Model Error Quantification in Turbulent Combustion Computations

Khachik Sargsyan, Xun Huan, Habib Najm

Sandia National Laboratories, Livermore, CA

SIAM CSE
Atlanta, GA
Feb 27 - Mar 3, 2017

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Further acknowledgements:
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DOE Office of Advanced Scientific Computing Research (ASCR), SciDAC
DOE Office of Basic Energy Sciences

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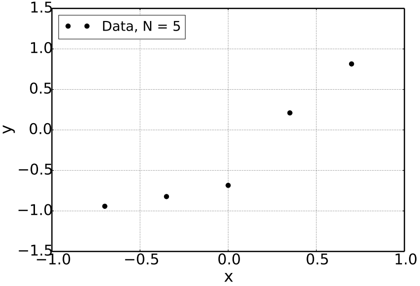
Main target

Model error = deviation from ‘truth’, or from a higher-fidelity model

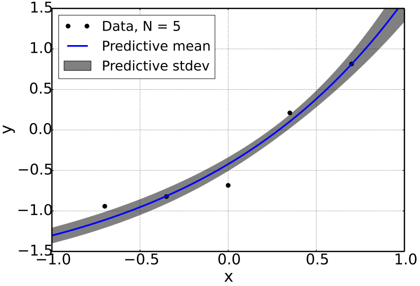
- Represent and estimate the error associated with
  - Simplifying assumptions, parameterizations
  - Mathematical formulation, theoretical framework
  - Numerical discretization
- ...will be useful for
  - Model validation
  - Model comparison
  - Scientific discovery and model improvement
  - Reliable computational predictions
- Inverse modeling context
  - Given experimental or higher-fidelity model data, estimate the model error

Motivation



Model-data fit

- Given noisy data – Gaussian noise
- $y = g_{\text{true}}(x) + \epsilon$



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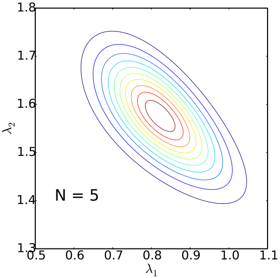
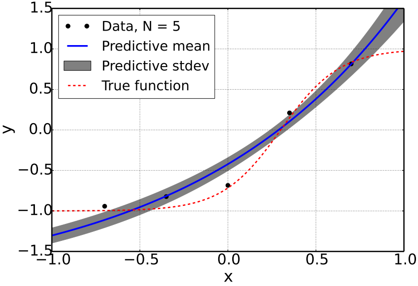


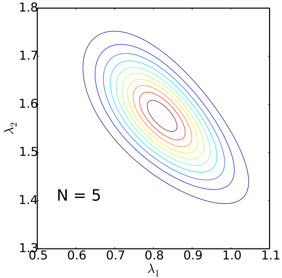
Posterior on parameters

- Employ Bayesian inference to fit an exponential model – $y_{\rm m} = f(x, \lambda)$
- Discrepancy between data and prediction presumed exclusively due to *i.i.d.* Gaussian data noise – $y = f(x, \lambda) + \epsilon_{\rm d}$
- Plotted:
  - Posterior density on the parameters
  - Predictive mean and standard deviation

Motivation



Model-data fit



Posterior on parameters

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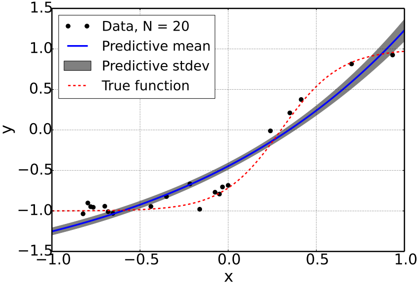
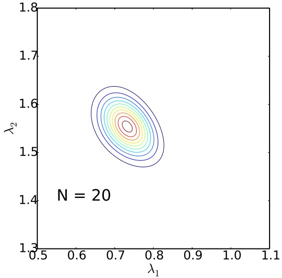
- Discrepancy between data and prediction presumed exclusively due to *i.i.d.* Gaussian data noise – $y = f(x, \lambda) + \epsilon_{\rm d}$
- True model $g(x)$ – dashed-red – differs from fit model $f(x, \lambda)$
- Actual discrepancy includes both data and model errors

Motivation



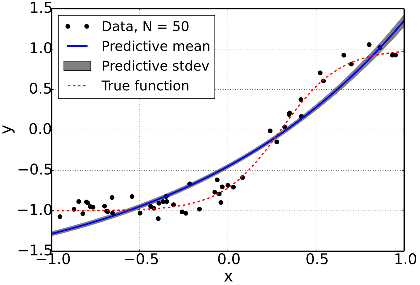
Model-data fit



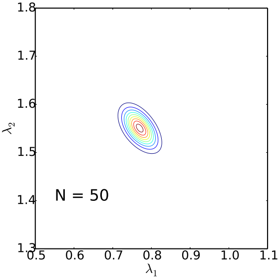
Posterior on parameters

- Increasing number of data points decreases posterior and predictive uncertainty
- We are increasingly sure about predictions based on the *wrong* model

Motivation



Model-data fit



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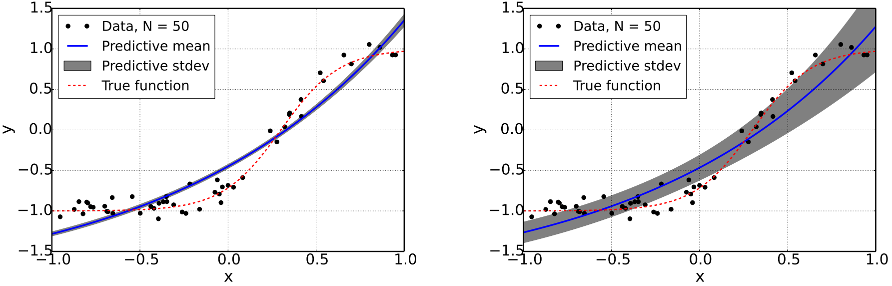


Model-data fit

What we want

- If the model has structural uncertainty, more data leads to biased and overconfident results
- We want to quantify model-vs-truth discrepancy in a rigorous and systematic way
  - Cannot ignore model error

Explicit model discrepancy: issues for physical models

$$y_i = \underbrace{f(x_i;\lambda) + \delta(x_i)}_{\text{truth}} + \epsilon_i$$

- Explicit additive statistical model for model error $\delta(x)$ [Kennedy-O'Hagan, 2001]
- Potential violation of physical constraints
- Disambiguation of model error $\delta(x_i)$ and data error ϵ_i^{d}
- Calibration of model error on measured observable does not impact the quality of model predictions on other QoIs
- Physical scientists are unlikely to augment their model with a statistical model error term on select outputs
  - Calibrated predictive model: $f(x;\lambda) + \delta(x)$ or $f(x;\lambda)$?
- Problem is highlighted in model-to-model calibration ($\epsilon_i = 0$)
  - no a priori knowledge of the statistical structure of $\delta(x)$

Model error embedding: key idea

Ideally, modelers want predictive *errorbars*:
inserting randomness on the outputs has issues, so...

- Cast input parameters λ as a random variable Λ

  Black-box $$y_i = f(x_i; \Lambda) + \epsilon_i$$

- Generalize parameter forms,

  Random field $$y_i = f(x_i; \Lambda(x_i)) + \epsilon_i$$

- More generally, explore additional parameterizations,

  Extra 'physics' $$y_i = \tilde{f}(x_i; \lambda, \Theta) + \epsilon_i$$

Model error embedding: key idea

Ideally, modelers want predictive *errorbars*:
inserting randomness on the outputs has issues, so...

