Embedded Model Error Representation

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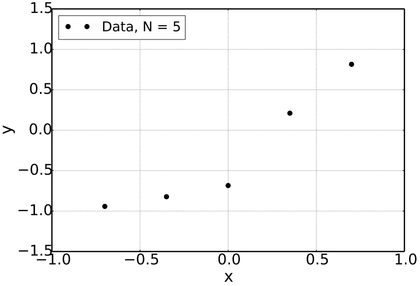
Main target

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

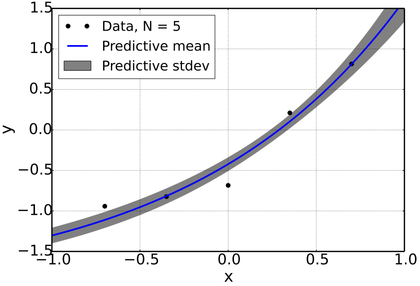
Motivation



Model-data fit

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

Motivation



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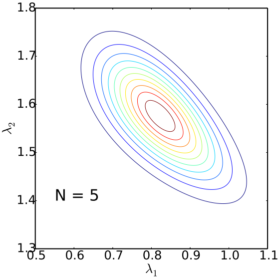
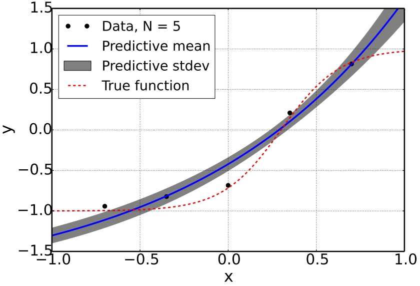


Posterior on parameters

- 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
  - Preditive mean and standard deviation

Motivation



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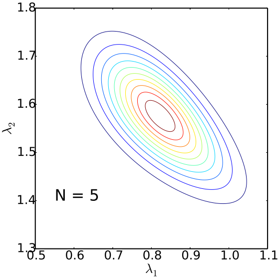

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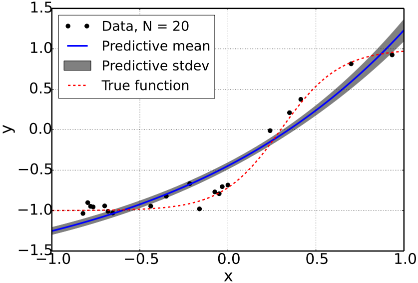
- Discrepancy between data and prediction presumed exclusively due to *i.i.d.* Gaussian data noise – $y = f(x, \lambda) + \epsilon_{\rm d}$
- True model $g(x)$ – dashed-red – differs from fit model $f(x, \lambda)$
- Actual discrepancy includes both data and model errors

Motivation



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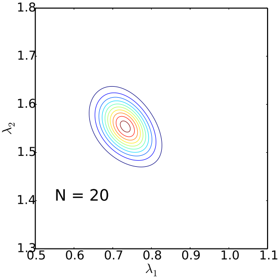

Posterior on parameters

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

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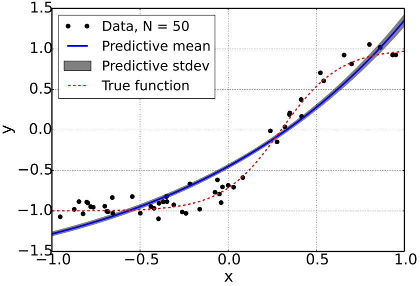

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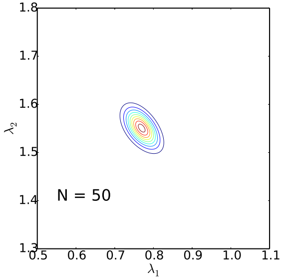

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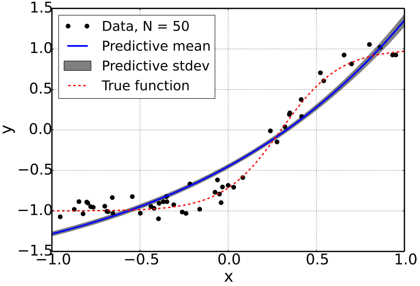

