 0, i = 1, \dots, N$
- Posterior maximization always finds one of these singularities, fitting one point perfectly, while misfitting the rest

⇒ can potentially be controlled via priors on  $\alpha$

# Approximate Bayesian Computation (ABC)

Employ a kernel density as a pseudo-likelihood to enforce select constraints:

Uncertain prediction  $p(y|D)$  is centered on the data

- With  $\mu_i(\alpha) = \mathbb{E}_\xi[f(x_i, \lambda(\xi; \alpha))]$ :

$$\text{minimize } \|\mu_i(\alpha) - y_{\text{data},i}\|$$

The width of the distribution  $p(y|D)$  is consistent with the spread of the data around the nominal model prediction

- With  $\sigma_i^2(\alpha) = \mathbb{V}_\xi[f(x_i, \lambda(\xi, \alpha))]$ :

$$\text{minimize } \|\sigma_i(\alpha) - \gamma |\mu_i(\alpha) - y_{\text{data},i}| \|$$

- $\gamma$  is a factor that specifies the desired match between  $\sigma_i$  and the discrepancy  $|\mu_i(\alpha) - y_{\text{data},i}|$ , on average

# ABC Likelihood

With  $\rho(\mathcal{S})$  being a metric of the statistic  $\mathcal{S}$ , use the kernel function as an ABC likelihood:

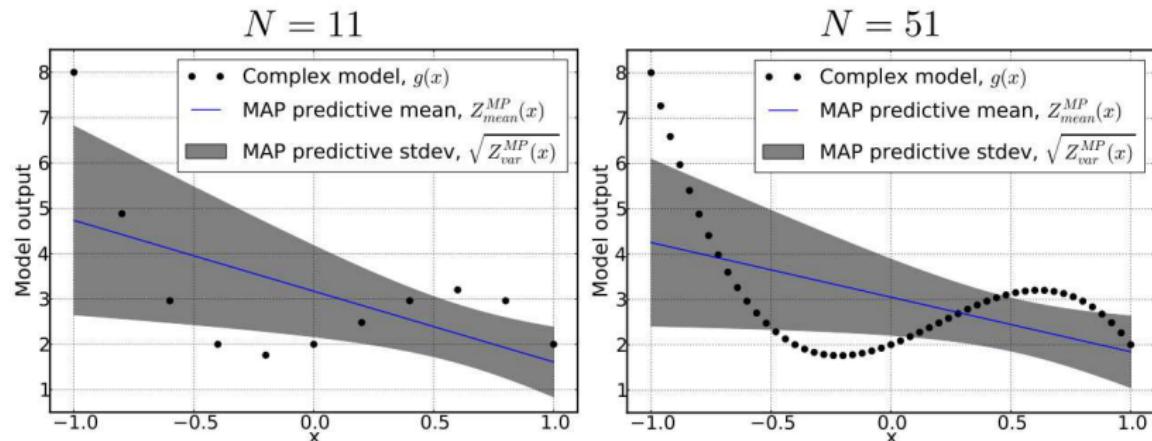
$$L_{\text{ABC}}(\alpha) = \frac{1}{\epsilon} K\left(\frac{\rho(\mathcal{S})}{\epsilon}\right)$$

where  $\epsilon$  controls the severity of the consistency control

Propose the Gaussian kernel density:

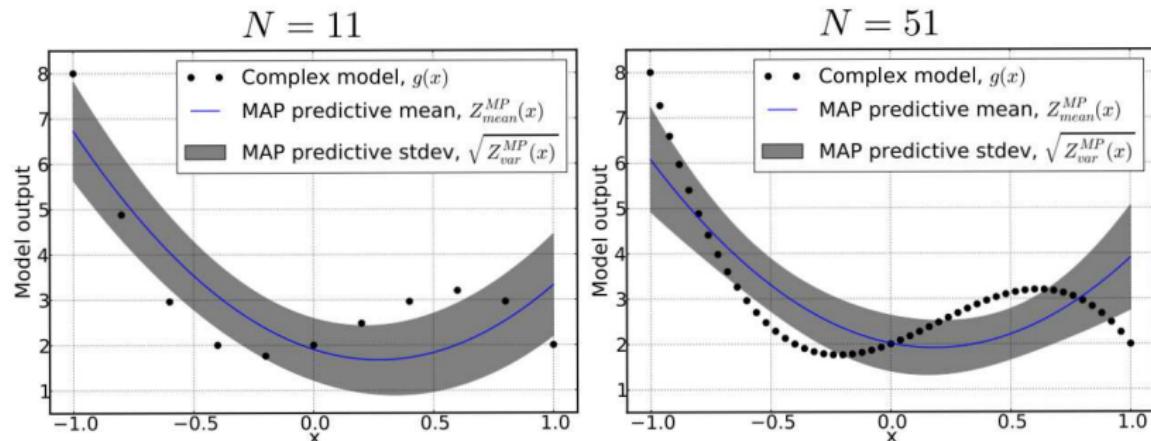
$$L_\epsilon(\alpha) = \frac{1}{\epsilon\sqrt{2\pi}} \prod_{i=1}^N \exp\left(-\frac{(\mu_i(\alpha) - y_{d,i})^2 + (\sigma_i(\alpha) - \gamma|\mu_i(\alpha) - y_{d,i}|)^2}{2\epsilon^2}\right)$$

## Test problem - Cubic data fit by a line - ABC



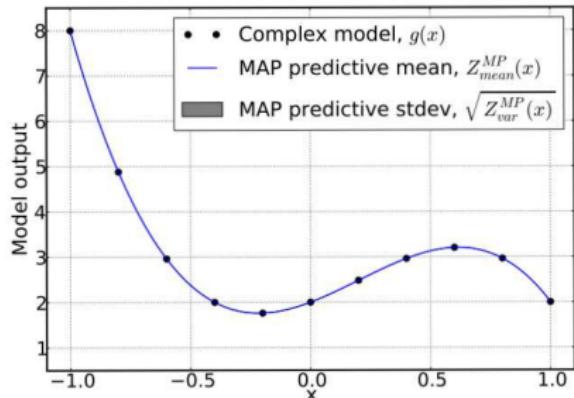
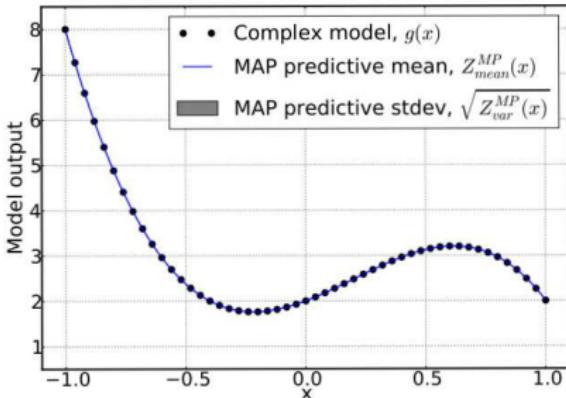
- MAP predictive (MP) mean centered on data
- MP standard deviation captures range of discrepancy
- Increasing number of data points has a small effect on both MP mean and stdev