- Cast input parameters λ as a random variable Λ

  Black-box

  $$\boxed{y_i = f(x_i; \Lambda) + \epsilon_i}$$

  ... even simpler, *additive correction term*

  $$\boxed{y_i = f(x_i; \lambda + \delta(\alpha, \xi)) + \epsilon_i}$$

- Infer the parameters of the correction (α) with the model parameters (λ)
- Stochastic dimension ξ corresponds to model error

Model error embedding: key idea

Augment input parameters λ with additive term $\delta(\alpha, \xi)$

$$\boxed{y_i = f(x_i; \lambda) + \delta(x_i) + \epsilon_i} \longrightarrow \boxed{y_i = f(x_i; \lambda + \delta(\alpha, \xi)) + \epsilon_i}$$

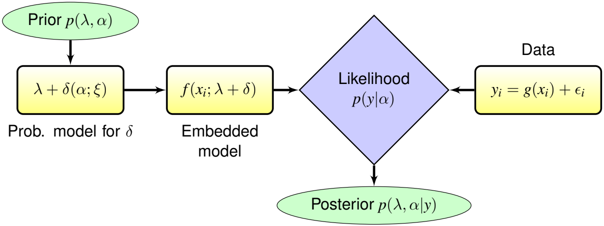
- Embed model error in specific submodel phenomenology
  - a modified transport or constitutive law
  - a modified formulation for a material property
- Allows placement of model error term in locations where key modeling assumptions and approximations are made
  - as a correction or high-order term
  - as a possible alternate phenomenology
- Naturally preserves model structure and physical constraints

Model error embedding – Bayesian density estimation

$$y_i = f(x_i; \lambda + \delta) + \epsilon_i$$

- Parametrize embedded random variable δ:
  - PDF form $\pi_\delta(\cdot;\alpha)$
  - Polynomial Chaos (PC): $\delta = \sum_k \alpha_k \Psi_k(\xi)$
  - Multivariate Normal (MVN): $\begin{cases} \delta_1 = \alpha_{11}\xi_1 \\ \delta_2 = \alpha_{21}\xi_1 + \alpha_{22}\xi_2 \\ \quad\vdots \\ \delta_d = \alpha_{d1}\xi_1 + \alpha_{d2}\xi_2 + \cdots + \alpha_{dd}\xi_d \end{cases}$
- Inverse modeling context
  - Parameter estimation of $\lambda \Rightarrow$ parameter estimation of $\tilde{\alpha} = (\lambda, \alpha)$
  - Bayesian formulation $\underbrace{p(\tilde{\alpha}|y)}_{\text{Posterior}} \propto \underbrace{L_y(\tilde{\alpha})}_{\text{Likelihood}} \underbrace{p(\tilde{\alpha})}_{\text{Prior}}$

Model error embedding – likelihood options



- Infer $\hat{\alpha} = (\lambda, \alpha, \sigma_{\mathcal{D}})$
- Data generation model; to aid likelihood $p(y|\hat{\alpha})$ construction

$$\begin{aligned} y_i &= f(x_i, \lambda + \delta(\alpha, \xi)) + \epsilon_i = \\ &= f\left(x_i, \lambda + \sum_k \alpha_k \Psi_k(\xi_1, \dots, \xi_d)\right) + \sigma_{\mathcal{D}} \xi_{d+i} = \\ \text{[NISP]} &\approx \sum_k f_{ik}(\alpha) \Psi_k(\xi_1, \dots, \xi_d) + \sigma_{\mathcal{D}} \xi_{d+i} = h_i(\hat{\xi}; \hat{\alpha}) \end{aligned}$$

- Full PC germ $\hat{\xi} = (\underbrace{\xi_1, \dots, \xi_d}_{\text{Model error}}, \underbrace{\xi_{d+1}, \dots, \xi_{d+N}}_{\text{Data noise}})$

Model error embedding – likelihood options

- Data generation model; to aid likelihood $p(y|\hat{\alpha})$ construction

$$
\begin{aligned}
y_i &= f(x_i, \lambda + \delta(\alpha, \xi)) + \epsilon_i = \\
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\text{[NISP]} &\approx \sum_k f_{ik}(\alpha) \Psi_k(\xi_1, \ldots, \xi_d) + \sigma_{\mathcal{D}} \xi_{d+i} = h_i(\hat{\xi}; \hat{\alpha})
\end{aligned}
$$

- Full Likelihood: $L(\hat{\alpha}) = p(y|\hat{\alpha}) = p(y_1, \ldots, y_N|\hat{\alpha}) = \pi(y)$
  - Degenerate if no data noise
  - Requires multivariate KDE or high-d integration
  - Gaussian approximation:
    $L(\hat{\alpha}) \propto \exp\left(-\frac{1}{2}(y - \mu(\hat{\alpha}))^T \Sigma^{-1}(\hat{\alpha})(y - \mu(\hat{\alpha}))\right)$
  - Non-intrusive spectral projection (NISP) relieves the expense and provides easy access to mean $\mu(\alpha)$ and covariance $\Sigma(\hat{\alpha})$

Model error embedding – likelihood options

- Data generation model; to aid likelihood $p(y|\hat{\alpha})$ construction

$$
\begin{aligned}
y_i &= f(x_i, \lambda + \delta(\alpha, \xi)) + \epsilon_i = \\
&= f\left(x_i, \lambda + \sum_k \alpha_k \Psi_k(\xi_1, \ldots, \xi_d)\right) + \sigma_{\mathcal{D}} \xi_{d+i} = \\
\text{[NISP]} &\approx \sum_k f_{ik}(\alpha) \Psi_k(\xi_1, \ldots, \xi_d) + \sigma_{\mathcal{D}} \xi_{d+i} = h_i(\hat{\xi}; \hat{\alpha})
\end{aligned}
$$

- Marginalized Likelihood:
  $L(\hat{\alpha}) = p(y|\hat{\alpha}) \approx \prod_{i=1}^N p(y_i|\hat{\alpha}) = \prod_{i=1}^N \pi(y_i)$
  - Requires univariate KDE
  - Neglects built-in correlations
  - Gaussian approximation:
    $L(\hat{\alpha}) \propto \exp\left(-\frac{1}{2} \sum_{i=1}^N \Sigma_{ii}^{-1}(\hat{\alpha})(y_i - \mu_i(\hat{\alpha}))^2\right)$

Model error embedding – likelihood options

- Data generation model; to aid likelihood $p(y|\hat{\alpha})$ construction

$$
\begin{aligned}
y_i &= f(x_i, \lambda + \delta(\alpha, \xi)) + \epsilon_i = \\
&= f\left(x_i, \lambda + \sum_k \alpha_k \Psi_k(\xi_1, \ldots, \xi_d)\right) + \sigma_{\mathcal{D}} \xi_{d+i} = \\
\text{[NISP]} &\approx \sum_k f_{ik}(\alpha) \Psi_k(\xi_1, \ldots, \xi_d) + \sigma_{\mathcal{D}} \xi_{d+i} = h_i(\hat{\xi}; \hat{\alpha})
\end{aligned}
$$

- Approximate Bayesian Computation (ABC): $L(\hat{\alpha}) = \frac{1}{\epsilon} K\left(\frac{\rho(\mathcal{S}_{\mathcal{M}}, \mathcal{S}_{\mathcal{D}})}{\epsilon}\right)$
  - Mean of $f(x_i; \lambda + \delta)$ is "centered" on the data
  - The width of the distribution of $f(x_i; \lambda + \delta)$ is consistent with the spread of the data around the nominal model prediction

$$
L(\hat{\alpha}) \propto \exp\left(-\frac{1}{2\epsilon^2} \sum_{i=1}^{N} \left[(\mu_i(\hat{\alpha}) - y_i)^2 + \left(\sqrt{\Sigma_{ii}(\hat{\alpha})} - \gamma|\mu_i(\hat{\alpha}) - y_i|\right)^2\right]\right)
$$

Model Error – Predictions

$$f(x;\lambda+\delta(\alpha,\xi)) = f\left(x;\lambda+\sum_k \alpha_k \Psi_k(\xi_{1:d})\right) = \sum_k f_k(x;\alpha)\Psi_k(\xi_{1:d})$$

- Non-intrusive spectral projection (NISP) will allow
  - Posterior/pushed-forward predictions
  - Easy access to first two moments:

$$\mu(x;\alpha) = f_0(x;\alpha), \qquad \sigma^2(x;\alpha) = \sum_{k>0} f_k^2(x;\alpha)||\Psi_k||^2$$

