Embedded Framework for Model Error Quantification and Propagation

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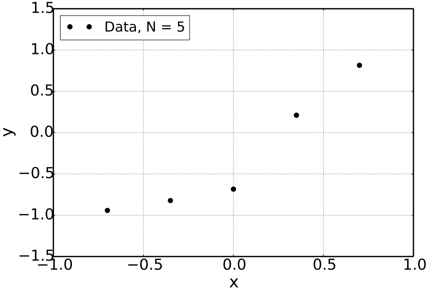
Main target: model error $g(x) \approx f(x; \lambda)$

deviation from 'truth' or from a higher-fidelity model

- ... otherwise called (with slightly altered meanings):
  model discrepancy, model structural error,
  model inadequacy, model misspecification,
  model form error, model uncertainty
- Inverse modeling context
  - Given experimental or higher-fidelity model data, estimate the model error
- Represent and estimate the error associated with
  - Simplifying assumptions, parameterizations
  - Mathematical formulation, theoretical framework
- ...will be useful for
  - Model validation
  - Model comparison
  - Scientific discovery and model improvement
  - Reliable computational predictions

Ignoring model error leads to overconfident and biased predictions



Model-data fit

- Given noisy data, calibrate an exponential model: $g(x) \approx f(x; \lambda)$

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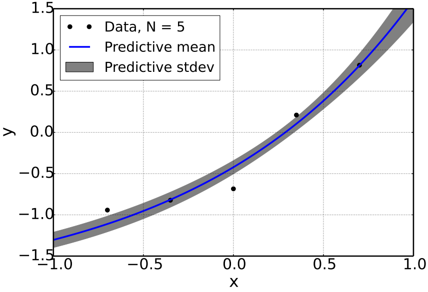

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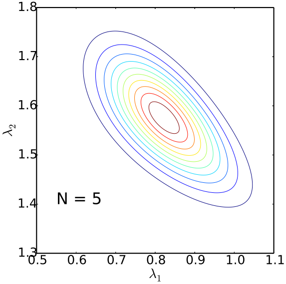

Posterior on parameters

- Given noisy data, calibrate an exponential model: $g(x) \approx f(x; \lambda)$
- Employ Bayesian inference to obtain posterior PDFs on λ

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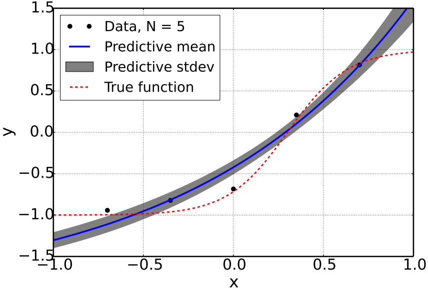

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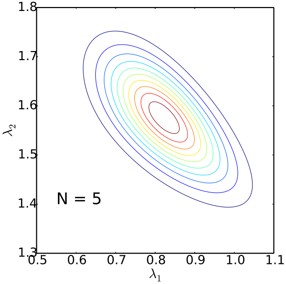

Posterior on parameters

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- True model – dashed-red – is *structurally* different from fit model $f(x,\lambda)$

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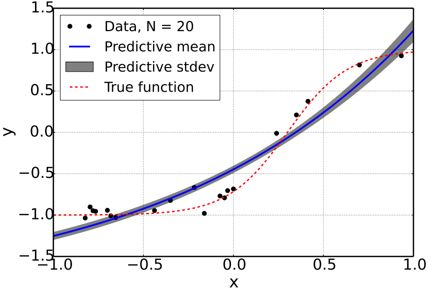

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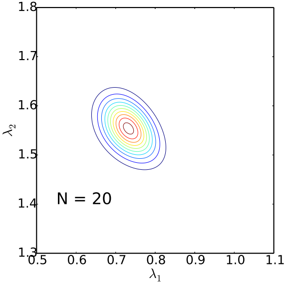

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- Higher data amount reduces posterior and predictive uncertainty
  - Increasingly sure about predictions based on the *wrong* model

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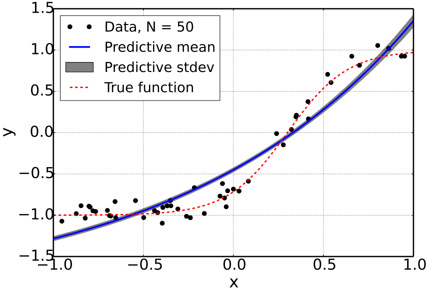

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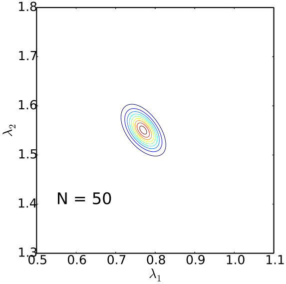