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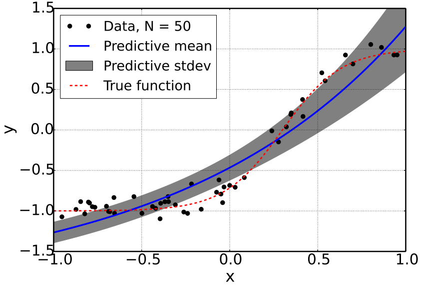


What we want

- 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
- 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

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

  ... even simpler, *additive correction term*

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

- 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 $\delta(\alpha, \xi)$

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

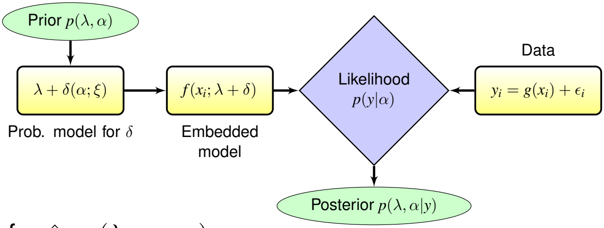
- Embed model error in specific submodel phenomenology
  - a modified transport or constitutive law
  - a modified formulation for a material property
- Allows placement of model error term in locations where key modeling assumptions and approximations are made
  - as a correction or high-order term
  - 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): $\begin{cases} \delta_1 = \alpha_{11}\xi_1 \\ \delta_2 = \alpha_{21}\xi_1 + \alpha_{22}\xi_2 \\ \vdots \\ \delta_d = \alpha_{d1}\xi_1 + \alpha_{d2}\xi_2 + \cdots + \alpha_{dd}\xi_d \end{cases}$
- 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

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

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

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\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

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\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

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

- 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

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

Model Error – Predictions

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

- 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

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

- 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

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

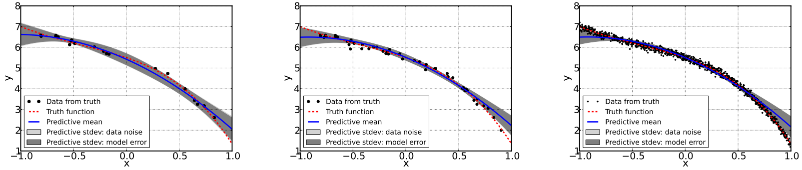
- Decomposition of predictive variance

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

More data leads to ‘leftover’ model error

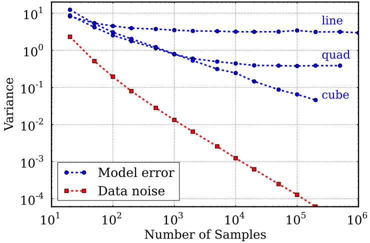
Calibrating a quadratic $f(x) = \lambda_0 + \lambda_1 x + \lambda_2 x^2$
w.r.t. ‘truth’ $g(x) = 6 + x^2 - 0.5(x+1)^{3.5}$ measured with noise $\sigma = 0.1$.

$N = 20$ $N = 50$ $N = 1000$



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



Challenges

- Density estimation is more challenging than parameter estimation
    - Inverse problem is ill-posed or intractable

  $\Rightarrow$ Employ approximate or empirical likelihoods

- Potentially a high-dimensional Bayesian problem
    - Full posterior may be inaccessible...