# Test problem - Cubic data fit by a quadratic - ABC



- Quadratic has better fit to the data
- Smaller MP stdev consistent with smaller discrepancy

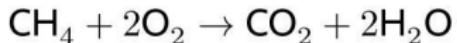
## Test problem - Cubic data fit by a cubic - ABC

 $N = 11$  $N = 51$ 

- Cubic has perfect fit to the data
- Negligible MP stdev consistent with negligible discrepancy

# Chemistry problem - ABC

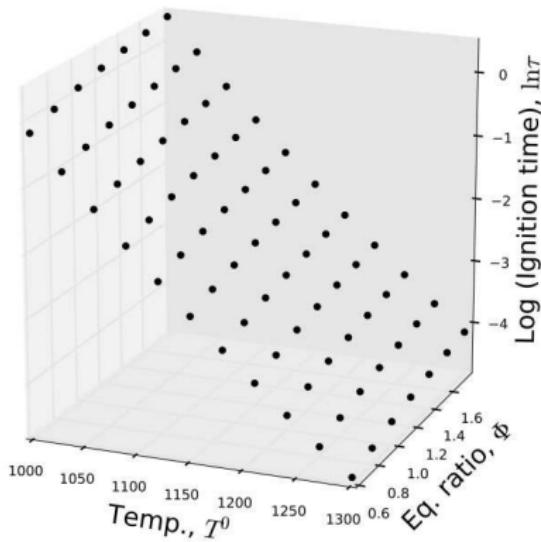
- Homogeneous ignition, methane-air mixture
- Single-step global reaction model calibrated against a detailed chemical kinetic model - ODE system
- Data: ignition time; range of initial  $T$  & equivalence ratio
- Single-step model:



$$\mathfrak{R} = [\text{CH}_4][\text{O}_2]k$$

$$k = A \exp(-E/R^\circ T)$$

$$\lambda = \begin{bmatrix} \ln A \\ E \end{bmatrix} = \sum_{k=0}^P \alpha_k \Psi_k(\xi)$$



# Constant Pressure Ignition – Problem Structure

- $N$  species,  $M$  reactions, rate parameter vector  $\lambda$
- State vector  $u = (X_1, \dots, X_N, T)$  – mole fractions, temperature
- ODE system

$$\begin{aligned}\frac{du_i(t; \lambda)}{dt} &= w_i(u; \lambda), \quad i = 1, \dots, N \\ u(0) &= u_0\end{aligned}$$

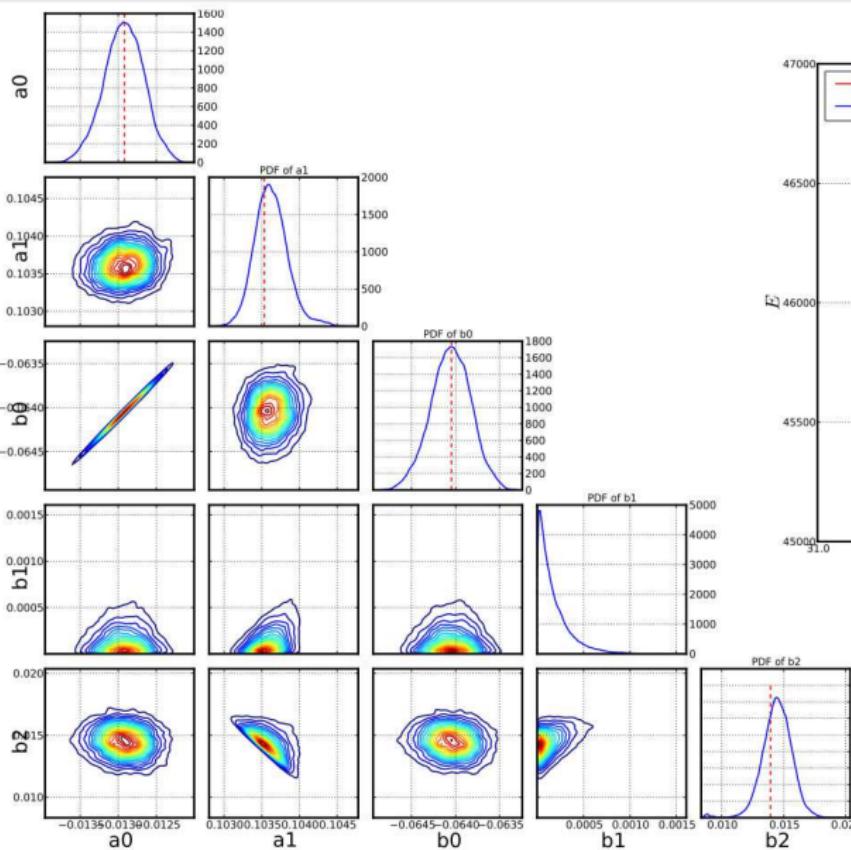
- Observable: ignition time  $\tau_{\text{ign}}(u_0, \lambda) = t \mid_{T(t; u_0, \lambda) = T_{\text{ign}}}$
- Challenge, for any proposed  $\lambda$ , computing  $\tau_{\text{ign}}(u_0, \lambda)$  is expensive
  - Large stiff ODE system for complex fuels
- Polynomial chaos formulation allows construction of a surrogate

$$\tau_{\text{ign}}(u_0, \lambda(\xi; \alpha)) = f(u_0, \xi; \alpha) = \sum_{k=0}^P f_k(u_0; \alpha) \Psi_k(\xi)$$

- Surrogate replaces the forward model in the Likelihood function

Posterior on  $\alpha$ 

-

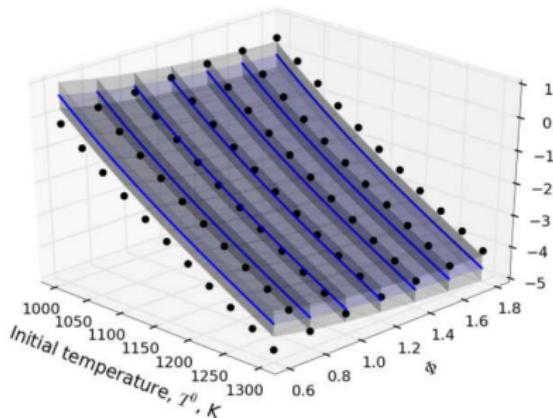
Posterior Predictive on  $(\ln A, E)$ 

# Quality of Uncertain Calibrated Model Predictions

Calibrated uncertain fit model  
is consistent with the  
detailed-model data.