- Predictive mean

$$\mathbb{E}[y(x)] = \mathbb{E}_\alpha[\mu(x;\alpha)]$$

- Decomposition of predictive variance

$$\mathbb{V}[y(x)] = \underbrace{\mathbb{E}_\alpha[\sigma^2(x;\alpha)]}_{\text{Model error}} + \underbrace{\mathbb{V}_\alpha[\mu(x;\alpha)]}_{\text{Posterior error}}$$

Model Error – Predictions at data locations

$$; \lambda + \delta(\alpha, \xi)) = f\,(x_i; \lambda + \textstyle\sum_k \alpha_k \Psi_k(\xi_{1:d}))\; + \sigma_D \xi_{i+d} = \textstyle\sum_k f_k(x_i; \alpha) \Psi_k(\xi_{1:d}) + \sigma_D$$

- Non-intrusive spectral projection (NISP) will allow
  - Likelihood computation
  - Easy access to first two moments:

$$\mu(x_i; \alpha) = f_0(x_i; \alpha), \qquad \sigma^2(x_i; \alpha) = \sum_{k>0} f_k^2(x_i; \alpha) ||\Psi_k||^2$$

- Predictive mean

$$\mathbb{E}[y(x_i)] = \mathbb{E}_\alpha[\mu(x_i; \alpha)]$$

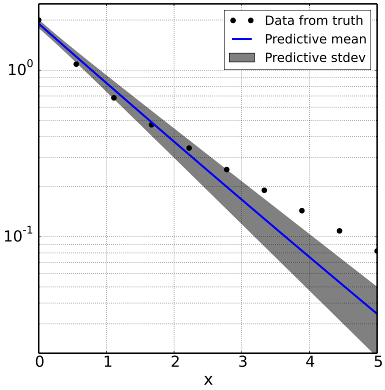
- Decomposition of predictive variance

$$\mathbb{V}[y(x_i)] = \underbrace{\mathbb{E}_\alpha[\sigma^2(x_i; \alpha)]}_{\text{Model error}} + \underbrace{\mathbb{V}_\alpha[\mu(x_i; \alpha)] + \sigma_d^2}_{\text{Posterior/Data error}}$$

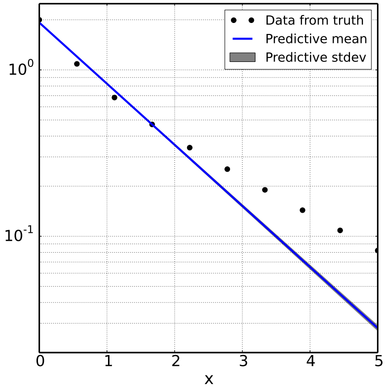
Predictions account for model error

Calibrating single-exponential models
with data from a double exponential model $g(x) = e^{-0.5x} + e^{-2x}$

Linear-exponential $f(x, \lambda) = e^{\lambda_1 + \lambda_2 x}$



Additive Gaussian error



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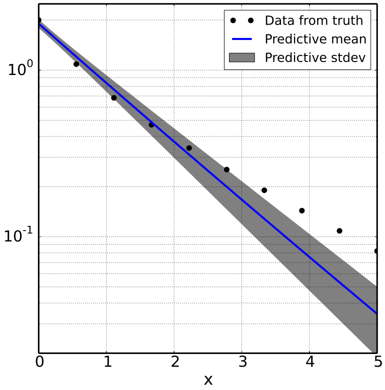
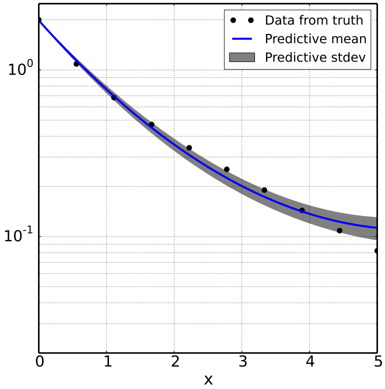


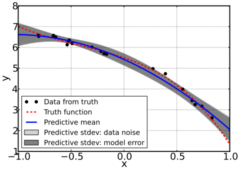
Quadratic-exponential $f_2(x,\lambda) = e^{\lambda_1+\lambda_2 x+\lambda_3 x^2}$



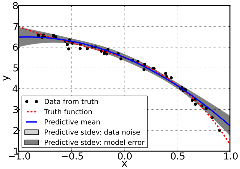
More data leads to 'leftover' model error

Calibrating a quadratic $f(x) = \lambda_0 + \lambda_1 x + \lambda_2 x^2$
w.r.t. 'truth' $g(x) = 6 + x^2 - 0.5(x+1)^{3.5}$ measured with noise $\sigma = 0.1$.

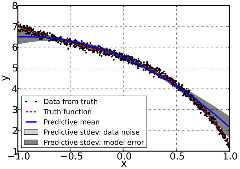
$N = 20$



$N = 50$

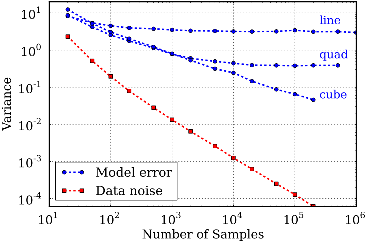


$N = 1000$



Summary of features:

- Well-defined model-to-model calibration
- Model-driven discrepancy correlations
- Respects physical constraints
- Disambiguates model and data errors
- Calibrated predictions of multiple QoIs

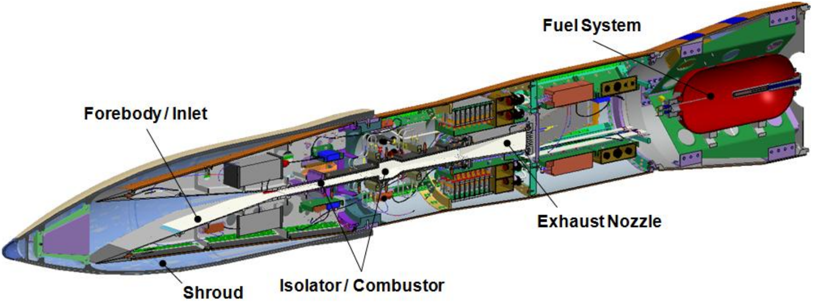


HIFiRE-II Scramjet

Development of scramjet engine involves

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

We focus on the HIFiRE-II*configuration:

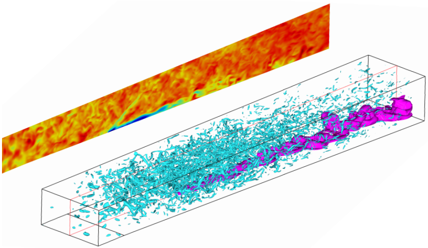


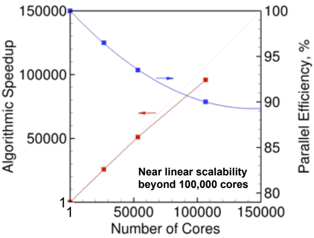
† Hypersonic International Flight Research and Experimentation-II

RAPTOR solver - direct UQ intractable

RAPTOR: code by Oefelein *et al.* at Sandia

- Fully-coupled, compressible conservation equations
- High Reynolds number, high-pressure, wide range of Mach number
- Real-fluid equation of state
- Detailed thermodynamics, transport and chemistry
- Non-dissipative, discretely conservative, staggered finite-volume
- Complex geometry treatment





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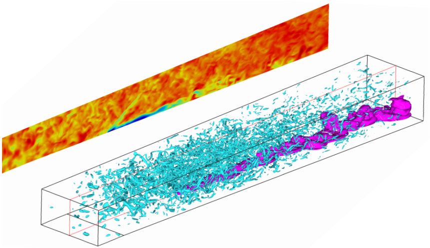

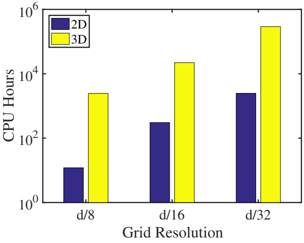

Model Error – Workflow

- ***Preprocess:*** Surrogate construction, GSA, select embedding
- ***Calibration:*** Prior selection, approximate likelihood+NISP
- ***Prediction:*** Forward propagation via NISP, possible extrapolation

