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Bayesian Model Calibration with an Embedded Statistical Characterization of Model Error

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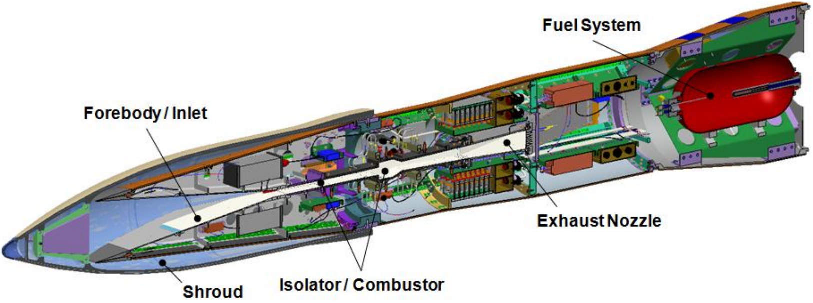
Motivation

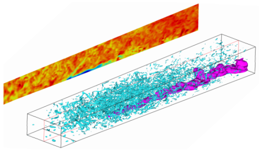


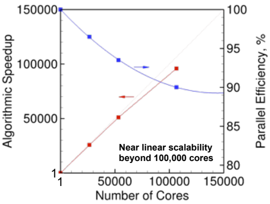
Design of scramjet engine involves many expensive flow simulations for

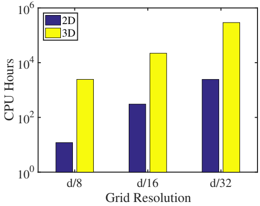
- uncertainty quantification (UQ)
- design optimization

Reactive turbulent flow

We use **RAPTOR**, a LES solver by Oefelein *et al.* at Sandia [Oefelein 06]







Highly-scalable but still **very expensive** for 3D high-resolution grids

"Model variants" trade off between solution accuracy and cost:

- Different grid resolutions
- Emulation using 2D geometry
- Modeling of near-wall properties
- ...

To use results from different models, need to **capture the error due to their model structure and assumptions**

Overview

Objective: capture uncertainty due to model error resulting from using lower-fidelity models

Plan: represent the model error stochastically, by embedding a discrepancy term in the low-fidelity model parameters in a non-intrusive manner

Traditional "external" representation of model error

Traditional additive form: [Kennedy & O'Hagan 01]

$$q_k = f_k(\lambda) + \delta_k + \epsilon_{d_k} \qquad \text{for } k\text{th QoI}$$

- Applies corrections on model output
- Flexible for fitting model error

- δ_k not transferable for prediction of QoIs outside calibration set
- Push-forward predictions generally no longer satisfy governing equations
- Difficult to distinguish uncertainty contributions between model error and measurement noise

Embedded model error representation

Embedded approach: [Sargsyan *et al.* 15]

$$q_k = f_k(\lambda + \delta_k) + \epsilon_{d_k}$$

$\Rightarrow$ physically-meaningful predictions that auto-satisfy governing equations

$\Rightarrow$ safer extrapolations of δ_k to other QoIs (to other k) since they all involve corrections on the same input parameter λ

Represent the discrepancy term δ in a stochastic manner:

$$\lambda + \delta(\alpha, \xi)$$

- α–calibration parameters for discrepancy term δ
- ξ–aleatoric source (representing model error)
- $\tilde{\alpha} \equiv (\lambda, \alpha)$–all parameters to be calibrated

$f_k(\lambda + \delta(\alpha, \xi))$ is now a **stochastic** model

Representing discrepancy via polynomial chaos expansion

Polynomial chaos expansion (PCE) in a nutshell:

an expansion for random variable:

$$\theta(\xi) = \sum_{\beta \in \mathcal{J}} c_\beta \Psi_\beta(\xi)$$

- c_β: PCE coefficients
- ξ: "germ" random vector (e.g., uniform, Gaussian)
- Ψ_β: multivariate orthonormal polynomial (e.g., Legendre, Hermite)
- β: multi-index, reflects order of polynomial basis

Embedded model becomes:

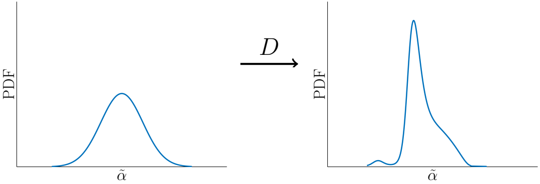
$$f_k\left(\lambda + \delta(\alpha, \xi)\right) = f_k\left(\lambda + \sum_{\beta \neq 0} \alpha_\beta \Psi_\beta(\xi)\right)$$

PCE convenient for uncertainty propagation and moment estimation

Bayesian calibration of model error

Calibrate model by performing statistical inference for $\tilde{\alpha} \equiv (\lambda, \alpha)$ via