  $\Rightarrow$ Resort to optimization algorithms in no-noise case
    - ... or hard to sample from

  $\Rightarrow$ Adaptive MCMC algorithms, Likelihood-informed subspaces

- Sparse data or expensive high-fidelity simulations
    - With low information content, calibration may struggle

  $\Rightarrow$ More informative priors/regularization

Summary

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

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

- Optimal design for maximum information
- Optimal embedding
- Bayesian problem still hard; MCMC, priors, ...
- Hierarchical Bayesian viewpoint
- More intrusive embedding; problem specific

Applications

Model-to-model calibration: ignition model

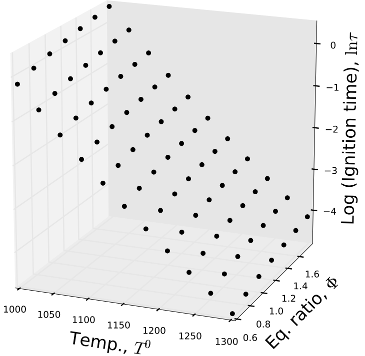
- Homogeneous ignition, methane-air mixture
- Single-step global reaction model calibrated against a detailed chemical kinetic model

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

$$\mathrm{CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O}$$

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

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

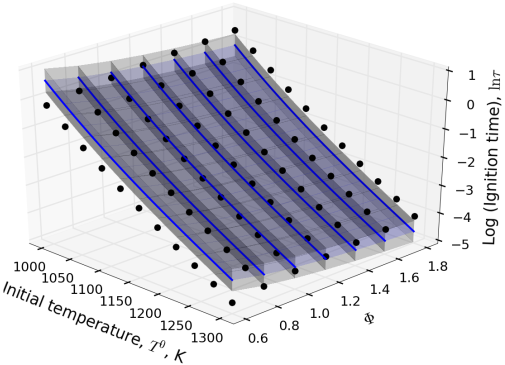


Model-to-model calibration: ignition model

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



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TransCom3 Experiment of CO_2 Flux Inversion

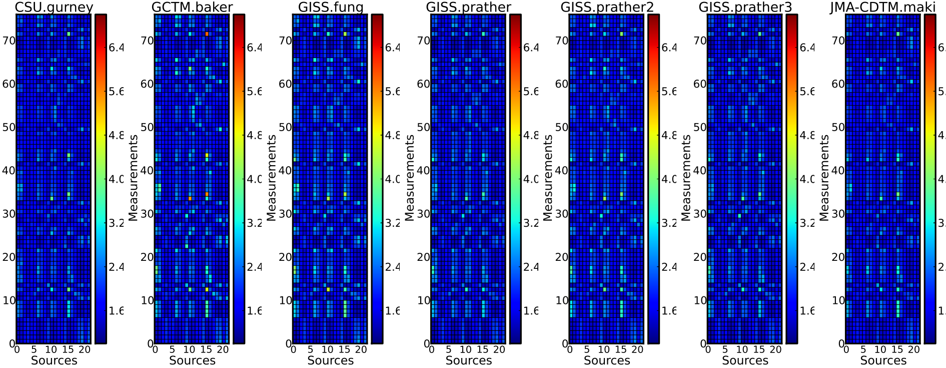
[Gurney *et al.*, Tellus B, 2003]

- 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 $\mathbf{d} \approx \mathbf{R}\mathbf{s}$

$$\mathbf{d} = \mathbf{R}\mathbf{s} + \epsilon_{\mathbf{d}}$$

- 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 $\boldsymbol{s}$: $\mathbf{d} = \mathbf{R}(\mu_\mathbf{s} + \mathbf{C}_\mathbf{s}\xi)$

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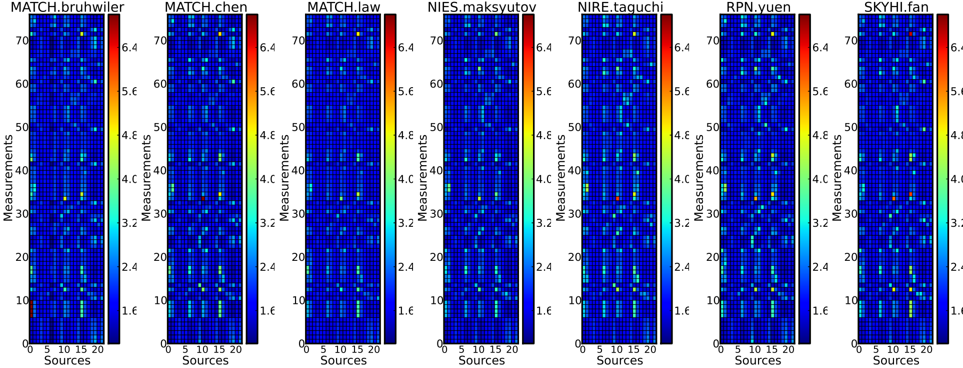