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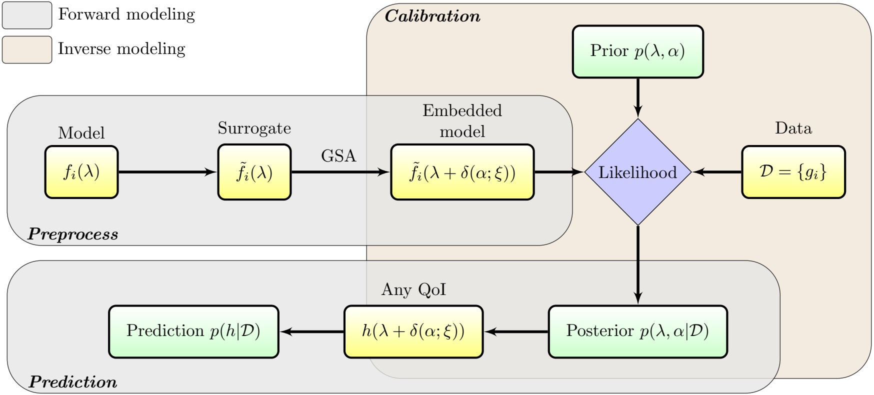

Static-vs-dynamic turbulence constants

Parameter	Notation	Range
Modified Smagorinsky constant	C_R	$[0.005, 0.08]$
(inverse) Turbulent Prandtl number	Pr_t^{-1}	$[0.25, 2.0]$
(inverse) Turbulent Schmidt number	Sc_t^{-1}	$[0.25, 2.0]$

- Jet in Crossflow problem – $3D$, $d/8$ grid resolution
- LES model fidelity
  - Dynamic: subgrid parameters variable in space/time, g_i
  - Static : subgrid parameters constant in space/time, $f_i(\lambda)$
- Embedding PCE for $\lambda = (C_R, Pr_t^{-1}, Sc_t^{-1})$ in static model governing equations
- Surrogate construction using $4^3 = 64$ simulations of $f(\lambda)$
  - Global sensitivity analysis: impact of $C_R \gg$ impact of Pr_t^{-1} and Sc_t^{-1}

Model Error – Embed it in turbulent closure constants

- Eddy Viscosity:

$$\mu_t = \overline{\rho} C_R \Delta^2 \Pi_{\tilde{\mathbf{S}}}^{\frac{1}{2}} \qquad \Pi_{\tilde{\mathbf{S}}} = \tilde{\mathbf{S}} : \tilde{\mathbf{S}} \qquad \tilde{\mathbf{S}} = \frac{1}{2}\left(\nabla\tilde{\mathbf{u}} + \nabla\tilde{\mathbf{u}}^T\right)$$

- Stress Tensor:

$$\vec{\vec{\mathcal{T}}} = (\overline{\tau} - \mathbf{T}) = (\mu_t + \mu)\frac{1}{Re}\left[-\frac{2}{3}(\nabla\cdot\tilde{\mathbf{u}})\mathbf{I} + \left(\nabla\tilde{\mathbf{u}} + \nabla\tilde{\mathbf{u}}^T\right)\right] \; - \; \overline{\rho}\left(\widetilde{\tilde{\mathbf{u}}\otimes\tilde{\mathbf{u}}} - \tilde{\tilde{\mathbf{u}}}\otimes\tilde{\tilde{\mathbf{u}}}\right) \; - \; \frac{1}{3}\overline{\rho} q_{\mathrm{sfs}}^2\, \mathbf{I}$$

- Energy Flux:

$$\vec{\mathcal{Q}}_e = (\overline{\mathbf{q}}_e - \mathbf{Q}) = \left(\frac{\mu_t}{Pr_t} + \frac{\mu}{Pr}\right)\frac{1}{Re}\nabla\tilde{h} + \sum_{i=1}^{N}\tilde{h}_i\vec{\mathcal{S}}_i \; - \; \overline{\rho}\left(\widetilde{\tilde{h}\tilde{\mathbf{u}}} - \tilde{\tilde{h}}\tilde{\tilde{\mathbf{u}}}\right)$$

- Mass Flux:

$$\vec{\mathcal{S}}_i = (\overline{\mathbf{q}}_i - \mathbf{S}_i) = \left(\frac{\mu_t}{Sc_{t_i}} + \frac{\mu}{Sc_i}\right)\frac{1}{Re}\nabla\tilde{Y}_i \; - \; \overline{\rho}\left(\widetilde{\tilde{Y}_i\tilde{\mathbf{u}}} - \tilde{\tilde{Y}}_i\tilde{\tilde{\mathbf{u}}}\right)$$

Model Error – Embed it in turbulent closure constants

- Eddy Viscosity:

$$\mu_t = \overline{\rho} C_R \Delta^2 \Pi_{\tilde{\mathbf{S}}}^{\frac{1}{2}} \qquad \Pi_{\tilde{\mathbf{S}}} = \tilde{\mathbf{S}} : \tilde{\mathbf{S}} \qquad \tilde{\mathbf{S}} = \frac{1}{2}\left(\nabla\tilde{\mathbf{u}} + \nabla\tilde{\mathbf{u}}^T\right)$$

- Stress Tensor:

$$\vec{\vec{\mathcal{T}}} = (\overline{\tau} - \mathbf{T}) = (\mu_t + \mu)\frac{1}{Re}\left[-\frac{2}{3}(\nabla\cdot\tilde{\mathbf{u}})\mathbf{I} + \left(\nabla\tilde{\mathbf{u}} + \nabla\tilde{\mathbf{u}}^T\right)\right] - \overline{\rho}\left(\widetilde{\tilde{\mathbf{u}}\otimes\tilde{\mathbf{u}}} - \tilde{\tilde{\mathbf{u}}}\otimes\tilde{\tilde{\mathbf{u}}}\right) - \frac{1}{3}\overline{\rho}q_{\mathrm{sfs}}^2\,\mathbf{I}$$

- Energy Flux:

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$$\begin{cases} C_R = \alpha_{10} + \alpha_{11}\xi_1 \\ Pr_t^{-1} = \alpha_{20} + \alpha_{21}\xi_1 + \alpha_{22}\xi_2 \\ Sc_t^{-1} = \alpha_{30} + \alpha_{31}\xi_1 + \alpha_{32}\xi_2 + \alpha_{33}\xi_3 \end{cases}$$

Model Error – Embed it in turbulent closure constants

- Eddy Viscosity:

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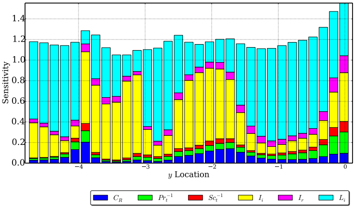
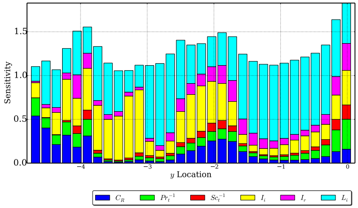
2D-vs-3D model configuration

Parameter	Notation	Range
Modified Smagorinsky constant	C_R	$[0.005, 0.08]$
(inverse) Turbulent Prandtl number	Pr_t^{-1}	$[0.25, 2.0]$
(inverse) Turbulent Schmidt number	Sc_t^{-1}	$[0.25, 2.0]$
Turbulence intensity (air)	$I_i = u_i'/U_i$	$[0.025, 0.075]$
Turbulence intensity ratio (air)	$I_r = v'/u'$	$[0.5, 1.0]$
Turbulence length scale (air)	L_i	$[0.0, 8.0]$

