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Quantifying Uncertainty from Model Error in Turbulent Combustion Applications

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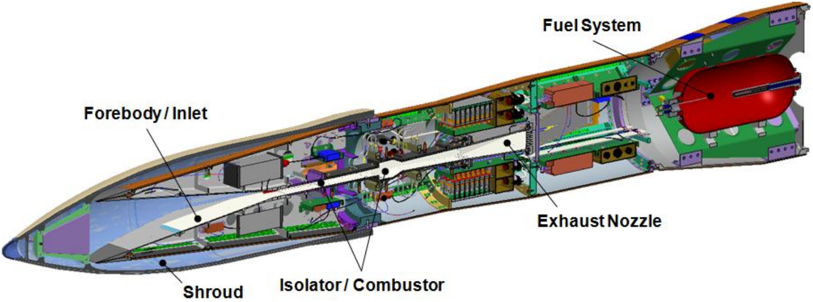
HIFiRE-II Scramjet

Development of scramjet[2] engine involves

- flow simulations
- uncertainty quantification (UQ)
- design optimization

We focus on the HIFiRE-II[3] configuration:



[2] supersonic combustion ramjet

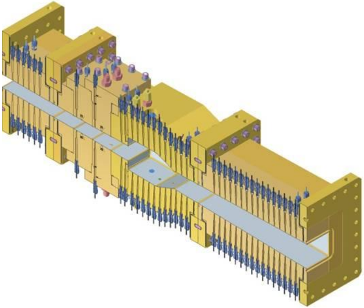
[3] Hypersonic International Flight Research and Experimentation-II

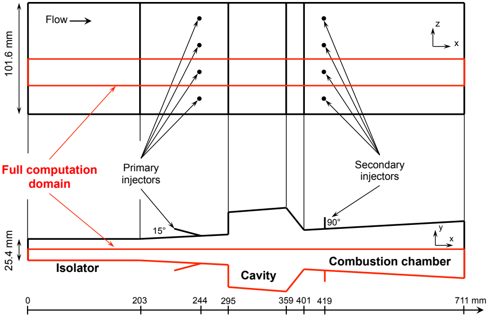
Computational domain of initial unit problem

Final: simulation of full combustor domain, match experimental setup —HIFiRE Direct Connect Rig (HDCR) [bottom-left figure]

Initial unit problem: primary injection section

- omit cavity
- no combustion
- focus on interaction of fuel jet and supersonic air crossflow





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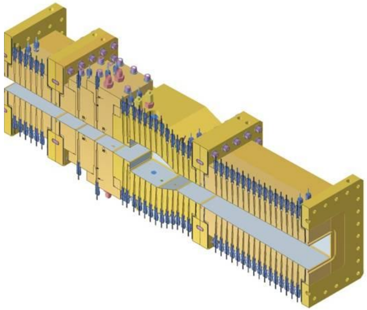
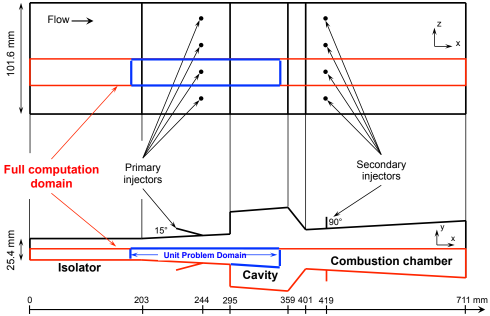
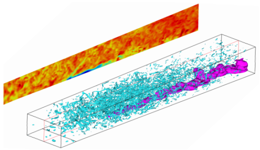
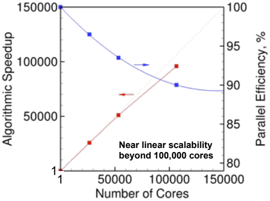


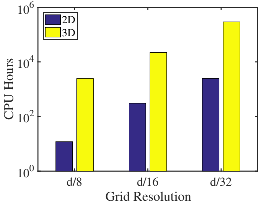


RAPTOR LES solver: model variants

RAPTOR: LES solver by Oefelein *et al.* at Sandia [Oefelein 06]







Highly-scalable but still **very expensive**

Motivation: different "model variants" are available under RAPTOR, trading off between solution accuracy and computational costs:

- Different grid resolutions
- Emulation using 2D geometry
- Static approximation of Smagorinsky model for SGS eddy viscosity
- Varying degree of detail in chemical mechanisms
- ...