Over the range of  $(T^0, \Phi)$ :

- MAP predictive mean ignition-time is centered on the data
- MAP predictive stdv is consistent with the scatter of the data



# Consider a noisy-data setting

- Calibration of a model  $y_m = f(x, \lambda)$  against noisy data
- Synthetic noisy data is generated from a “truth” model + Gaussian noise
- Discrepancy between fit model prediction and data is due to both model error & data noise

$$y = y_{\text{data}} = y_{\text{truth}} + \epsilon = f(x, \lambda) + \epsilon$$

- Modeling strategy:
  - Model  $\lambda$  as a random vector, represented with PC
  - Represent the noise similarly using PC
  - Estimate all PC coefficients using Bayesian inference

# Model Error formulation - noisy data

$$y = f(x, \lambda) + \epsilon$$

Let  $\epsilon \sim N(0, \sigma^2)$ . With  $N$  i.i.d. data points we have

$$y_i = f(x_i, \lambda) + \epsilon_i, \quad i = 1, \dots, N$$

For Hermite-Gaussian PC:

$$\begin{aligned}\lambda &= \sum_{k=0}^P \alpha_k \Psi_k(\xi_1, \dots, \xi_d), \quad \alpha \equiv (\alpha_0, \dots, \alpha_P) \\ f(x, \lambda) &= \sum_{k=0}^P f_k(x, \alpha) \Psi_k(\xi_1, \dots, \xi_d) \\ y_i &= \sum_{k=0}^P f_k(x_i, \alpha) \Psi_k(\xi_1, \dots, \xi_d) + \sigma \xi_{d+i}\end{aligned}$$

Augmented PC germ  $\xi = (\underbrace{\xi_1, \dots, \xi_d}_{\epsilon_m}, \underbrace{\xi_{d+1}, \dots, \xi_{d+N}}_{\epsilon_d})$

# Model Error Estimation - noisy data

Inverse problem:

- Given:
  - data:

$$D = \{(x_i, y_i)\}_{i=1}^N$$

- data model:

$$y_i = \underbrace{\sum_k f_k(x_i, \alpha) \Psi_k(\xi_1, \dots, \xi_d)}_{y_{\text{model}}(\epsilon_m)} + \underbrace{\sigma \xi_{d+i}}_{\epsilon_d}, \quad i = 1, \dots, N$$

- Estimate parameters  $(\alpha, \sigma)$

Bayesian context:

- posterior:  $p(\alpha, \sigma | D)$
- options: Full Bayesian likelihood; Marginalized; ABC
- All are viable here in principle, as the data noise introduces regularity
- We illustrate the case with a Marginalized Gaussian approximation

# Calibrated Uncertain Model Posterior Predictive

- Calibrated data model:  $y_i = f(x_i; \lambda(\xi; \alpha)) + \sigma \xi_{d+i}$
- Full posterior on  $\alpha, \sigma$ :  $\alpha, \sigma \sim p(\alpha, \sigma | D)$
- Marginal posteriors:  $\alpha \sim p(\alpha | D), \sigma \sim p(\sigma | D)$
- Posterior Predictive (PP):

$$p(y|D) = \int p(y|\alpha, \sigma)p(\alpha, \sigma|D)d\alpha d\sigma = \mathbb{E}_{\alpha, \sigma}[p(y|\alpha, \sigma)]$$

- PP Mean :

$$\mathbb{E}_{\text{PP}}[y] = \mathbb{E}_{\alpha}[\mathbb{E}_{\xi}[f]]$$

- PP Variance:

$$\mathbb{V}_{\text{PP}}[y] = \underbrace{\mathbb{E}_{\alpha}[\mathbb{V}_{\xi}[f]]}_{\text{model error}} + \underbrace{\mathbb{E}_{\sigma}[\sigma^2]}_{\text{data noise}} + \mathbb{V}_{\alpha}[\mathbb{E}_{\xi}[f]]$$

# Calibrated Uncertain Model Predictions

- Calibrated model:  $y = f(x; \lambda(\xi; \alpha))$
- Marginal posterior on  $\alpha$ :  $\alpha \sim p(\alpha|D)$
- Pushed forward posterior (PFP):

$$p(f|D) = \int p(f|\alpha)p(\alpha|D)d\alpha = \mathbb{E}_\alpha[p(f|\alpha)]$$

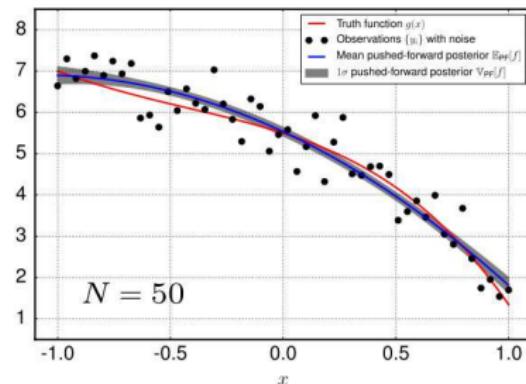
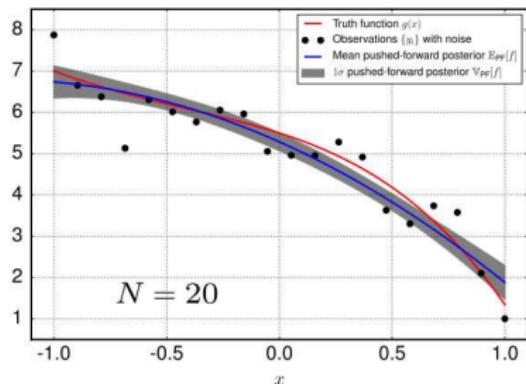
- PFP Mean:

$$\mathbb{E}_{\text{PFP}}[f] = \mathbb{E}_\alpha[\mathbb{E}_\xi[f]]$$

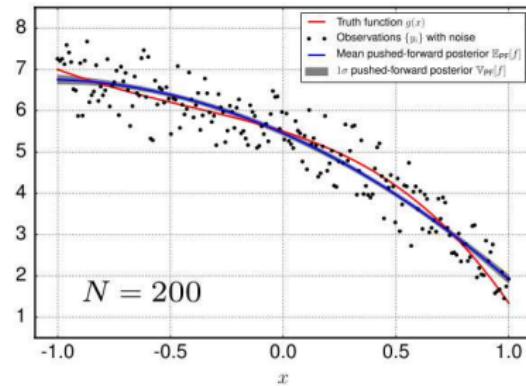
- PFP Variance:

$$\mathbb{V}_{\text{PFP}}[f] = \underbrace{\mathbb{E}_\alpha[\mathbb{V}_\xi[f]]}_{\text{model error}} + \underbrace{\mathbb{V}_\alpha[\mathbb{E}_\xi[f]]}_{\text{data noise}}$$

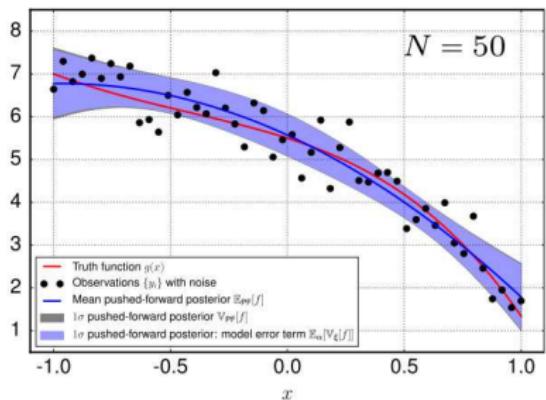
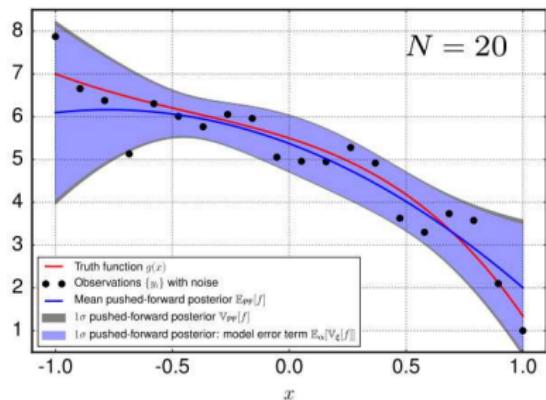
# Quadratic-fit - Classical Bayesian likelihood



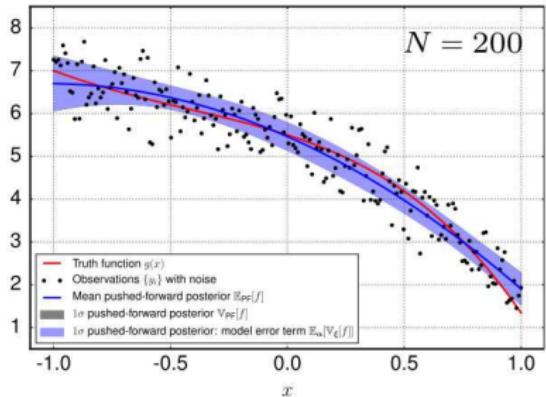
- With additional data, predictive uncertainty around the wrong model is indefinitely reducible
- Predictive uncertainty not indicative of discrepancy from truth



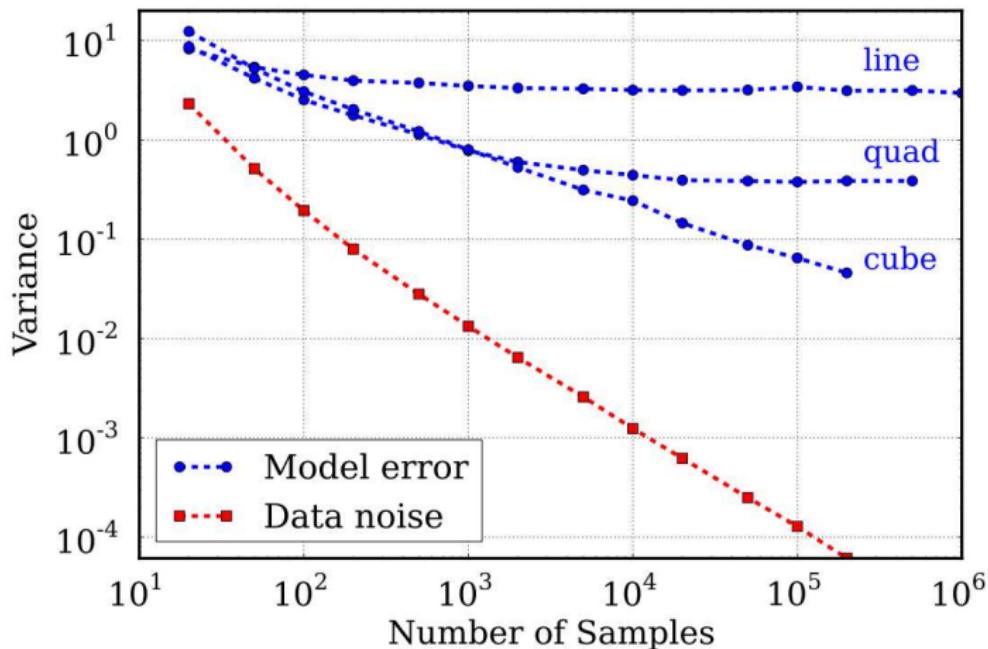
# Quadratic-fit - ModErr - MargGauss



- With additional data, predictive uncertainty due to data noise is reducible
- Predictive uncertainty due to model error is not reducible