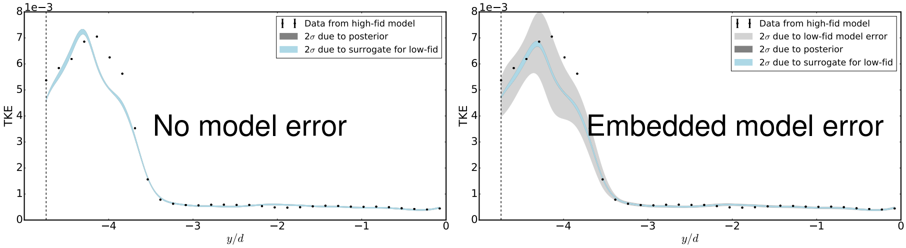
Pressure



Temperature

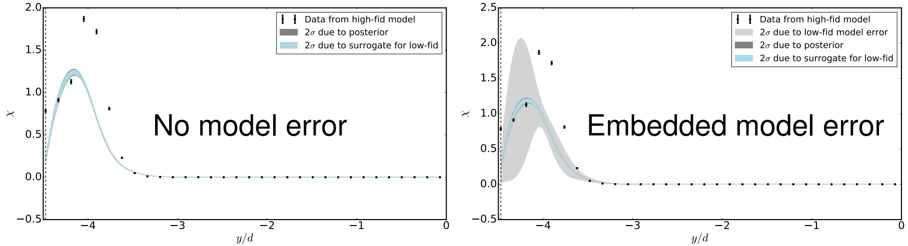


Model Error – Static-vs-Dynamic Jet-in-Crossflow



- High-fidelity model data noise is small in these cases
- Model error is the highest contributor of predictive uncertainty
- Embedded form allows prediction of other QoIs (i.e. ones not used for calibration)
- Results using model error treatment capture discrepancy much better than results without model error treatment

Model Error – 2D-vs-3D Jet-in-Crossflow



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Summary and Future

Thank You

- Represent, quantify and propagate physical model errors
- Parameter estimation $\Rightarrow$ density estimation
- Bayesian machinery to find parameters of the embedded PDFs
- Approximate/empirical likelihoods impose constraints of interest
- Differentiates from data noise; allows model-to-model calibration
- Implemented in UQTk (www.sandia.gov/UQToolkit)

- K. Sargsyan, H. Najm, and R. Ghanem. “On the Statistical Calibration of Physical Models”. *International Journal for Chemical Kinetics*, 47(4): 246-276, 2015.

- Bayesian model selection for optimal embedding
- Challenging Bayesian problem: MCMC sampling, prior dependence
- More intrusive embedding; problem specific

Additional Material
(Core Dump)

Likelihood construction – variants

- Full Likelihood

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

- Marginalized Likelihood

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

- Approximate Bayesian Computation (ABC)
  – seek to satisfy the constraints:
  - $p(y|D)$ is “centered” on the data
  - The width of the distribution $p(y|D)$ is “consistent” with the spread of the data around the nominal model prediction

Full Likelihood

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

where:
$\pi_f(\cdot, \alpha)$: N-variate density of the random variable $(f_1, \ldots, f_N)$
with $f_i = f(x_i, \lambda(\alpha))$

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

Consider a case with $M = 1$, $\lambda \sim N(\mu, \sigma^2)$, and $f = \lambda x$
Let $N = 2$, hence $(f_1, f_2) = (\lambda x_1, \lambda x_2)$ for any λ sample
With $f_1/x_1 = f_2/x_2 = \lambda$, (f_1, f_2) are dependent and
$\pi_f(\cdot|\mu, \sigma)$ is non-zero only along the line $f_2 = (x_2/x_1)f_1$

hence $\pi_f(y_{\text{data},1}, y_{\text{data},2}|\mu, \sigma)$ is non-zero only along the line
$y_{\text{data},2}/x_2 = y_{\text{data},1}/x_1$

Marginalized Likelihood

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

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 α values leading to vanishing marginal variances at each x_i

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

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

Multiple singularities, $\sigma_i(\alpha) = 0$, $i = 1, \ldots, N$

Posterior maximization always finds one of these singularities, fitting one point perfectly, while misfitting the rest   ($\Rightarrow$ priors)

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 $\mu_i(\alpha) = \mathrm{E}_\xi[f(x_i, \lambda(\xi;\alpha))]$: minimize $\|\mu_i(\alpha) - y_{\mathrm{data},i}\|_2^2$
- The width of the distribution $p(y|D)$ is consistent with the spread of the data around the nominal model prediction
  - With $\sigma_i(\alpha)^2 = \mathrm{V}_\xi[f(x_i, \lambda(\xi, \alpha))]$:
    minimize $\|(\sigma_i(\alpha) - \gamma|\mu_i(\alpha) - y_{\mathrm{data},i}|)\|_2^2$
  - γ is a factor that specifies the desired match between σ_i and the discrepancy $|\mu_i(\alpha) - y_{\mathrm{data},i}|$, 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 ϵ controls the severity of the consistency control

Propose the Gaussian kernel density:

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

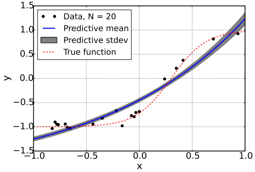
Data-Model-Truth

- Measurements

$$\overset{\text{data}}{y_i} = \overset{\text{truth}}{g(x_i)} + \overset{\text{data error}}{\epsilon_i^{\mathrm{d}}}$$

- Model

$$\overset{\text{truth}}{g(x_i)} = \overset{\text{model}}{f(x_i;\lambda)} + \overset{\text{model error}}{\delta(x_i)}$$



- Total error budget

$$y_i = \underbrace{f(x_i;\lambda) + \delta(x_i)}_{\text{truth } g(x_i)} + \epsilon_i^{\mathrm{d}}$$

Explicit statistical modeling of model discrepancy/error $\delta(x)$

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

Data Error: $\epsilon_i^{\mathrm{d}} \sim \mathrm{N}(0,\sigma^2)$

Estimate model parameters λ along with those of $\delta(x)$, ϵ_i^{d}

Attribution of error components

$$y_i = \underbrace{\sum_k f_{ik}(\alpha)\Psi_k(\xi_1,\ldots,\xi_d) + \sigma_{\mathcal{D}}\xi_{d+i}}_{h_i(\hat{\xi};\hat{\alpha})}$$

Stochastic dimensions:

- Model error $\xi_1,\ldots,\xi_d$
- Measurement error $\xi_{d+1},\ldots,\xi_{d+N}$
- Posterior uncertainty (α): can be represented via its own PC expansion (using MCMC samples and Rosenblatt transformation)

Full PC expansion: $y_i = \sum f_j \Psi_j(\hat{\hat{\xi}})$

Full stochastic *germ*:

$$\hat{\hat{\xi}} = (\underbrace{\xi_1,\ldots,\xi_d}_{\text{Model error}}, \underbrace{\xi_{d+1},\ldots,\xi_{d+N}}_{\text{Measurement error}}, \underbrace{\xi_{d+N+1},\ldots,\xi_{d+N+N_\alpha}}_{\text{Posterior uncertainty}})$$

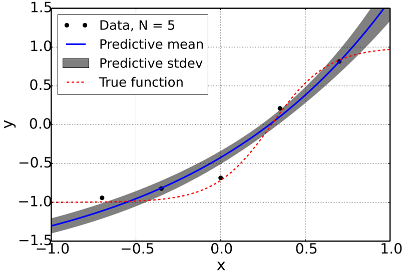
Posterior predictive variance:

$$\sigma^2_{\mathrm{PP}}(x_i) = \mathbb{E}_\alpha[\sigma^2(x_i,\alpha)] + \mathbb{E}_{\sigma_{\mathcal{D}}}[\sigma^2_{\mathcal{D}}] + \mathbb{V}_\alpha[\mu(x_i,\alpha)]$$

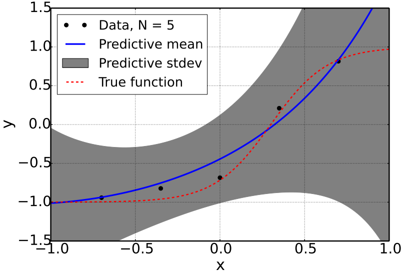
Predictions account for model error: example 1

Calibrating an exponential model $f(x;\lambda_1,\lambda_2) = \lambda_2 e^{\lambda_1 x} - 2$
with data from a hyperbolic tangent model $g(x) = \tanh(3(x-0.3))$