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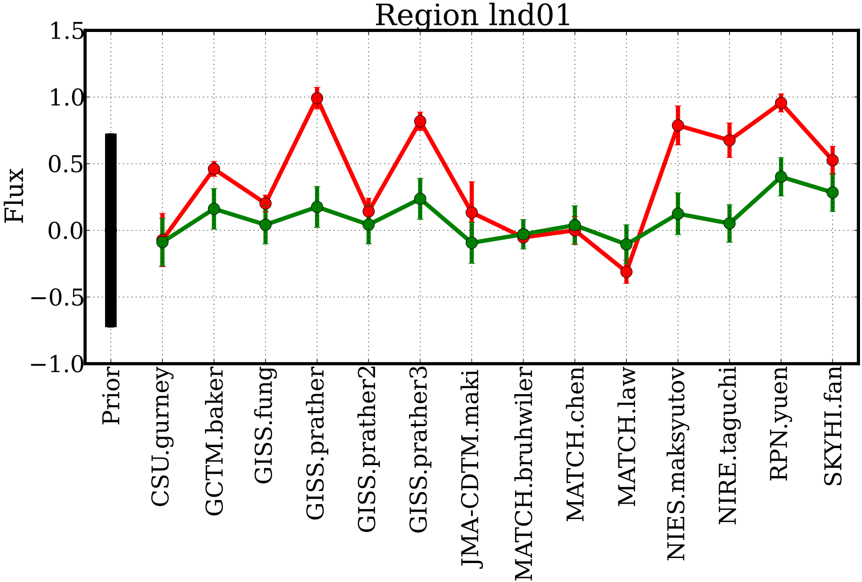
Inferred fluxes show less variability across models



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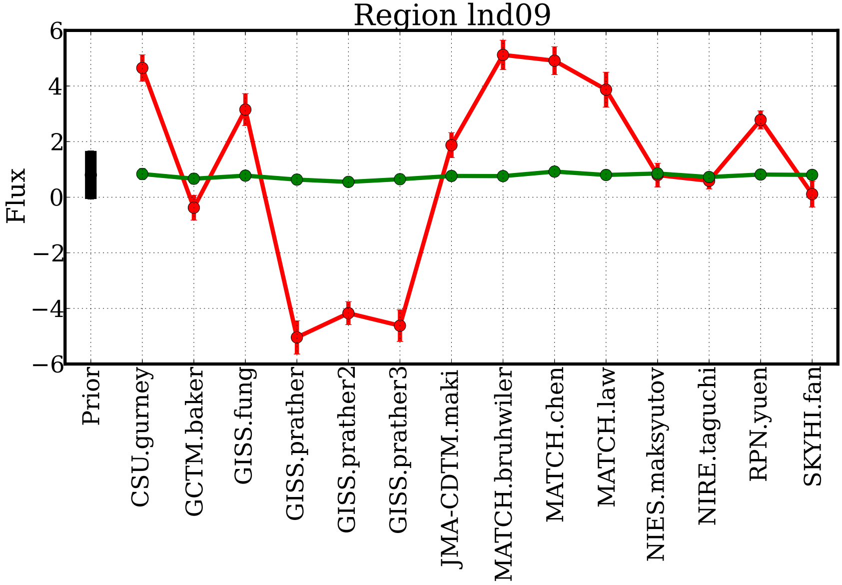