⇒ to use/combine them, need to quantify the error due to model structure

Overview

Challenge:
LES is expensive, many flow solves needed to perform UQ and design

Would like to:
incorporate results from less expensive simulations of lower-fidelity models, while capturing model errors

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

Plan: represent the model error stochastically, by embedding a discrepancy term in the model parameters in a non-intrusive manner, where predictions automatically satisfy the governing equations

Embedded representation of model error

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

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

- Flexible for fitting model discrepancy
- Only applies corrections on model output, not on input parameters
- δ_k not transferable for prediction of QoIs outside calibration set
- Predictions generally do not obey governing equations
- Difficult to distinguish uncertainty contributions between model error and measurement noise

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

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

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

Model error representation via polynomial chaos

Represent the discrepancy term δ in a stochastic manner using a polynomial chaos expansion (PCE):

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

$\tilde{\alpha} \equiv (\lambda, \alpha)$–calibration parameters ξ–aleatoric source (rep. model error)

Safer extrapolation of δ over k since is always a λ correction

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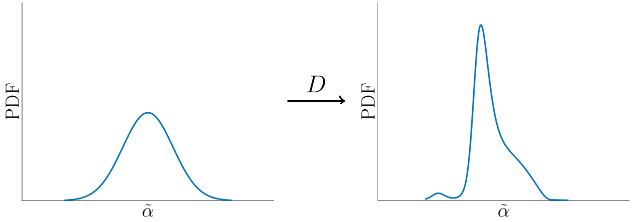
PCE in a nutshell: an expansion for a random variable:

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

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

Calibrate by inferring all parameters $\tilde{\alpha} \equiv (\lambda, \alpha)$ via

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



Calibration data D is often higher-fidelity model simulations

$\Rightarrow$ capturing model error of **low-fidelity model w.r.t. high-fidelity model**

True likelihood is intractable

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

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

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

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Enable tractable likelihood evaluation via two approximations:

1. Deterministic surrogate for low-fidelity model, built using 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 average leave-one-out cross validation error

Purpose: to replace the many subsequent low-fidelity model evaluations needed in MCMC; can skip if low-fidelity model inexpensive

Approximate likelihood using Gauss-marginal form

2 Gauss-marginal approximation to likelihood

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

where $\mu_k(\tilde{\alpha})$ and $\sigma_k^2(\tilde{\alpha})$ are obtained by constructing a PCE for $\hat{f}_k$ at given $\tilde{\alpha}$ and in the argument of ξ:

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

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

This PCE needs to be constructed at every $\tilde{\alpha}$ encountered in the MCMC, but not too expensive if we are working with $\hat{f}_k$ instead of f_k (use NISP)

Attribution of total predictive variance

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

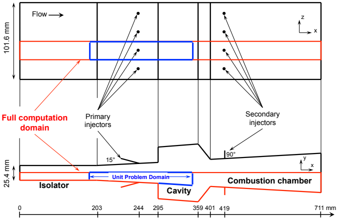
Recall
$$\begin{aligned} q_k &= f_k(\lambda + \delta(\alpha, \xi)) + \epsilon_{d_k} \\ &\approx \hat{f}_k(\lambda + \delta(\alpha, \xi)) + \epsilon_{k,\mathrm{LOO}} + \epsilon_{d_k} \\ &\approx \sum_{\beta} \hat{f}_{k,\beta}(\tilde{\alpha})\Psi_{\beta}(\xi) + \epsilon_{k,\mathrm{LOO}} + \epsilon_{d_k} \end{aligned}$$

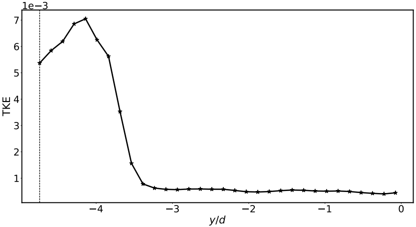
$$\mathrm{Var}[q_k] = \underbrace{\mathbb{E}_{\tilde{\alpha}}\left[\sigma_k^2(\tilde{\alpha})\right]}_{\text{model error}} + \underbrace{\mathrm{Var}_{\tilde{\alpha}}\left[\mu_k(\tilde{\alpha})\right]}_{\text{posterior uncertainty}} + \underbrace{\sigma_{k,\mathrm{LOO}}^2}_{\text{surrogate error}} +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