Additive Gaussian error



Embedded model error



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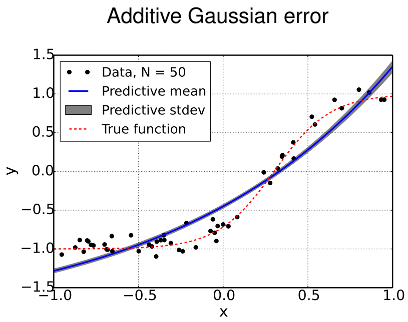
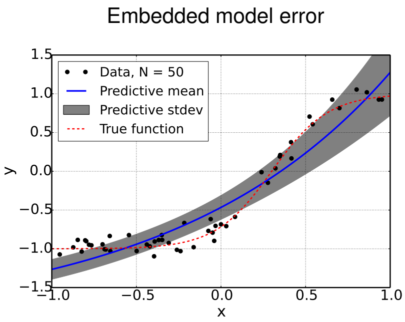


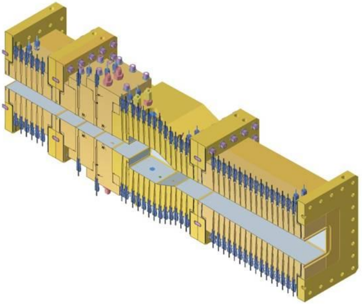


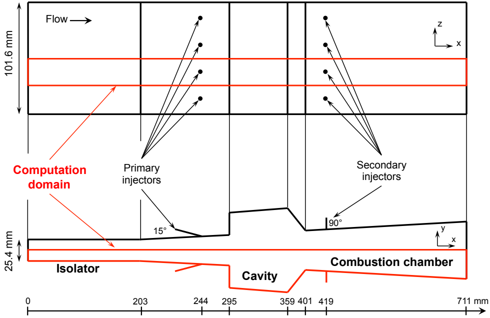
Computational domain of initial unit problem

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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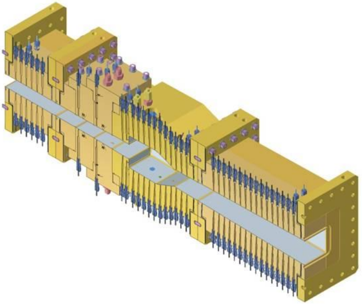
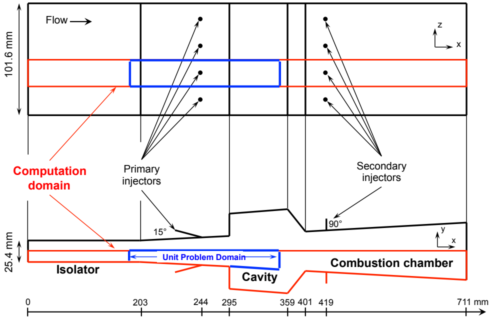
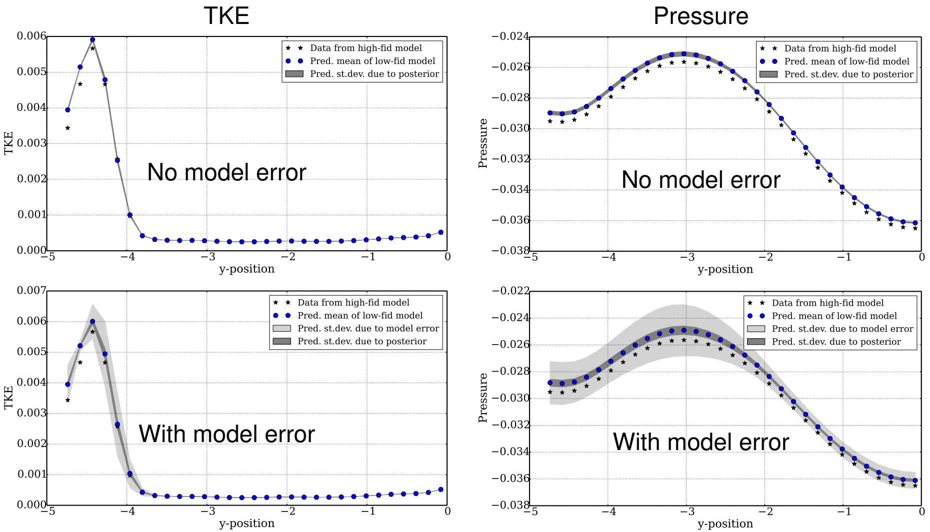




LES computation in Scramjet engine: static-vs-dynamic SGS model calibration

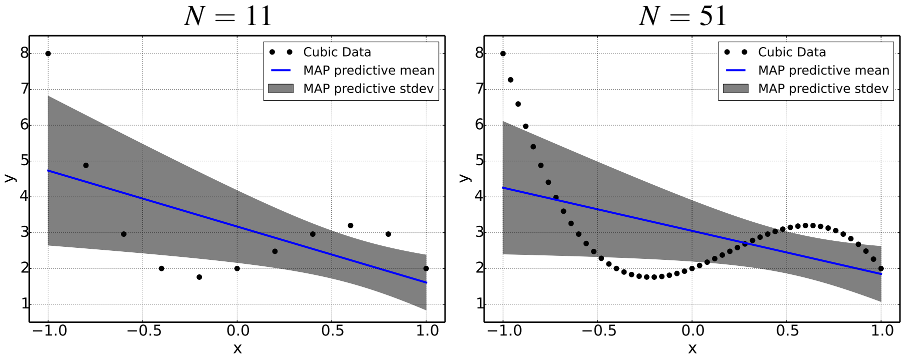
Calibrate with Turbulent Kinetic Energy (TKE) data, predict both TKE and Pressure



Model error – Study 2: quantify error due to 2D grid

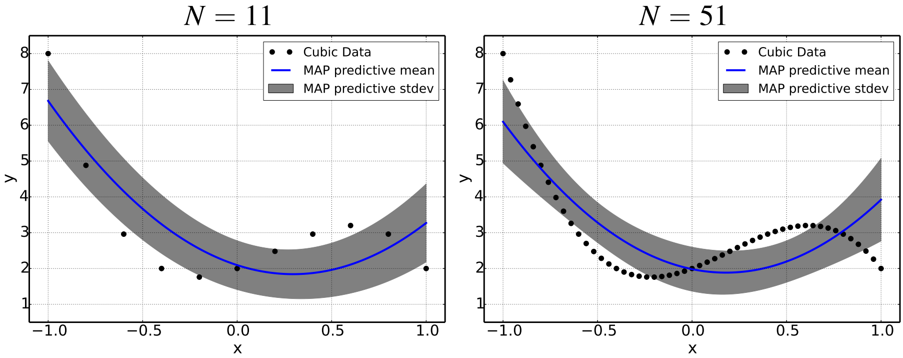
- Problem Focus: P1 Jet in Crossflow problem
  – static SGS constant, $d/8$ grid resolution
  - Calibrate a $2D$ model using $3D$ benchmark simulations as data
  - Quantify the model error associated with 2D treatment
  - Can 2D-grid model mimick 3D solution with acceptable accuracy?
- Surrogate construction
  - Model still expensive; direct evaluations in MCMC infeasible
  - Selected 6 parameters
  - Ensemble of 500 simulations of the 2D model $f(\lambda)$
  - Legendre polynomial expansion surrogate
  - Initial GSA suggests how to embed model error, see next slide
- Benchmark run taken from Study 1, run #42/64
  - 3D QoI selection for 2D comparison: (a) centerline, (b) spanwise average

Test problem – Cubic data fit by a line – ABC



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

Test problem – Cubic data fit by a quadratic – ABC



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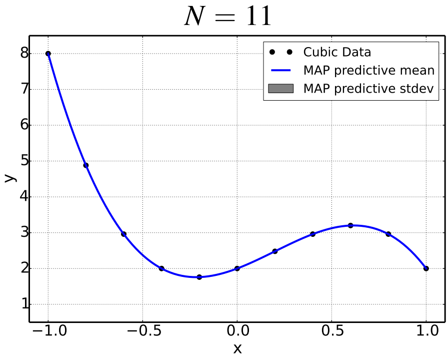