# Model Error - Fit with Different Models



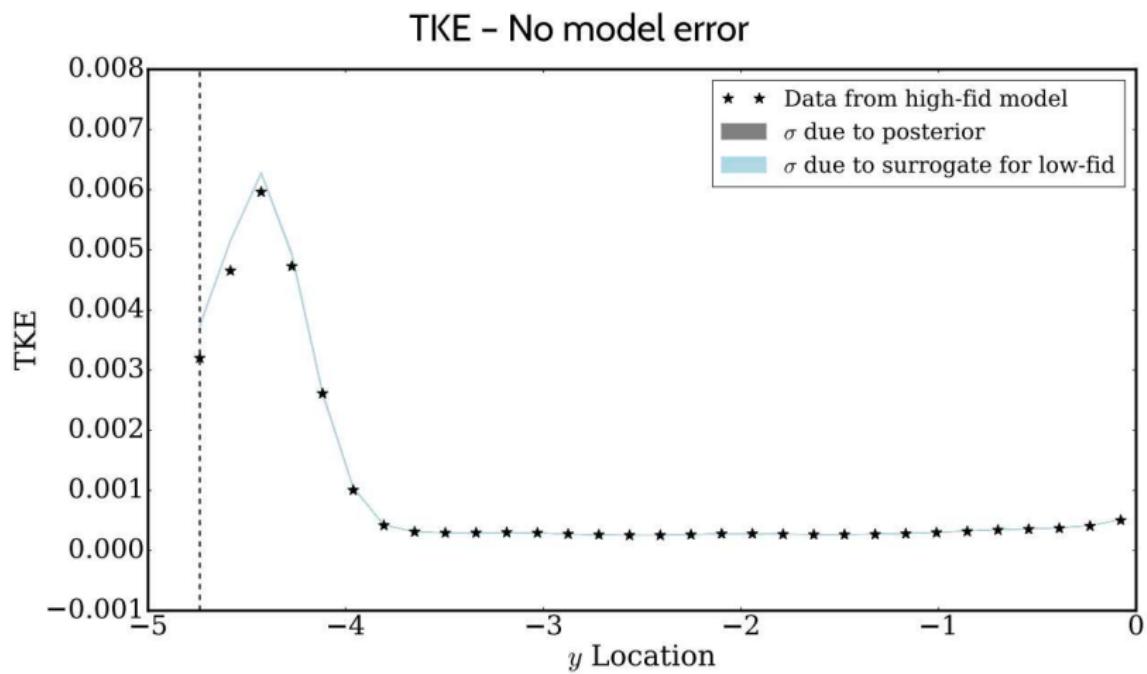
# LES subgrid static-vs-dynamic – Jet-in-crossflow

- Large Eddy Simulation (LES) subgrid model fidelity
  - Dynamic: subgrid parameters variable in space/time,  $g_i$
  - Static : subgrid parameters constant in space/time,  $f_i(\lambda)$
- Target: Calibrate a static model against a dynamic model
  - Fit parameters  $\lambda = (C_R, Pr_t^{-1}, Sc_t^{-1})$  of static model  $f(\lambda)$  to data from dynamic model simulations, accounting for model error
- Static model surrogate construction using  $4^3 = 64$  simulations of  $f(\lambda)$ 
  - Legendre polynomial expansion surrogate of 3-rd order
    - Account for surrogate error: *i.i.d.* zero-bias Gaussian noise
  - Global sensitivity analysis: impact of  $C_R \gg$  impact of  $Pr_t^{-1}$  and  $Sc_t^{-1}$ 
    - Selected only  $C_R$  for model error embedding

$$\mathbb{V}_{\text{PFP}}[f] = \underbrace{\mathbb{E}_\alpha[\mathbb{V}_\xi[f]]}_{\text{model error}} + \underbrace{\mathbb{V}_\alpha[\mathbb{E}_\xi[f]]}_{\alpha \text{ posterior}} + \underbrace{\mathbb{E}_{\sigma_S}[\sigma_S^2]}_{\text{surrogate error}}$$

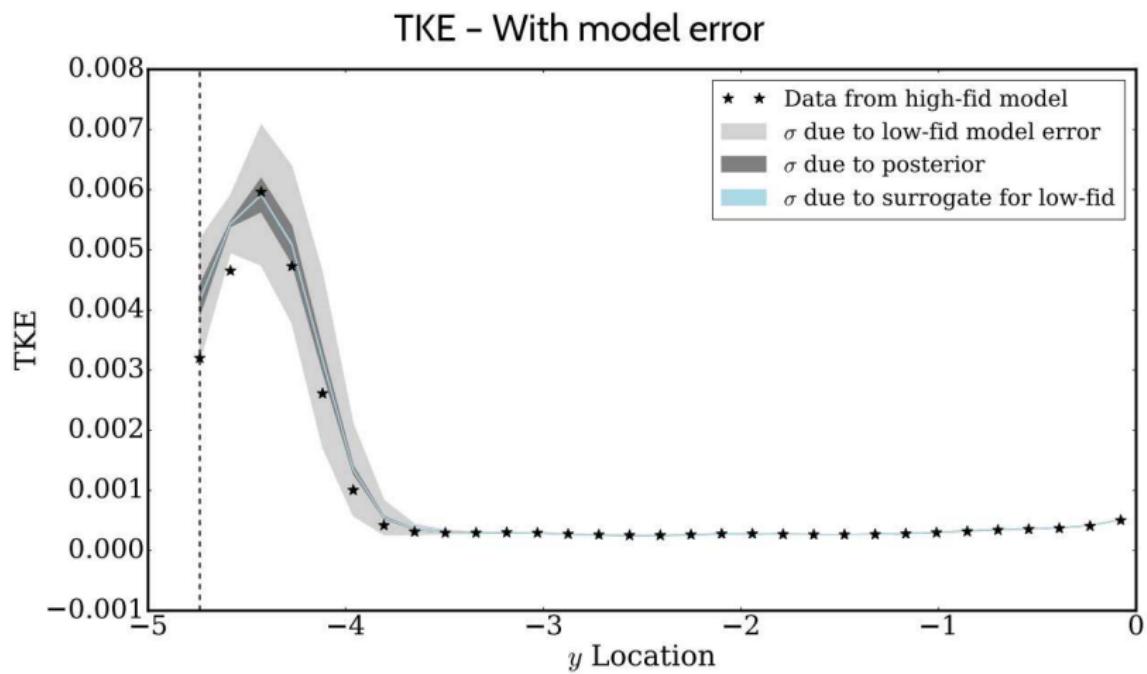
# Calibrate with TKE data; Predict both TKE and Pressure