Dynamic-vs-Static Smagorinsky turbulence model

Calibrate static Smagorinsky model with dynamic treatment simulations

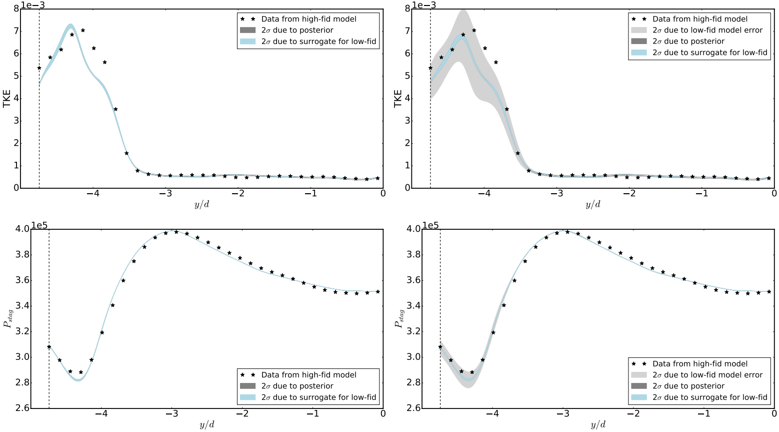
- 3D geometry
- Calibrate using TKE y-profile (t-averaged, at fixed x, centerline z)





- 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



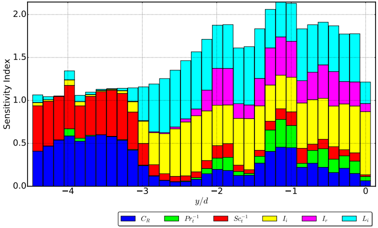
No model error treatment

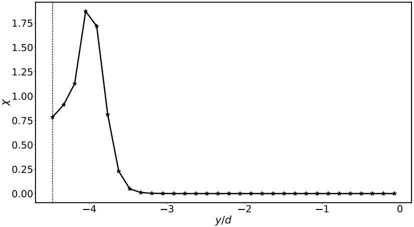
Embedded model error treatment

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
    - Employ triangular form of PCE for multivariate embedding
    - 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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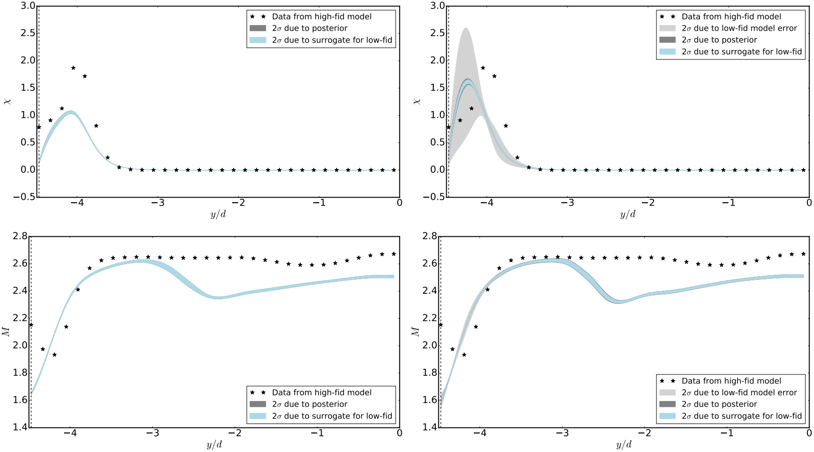
$\Rightarrow$ embed in C_R and Sc_t^{-1}

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

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
- Illustrated good capture of model-to-model discrepancy, and also limitations when models are too different
- Demonstrated method in a non-reactive unit problem in scramjet design involving expensive LES:
  - Dynamic vs. static Smagorinsky model treatment
  - 2D vs. 3D geometry

Future work:

- Bayesian model selection for optimal model error embedding
- More sophisticated forms of embedding
- Full HDCR geometry with combustion

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