Bayesian inference: $$\underbrace{p(\tilde{\alpha}|D)}_{posterior} \propto \underbrace{p(D|\tilde{\alpha})}_{likelihood} \underbrace{p(\tilde{\alpha})}_{prior}$$



Calibration data D from higher-fidelity model simulations
$\Rightarrow$ capturing discrepancy between **low- and high-fidelity models**

Posterior explored via **Markov chain Monte Carlo (MCMC)**

- adaptive Metropolis [Haario 01]
- efficient Gaussian proposal constructed from chain samples

MCMC requires likelihood evaluations $p(D|\tilde{\alpha})$, but no analytical form

True likelihood is intractable

Gauss-marginal approximation to likelihood:

$$p(D|\tilde{\alpha}) \approx \frac{1}{(2\pi)^{\frac{N}{2}}} \prod_{k=1}^{N} \frac{1}{\sigma_k(\tilde{\alpha})} \exp\left[-\frac{(\mu_k(\tilde{\alpha}) - D_k)^2}{2\sigma_k^2(\tilde{\alpha})}\right]$$

$\mu_k(\tilde{\alpha})$, $\sigma_k^2(\tilde{\alpha})$: mean and variance of $f_k(\lambda + \delta(\alpha, \xi))$ given $\tilde{\alpha}$

Estimate them by constructing PCE (e.g., using NISP)

$$f_k(\lambda + \delta(\alpha, \xi)) = f_k\left(\lambda + \sum_{\beta \neq 0} \alpha_\beta \Psi_\beta(\xi)\right) \approx \sum_{\beta} f_{k,\beta}(\tilde{\alpha})\Psi_\beta(\xi)$$

and so $\mu_k(\tilde{\alpha}) \approx f_{k,0}(\tilde{\alpha})$ and $\sigma_k^2(\tilde{\alpha}) \approx \sum_{\beta \neq 0} f_{k,\beta}^2(\tilde{\alpha})$

Surrogate acceleration for tractable likelihood

A PCE needs to be constructed at every $\tilde{\alpha}$ encountered in the MCMC, can be expensive using f_k

To accelerate PCE construction, pre-build surrogate for f_k (e.g., regression)

$$f_k(\cdot) \approx \hat{f}_k(\cdot) + \epsilon_{k,\mathrm{LOO}}$$

$\epsilon_{k,\mathrm{LOO}} \sim \mathcal{N}(0, \sigma^2_{k,\mathrm{LOO}})$ models the discrepancy between $\hat{f}_k$ and f_k, $\sigma^2_{k,\mathrm{LOO}}$ approximated from leave-one-out cross validation

Attribution of total predictive variance

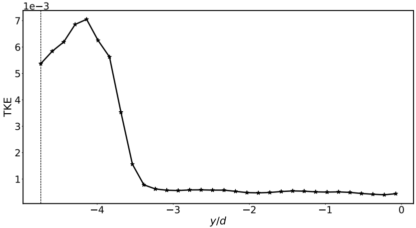
A nice result: **attribute total predictive variance** to different sources

$$\mathrm{Var}\left[q_k\right] = \underbrace{\mathbb{E}_{\tilde{\alpha}}\left[\sigma_k^2(\tilde{\alpha})\right]}_{\text{model error}} + \underbrace{\mathrm{Var}_{\tilde{\alpha}}\left[\mu_k(\tilde{\alpha})\right]}_{\text{posterior uncertainty}} + \underbrace{\sigma_{k,\mathrm{LOO}}^2}_{\text{surrogate error}} + \underbrace{\sigma_{d_k}^2}_{\text{data noise}}$$

Dynamic-vs-Static Smagorinsky turbulence model

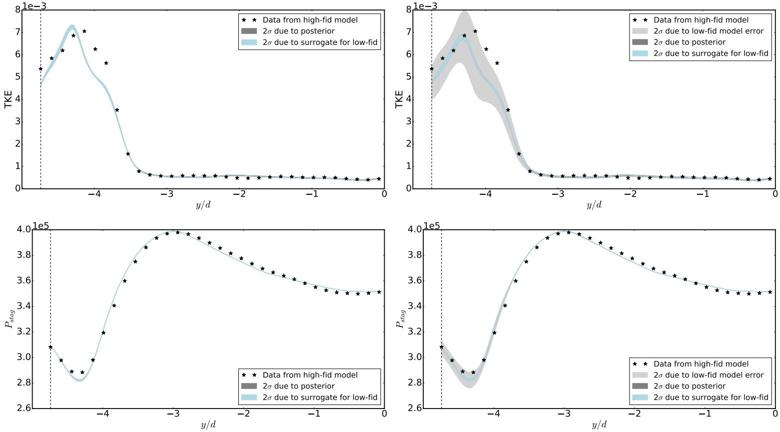
Calibrate static Smagorinsky model with dynamic simulations