Pushed forward posterior



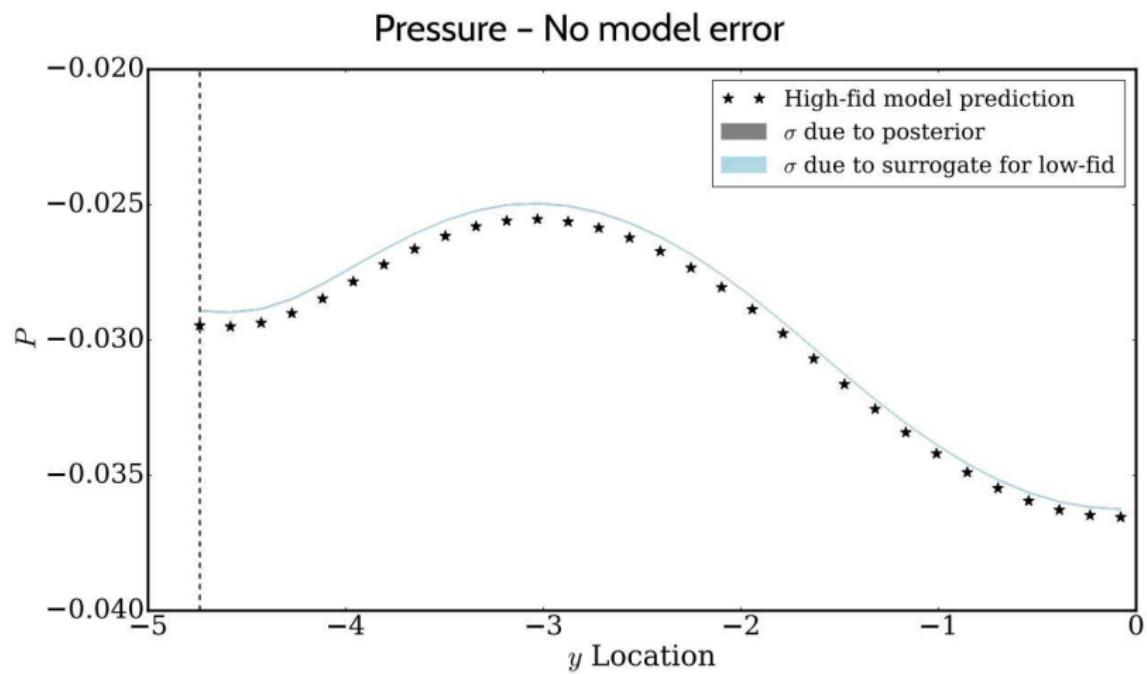
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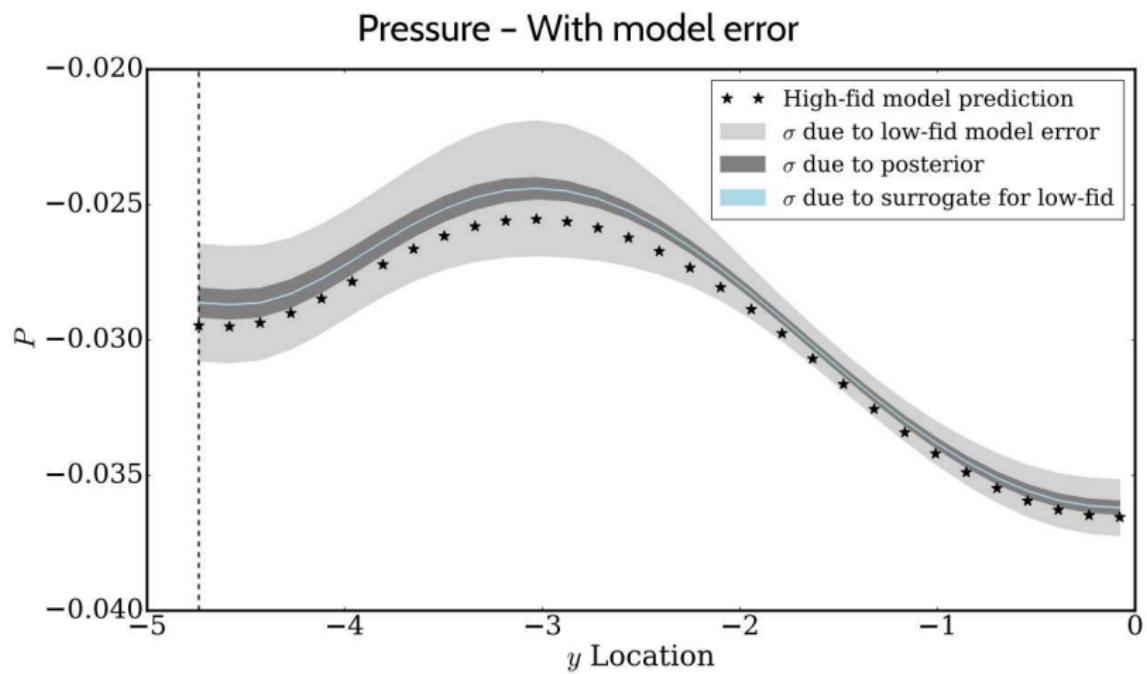
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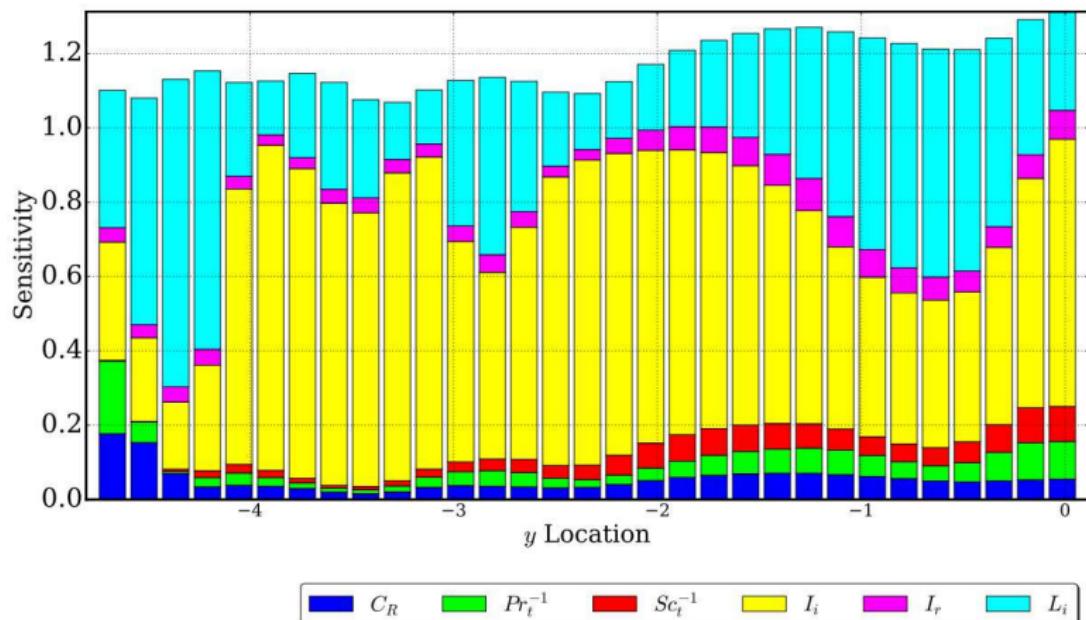
Pushed forward posterior