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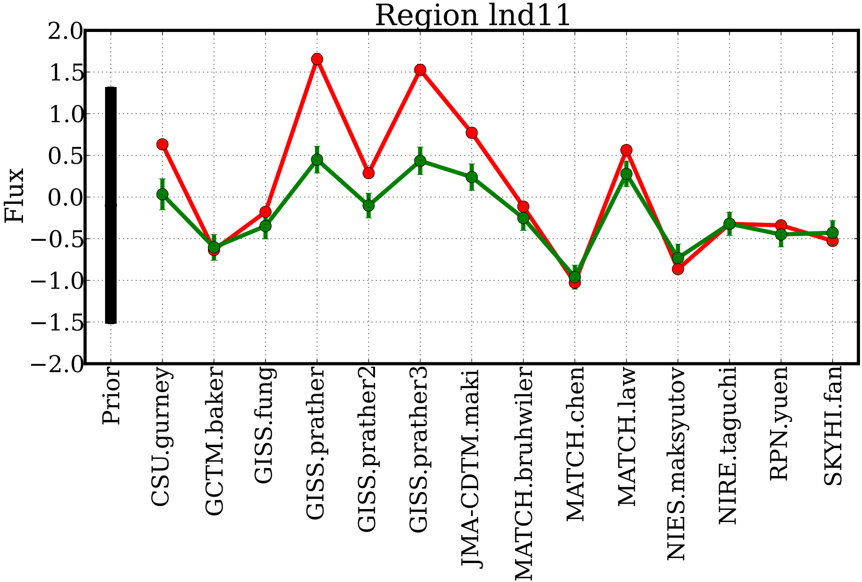

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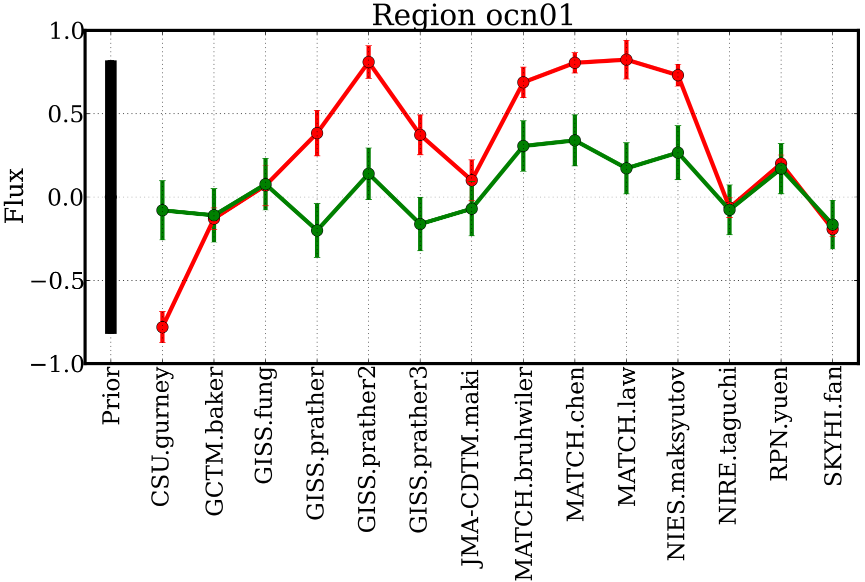

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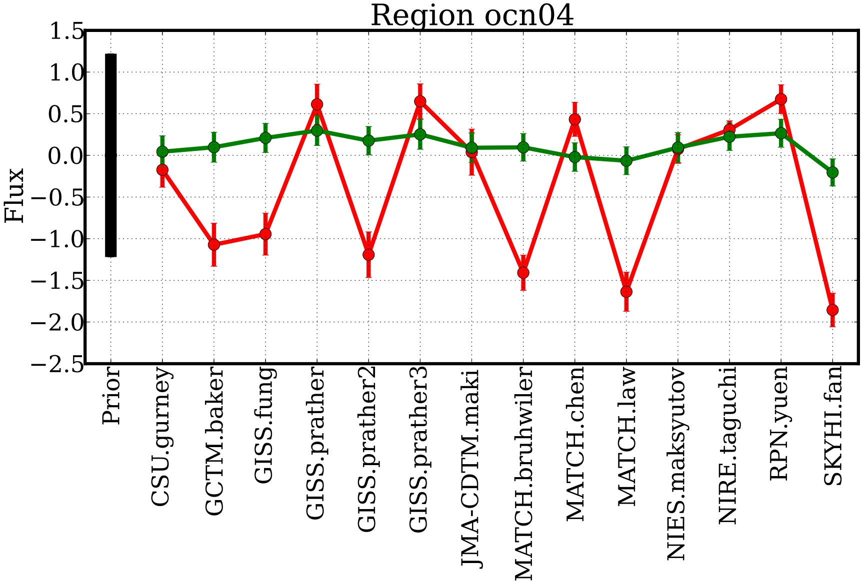