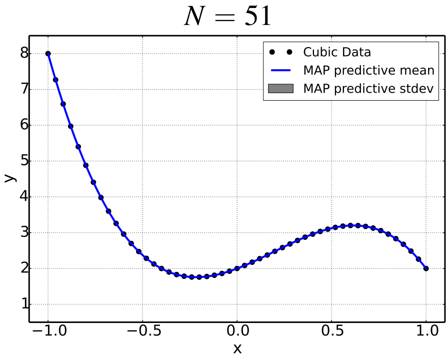

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Scenarios of interest

- Model-to-model calibration
  - Chemical reaction model
- Multi-model analysis
  - Atmospheric transport
- Prediction of other QoIs
  - LES computation

Model-to-model calibration: ignition model

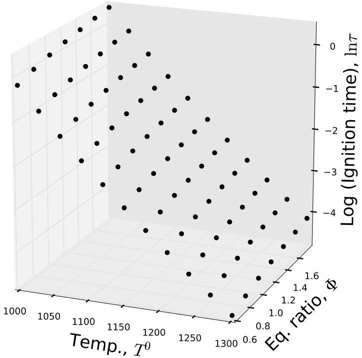
- Homogeneous ignition, methane-air mixture
- Single-step global reaction model calibrated against a detailed chemical kinetic model

- Data: ignition time; range of initial T & equivalence ratio
- Single-step model:

$$CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O$$

$$\begin{aligned} \mathfrak{R} &= [CH_4][O_2]k_f \\ k_f &= A\exp(-E/R^oT) \end{aligned}$$

- $(\ln A, E) = \sum_k \boldsymbol{\alpha}_k \Psi_k(\xi)$

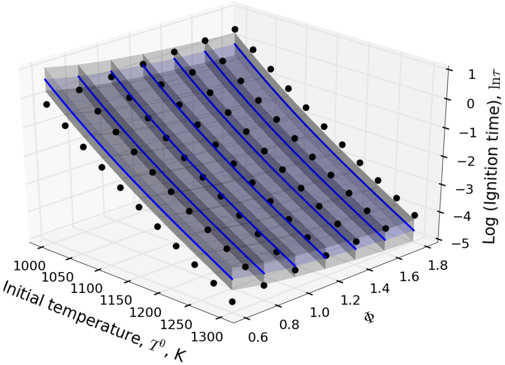


Model-to-model calibration: ignition model

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

Over the range of (T^0, Φ):

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



K. Sargsyan, H.N. Najm, and R. Ghanem
"On the Statistical Calibration of Physical Models"
Int. J. Chem. Kin., 47(4): 246-276, 2015

TransCom3 Experiment of CO_2 Flux Inversion

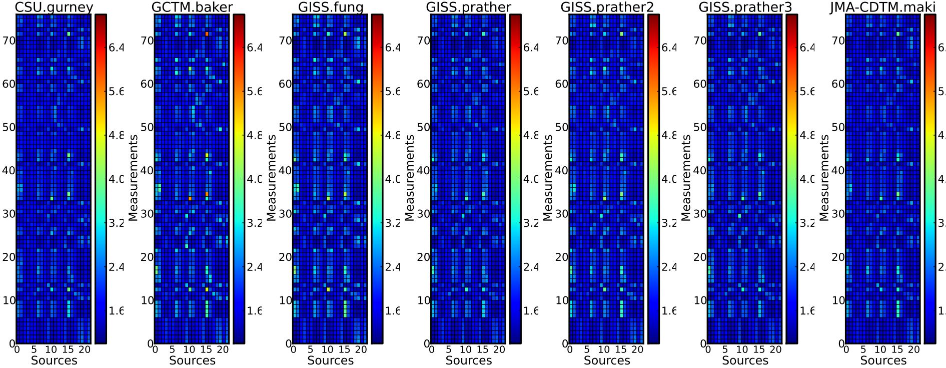
[Gurney *et al.*, Tellus B, 2003]

- Observations $\mathbf{d}$ at $N = 77$ sites around the world
- Inverse problem: find fluxes $\mathbf{s}$ at $M = 22$ locations
- Linearized 'response' model $\mathbf{R}$, such that $\mathbf{d} \approx \mathbf{Rs}$

$$\boxed{\mathbf{d} = \mathbf{Rs} + \epsilon_{\mathbf{d}}}$$

- Model $\mathbf{R}$ is never perfect thus contaminating the inversion
- The inferred values of $\mathbf{s}$ compensate for model deficiencies
- $\epsilon_{\mathbf{d}}$ is meant to capture data errors, but is 'entangled' with model errors

Consider 14 different response models $\mathbf{R}$



Infer fluxes $\mathbf{s}$, given measurements $\mathbf{d}$ to satisfy $\mathbf{d} \approx \mathbf{R}\mathbf{s}$

- Conventional additive Gaussian error (least-squares): $\mathbf{d} = \mathbf{R}\mathbf{s} + \xi$
- Embed probabilistic model for fluxes s: $\mathbf{d} = \mathbf{R}(\mu_\mathbf{s} + \mathbf{C}_\mathbf{s}\xi)$

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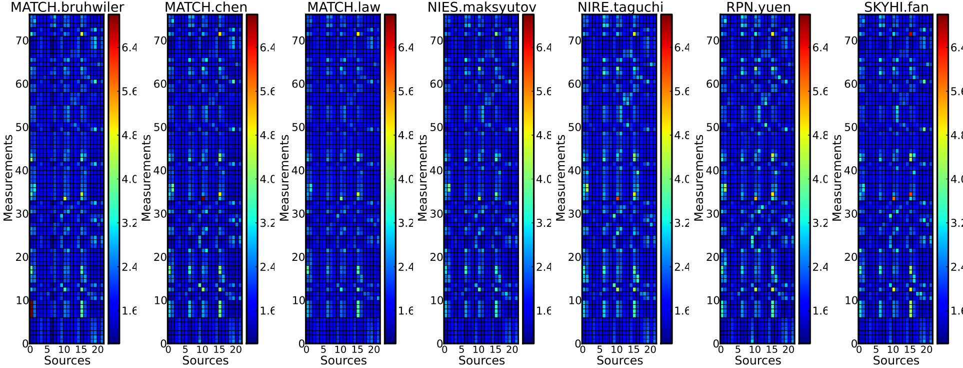

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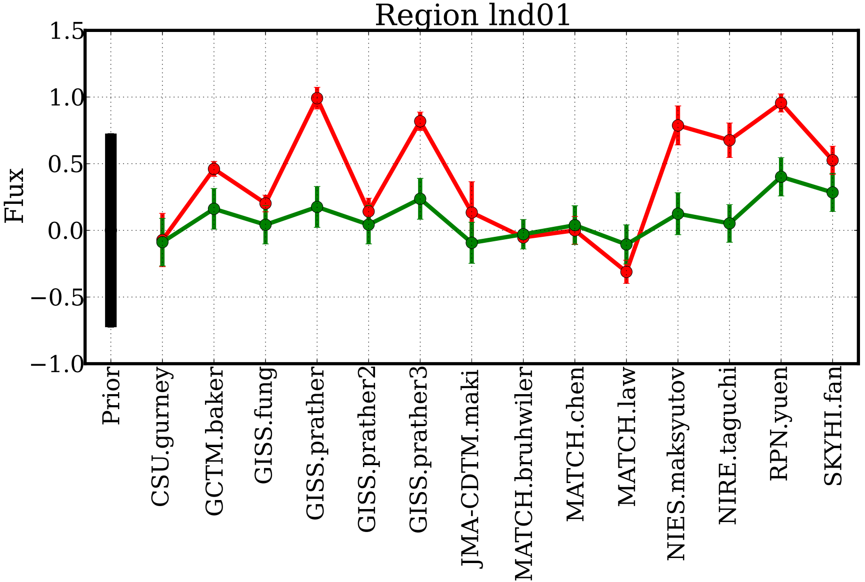
Inferred fluxes show less variability across models