- 3D geometry
- Combustion turned off for initial demonstration
- Calibrate using TKE y-profile (t-averaged, at fixed x, centerline z)



- Embed in parameter $\lambda = C_R$
  - 1st-order expansion for $\delta = \alpha\xi$ (i.e., Gaussian)
- Surrogates: 500 regression points, 3rd-order PCEs

Dynamic-vs-Static Smagorinsky turbulence model

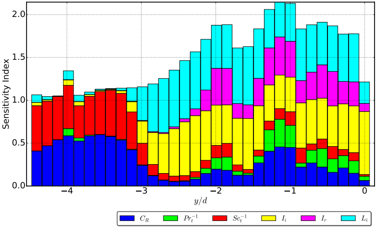


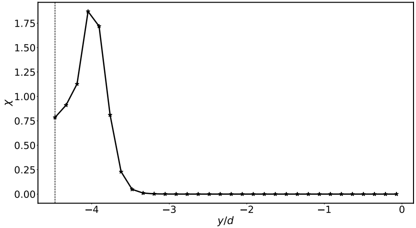
No model error treatment | Embedded model error treatment

2D-vs-3D: choice of embedding parameters

Calibrate 2D model using 3D model simulations

- Calibrate using χ profile
- $\lambda = (C_R, Pr_t^{-1}, Sc_t^{-1}, I_i, I_r, L_i)$
- We do not want to embed δ for all λ, too many terms
  - Embed δ in select parameters
  - Target parameters where embedding is most "effective"
    - Global sensitivity analysis on calibration QoIs
    - Bayesian model selection (evidence computation)





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Embed Param	GSA $\bar{S}_{T_i}$	Log-evidence
$\mathbf{C_R}$	$\mathbf{5.24 \times 10^{-1}}$	$\mathbf{2.82 \times 10^{2}}$
Pr_t^{-1}	1.58×10^{-2}	-2.55×10^{3}
$\mathbf{Sc_t^{-1}}$	$\mathbf{4.90 \times 10^{-1}}$	$\mathbf{2.30 \times 10^{2}}$
I_i	3.63×10^{-2}	-9.68×10^{2}
I_r	2.24×10^{-3}	-3.74×10^{3}
L_i	5.32×10^{-2}	-4.15×10^{2}
C_R, Sc_t^{-1}		2.79×10^{2}

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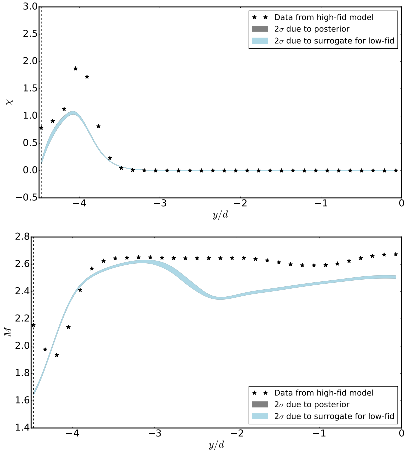
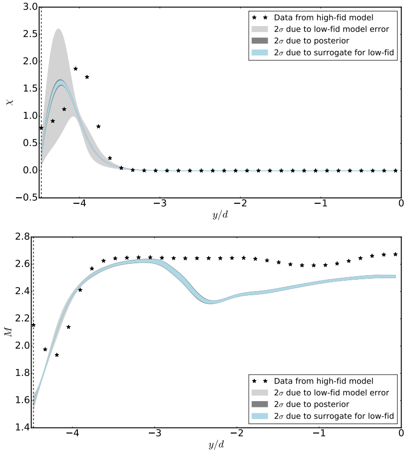
$\Rightarrow$ embed in C_R and Sc_t^{-1}, employ triangular multivariate PCE form

$$(\lambda + \delta(\alpha, \xi)) = \begin{cases} C_R + \alpha_{(1)}\xi_1 \\ Pr_t^{-1} \\ Sc_t^{-1} + \alpha_{(1,0)}\xi_1 + \alpha_{(0,1)}\xi_2 \\ I_i \\ I_r \\ L_i \end{cases}$$

2D-vs-3D: predictive quantities



No model error treatment



Embedded model error treatment

Conclusions

Conclusions:

- Introduced a framework for characterizing uncertainty from model error
  - embed discrepancy in model parameters; non-intrusive
  - predictions automatically satisfy governing equations
- Attributed total predictive variance to different contributing sources
- Demonstrated method in a non-reactive demonstration unit problem in scramjet design involving expensive LES:
  - Static vs. dynamic Smagorinsky turbulence treatments
  - 2D vs. 3D geometry
- Illustrated good capturing of model-to-model discrepancy, and also limitations when models are too different

Future work:

- Bayesian model selection for optimal model error embedding
- More sophisticated forms of embedding
- Combine with multifidelity and multilevel methods

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