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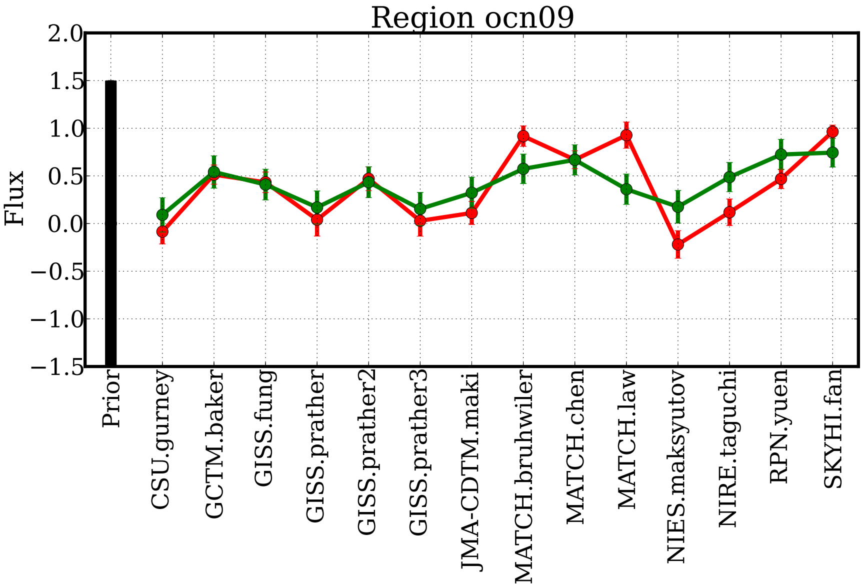

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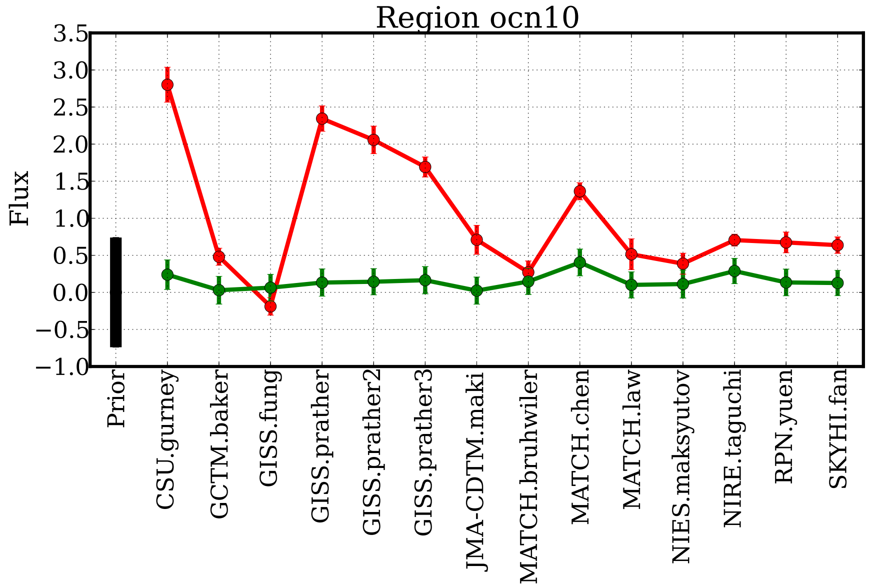

LES computation in Scramjet engine: static-vs-dynamic SGS model calibration

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