# LES subgrid 2D-vs-3D - Jet-in-crossflow

- Target: Calibrate a 2D LES model against a 3D model
  - Fit parameters  $\lambda = (C_R, Pr_t^{-1}, Sc_t^{-1}, I_i, I_r, L_i)$  of 2D model to data from 3D model simulations, accounting for model error
  - Parameters:
    - $C_R$  : Smagorinsky constant
    - $Pr_t$  : Turbulent Prandtl number
    - $Sc_t$  : Turbulent Schmidt number
    - $I_i$  : Turb. intensity (inflow air) horizontal component
    - $I_r$  : Turb. intensity (inflow air) ratio: vertical/horizontal
    - $L_i$  : Length scale of most energetic eddies
- 2D model surrogate construction
  - Account for surrogate error: *i.i.d.* zero-bias Gaussian noise
  - Global sensitivity analysis
    - Selected one parameter ( $I_i$ ) for model error embedding
  - Calibrate 2D model with observable: Mach no.  $M(y)$  at a given  $x$ -location
  - Predict both  $M(y)$  and pressure  $P(y)$ , and compare to 3D model

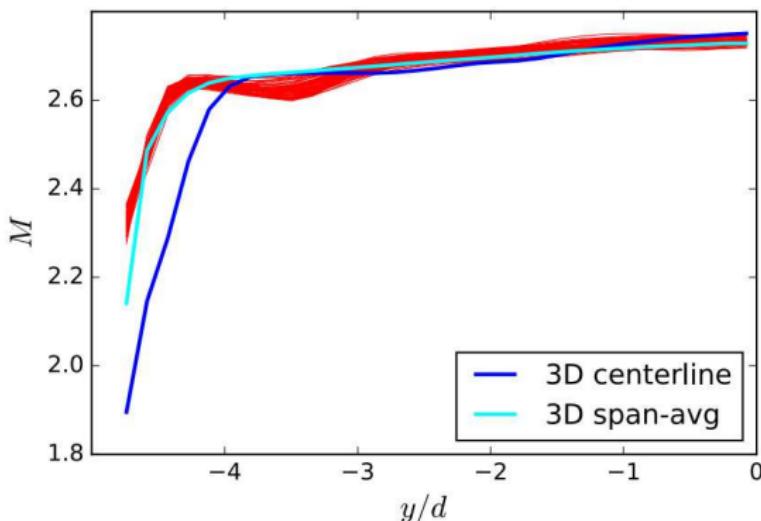
# Global Sensitivity Analysis Results



Dominant parameter is  $I_i$ : employ it to embed model error

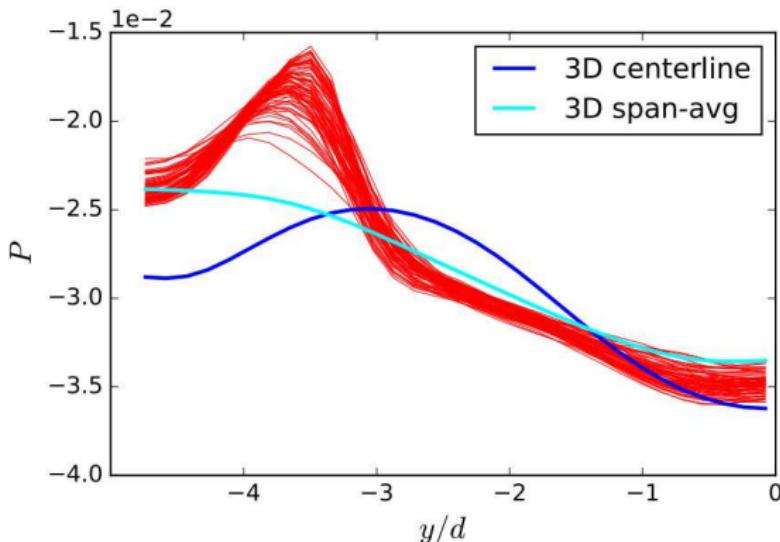
# Model Error - Case study: 2D-vs-3D

- Problem Focus: P1 Jet in Crossflow problem
  - static SGS constants,  $d/8$  grid resolution
- Calibrate a 2D model using 3D benchmark simulations as data
- Quantify the model error associated with 2D treatment
- Red curves show ensemble of 2D runs over  $\lambda$ -range
- 3D QoI selection for 2D comparison: (a) centerline, (b) spanwise average