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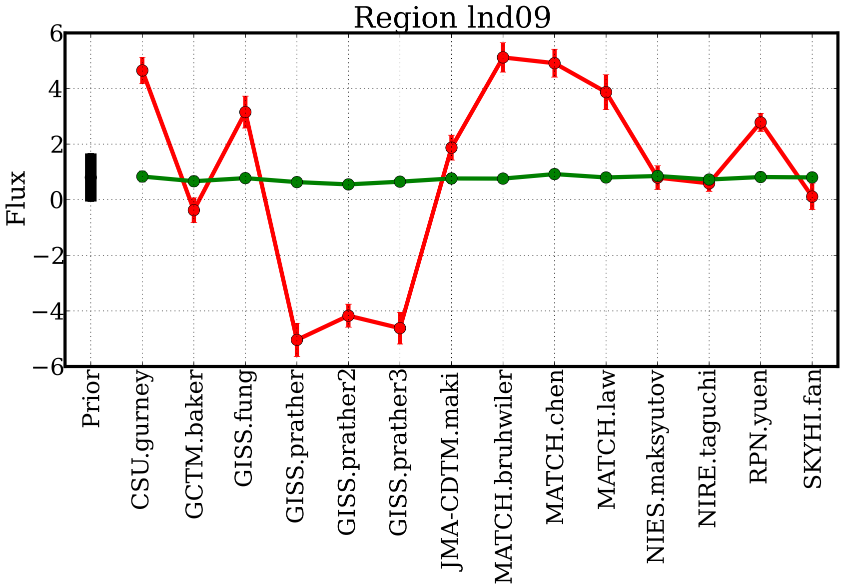

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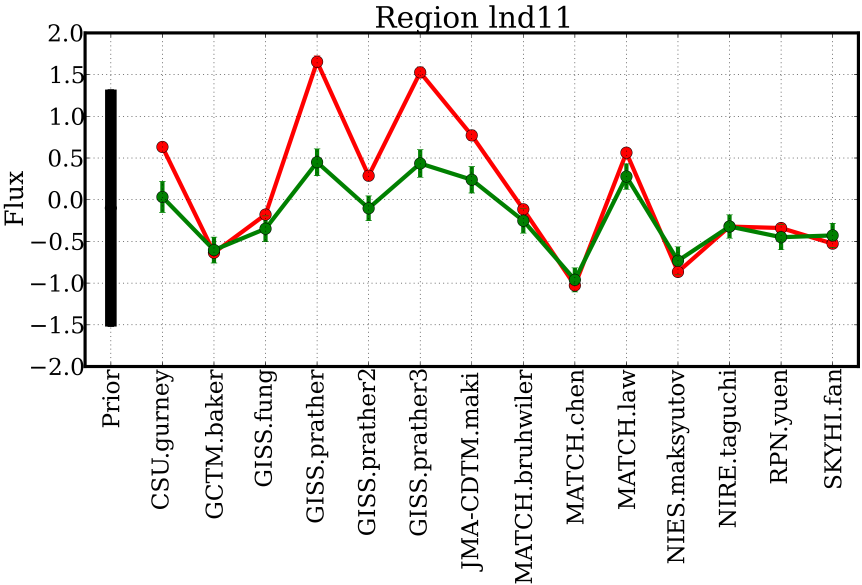

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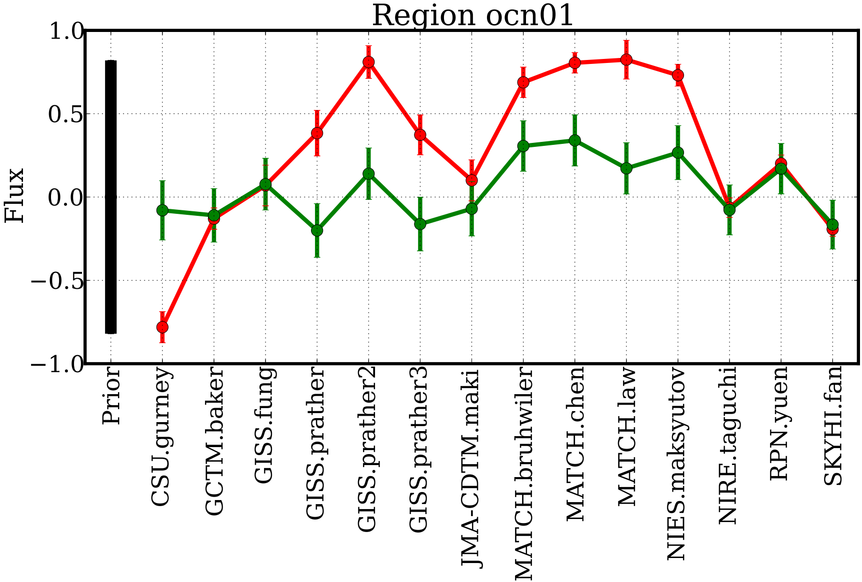

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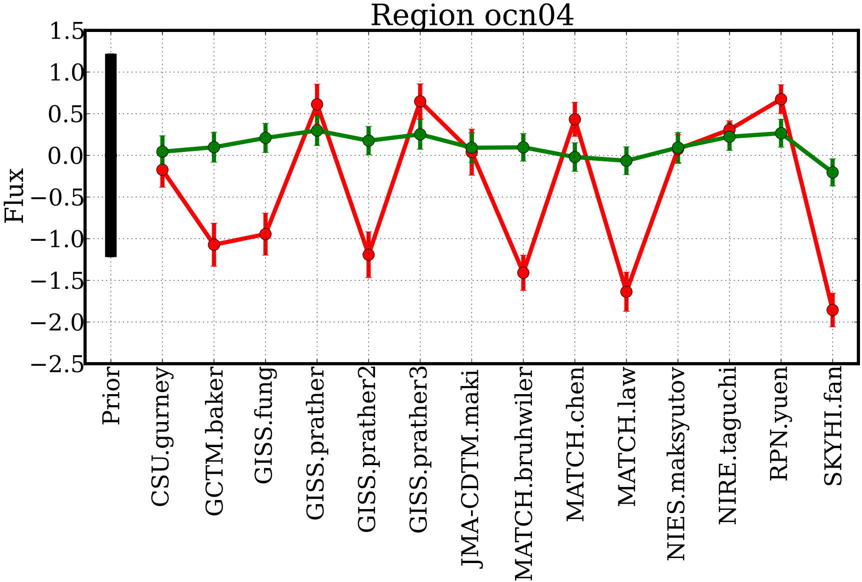

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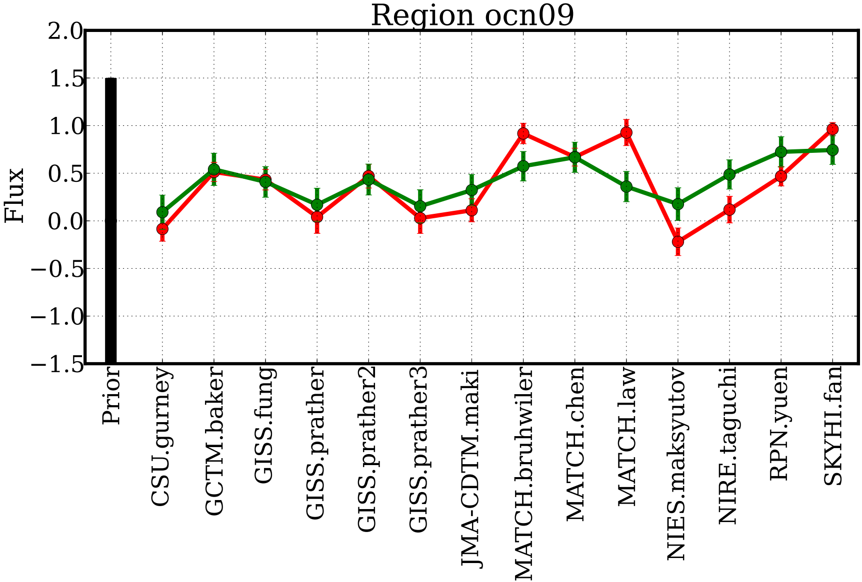

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