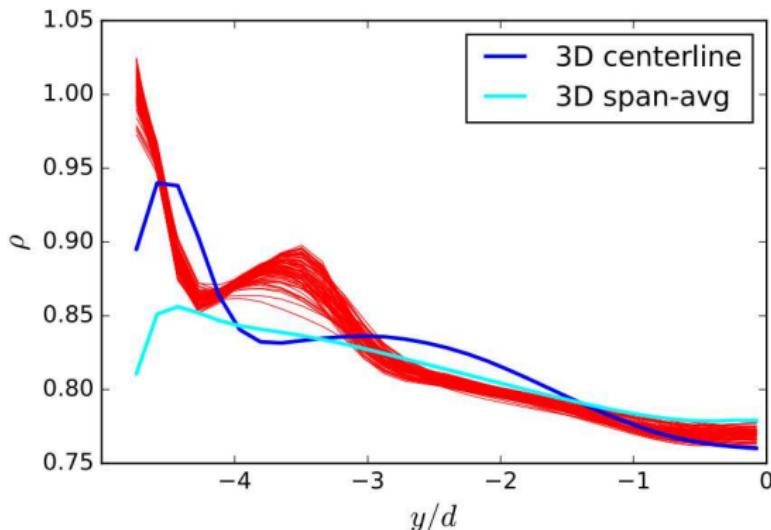
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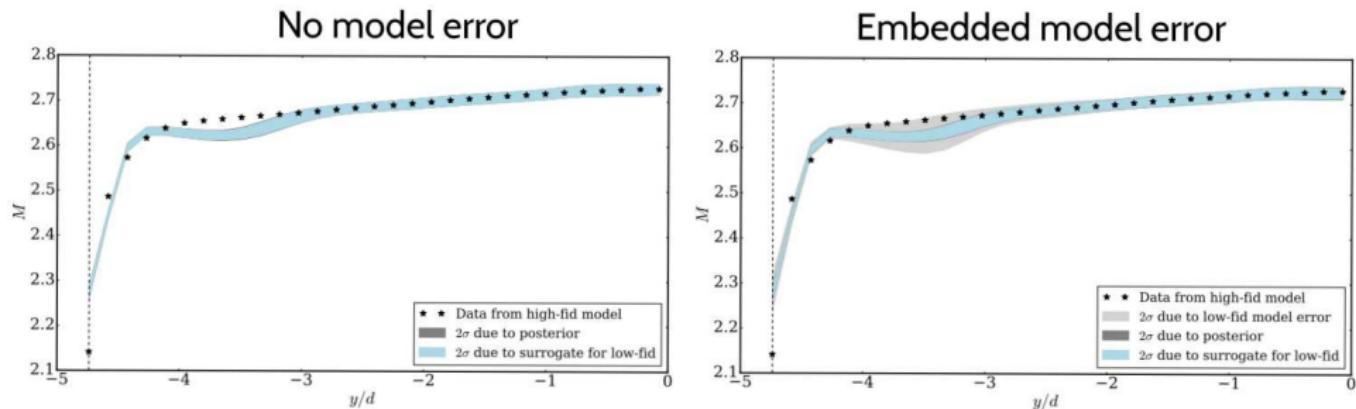
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# Model Error - Mach Number spanwise-average

- Model error contribution captures the discrepancy

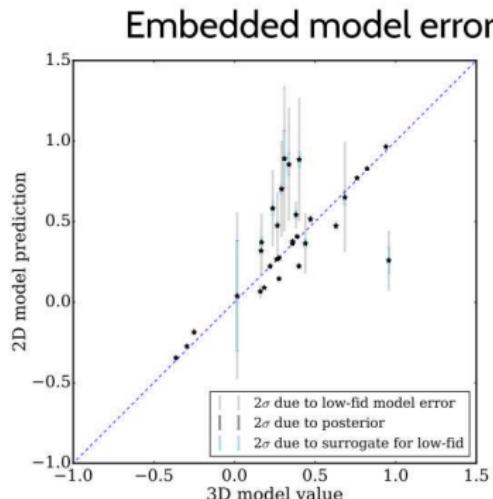
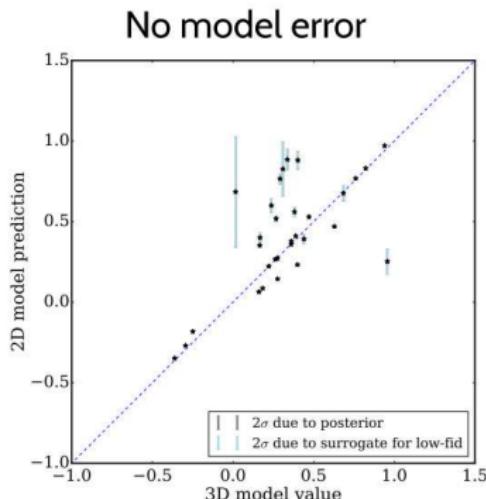


$$\sigma_i^2 = \underbrace{\mathbb{E}_{\tilde{\lambda}} \left[ \sigma_i^2(\tilde{\lambda}) \right]}_{\text{Model error}} + \underbrace{\mathbb{V}_{\tilde{\lambda}} \left[ \mu_i(\tilde{\lambda}) \right]}_{\text{Posterior uncertainty}} + \underbrace{(\sigma_i^{LOO})^2}_{\text{Surrogate error}}$$



# Model Error - Select Qols

- Model error contribution captures the discrepancy for averaged quantities across a wide range of observables



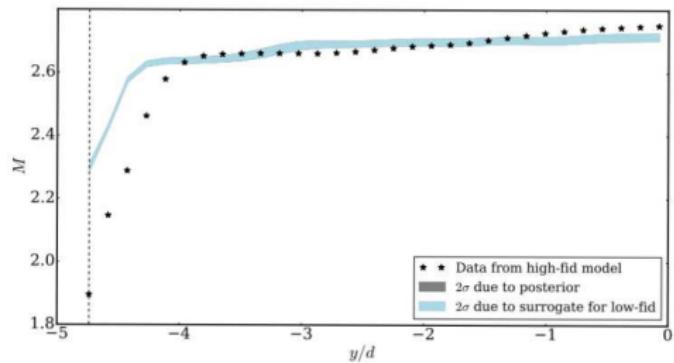
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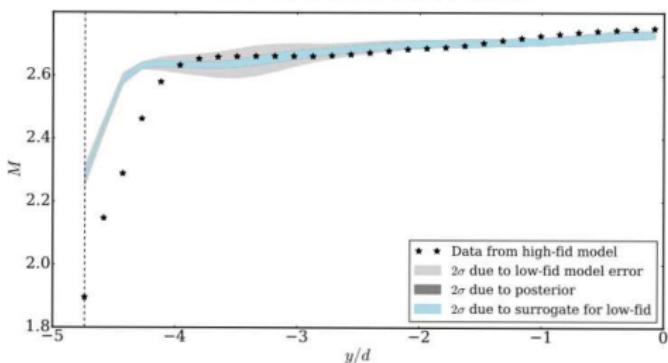
# Model Error - Mach Number centerline

- Model error contribution extends as much as prior allows

No model error



Embedded model error



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# Closure

- Presented a strategy for dealing with model error
  - targeted at physical models
- Density estimation framework -  $y = f(x; \lambda(\xi; \alpha))$
- Uncertain predictions with the calibrated model include uncertainty due to both model-error and data-noise
- Results suggest disambiguation of the two components
- Demonstrations in chemical ignition and LES of jet-in-crossflow
  - Including accounting for PC surrogate error
- Limitation of model-error embedding: when no variation of the chosen parameter in the simple model could reproduce results of the detailed model
  - Expand parameter prior range(s)
  - Consider other parameters
  - Propose a modification in the model