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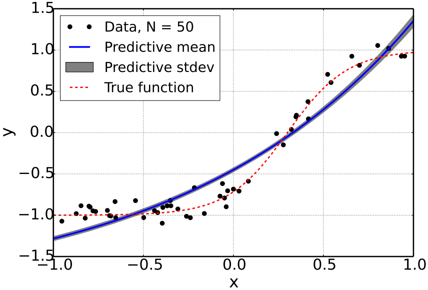
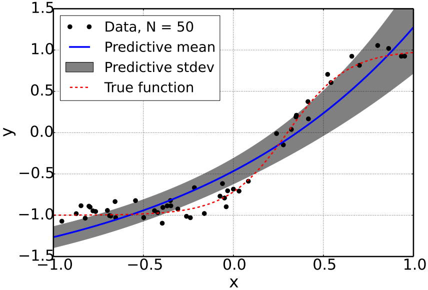


No model error treatment



Model error accounted for

- Given noisy data, calibrate an exponential model: $g(x) \approx f(x;\lambda)$
- Employ Bayesian inference to obtain posterior PDFs on λ
- True model – dashed-red – is *structurally* different from fit model $f(x, \lambda)$
- Accounting for model error allows extra uncertainty component to propagate through predictions

Where to put model error?

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

- Outside:
  - Explicit GP representation [Kennedy-O'Hagan, 2001]
  - See also [Higdon et. al, 2004], [Bayarri et. al, 2007]
  - Usage: too many to cite
  - Issues: see next slide
  - Variants exist: multiplicative noise, non-linear maps etc.

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

- Inside:
  - Increased use, especially in physical models: [Emory et. al, 2011] [Oliver and Moser, 2011], [Morrison et. al, 2016], [Sondak et. al, 2017], [Huan et. al, 2017], [Rizzi et. al, 2018]...
  - Engineering/statistical adjustment [Joseph and Melkote, 2009]
  - Additive corrections to submodels [Strong et. al, 2011]
  - Validation of extrapolative predictions [Oliver et. al, 2014]
  - Field inversion and machine learning [Duraisamy et. al, 2015-]
  - Hybrid correction [He and Xiu, 2016]
  - Random field correction [Brown and Atamturktur, 2016]
  - Hierarchical mixture model [Feng, 2017]
  - Parameter inflation [Pernot et. al, 2017]
  - Hierarchical stochastic model [Wu et. al, 2017]
  - Dynamic discrepancy [Bhat et. al., 2017]

External correction often not satisfactory for physical models

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

- Explicit additive statistical model for model error [KOH, 2001]
- Potential violation of physical constraints
- Disambiguation of model error $\delta(x_i)$ and data error ϵ_i
- Yes, priors help: [Brynjarsdottir and O'Hagan, 2014], [Plumlee, 2017]
- 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 $\delta(x)$

Case for Model Error Embedding

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

$$y_i = \tilde{f}(x_i; \lambda, \delta_\alpha) + \epsilon_i$$

- Embed model error in specific submodel phenomenology
  - a modified transport or constitutive law
  - a modified formulation for a material property
  - turbulent model constants
- 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
- Disambiguates model/data errors

Embedded Model Error Options

- Explore different model forms,

Intrusive

$$y_i = \tilde{f}(x_i; \lambda, \delta_\alpha(x_i)) + \epsilon_i$$

- Additive stochastic corrections to existing inputs

Non-intrusive

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

- ... even simpler, x-independent

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

Bayesian Framework for Model Error Estimation

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

- Given data y_i, perform *simultaneous* estimation of $\tilde{\alpha} = (\lambda, \alpha)$, i.e. model parameters λ and model-error parameters α.
- Bayes' theorem

$$\overbrace{p(\tilde{\alpha}|y)}^{\text{Posterior}} = \frac{\overbrace{p(y|\tilde{\alpha})}^{\text{Likelihood}}\ \overbrace{p(\tilde{\alpha})}^{\text{Prior}}}{\underbrace{p(y)}_{\text{Evidence}}}$$

- In order to estimate the likelihood $L_y(\tilde{\alpha}) = p(y|\tilde{\alpha}) = p(y|\lambda, \alpha)$, one needs uncertainty propagation through $f(x_i; \underbrace{\lambda + \delta_\alpha}_{\text{stochastic}})$,
- ... hence, we employ Polynomial Chaos (PC) representation for δ_α.

Polynomial Chaos Representation of Augmented Input

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

- Zero-mean PC form $\delta_\alpha = \sum_{k=1}^{K} \alpha_k \Psi_k(\xi)$
- Functional representation of a large class of random variables
- The PC *germ* ξ is a standard random variable
  - e.g. Uniform$(-1, 1)$ or Normal$(0, 1)$
- The PC bases (e.g. Legendre or Hermite polynomials) are orthogonal w.r.t. PDF of ξ

$$\int \Psi_m(\xi)\Psi_k(\xi)\pi_\xi(\xi)d\xi = 0 \quad \text{for } m \neq k.$$

- PC representation allows efficient
  - Sampling
  - Moment estimation
  - Variance-based decomposition
  - Uncertainty propagation (via NISP)

Model Error – Likelihood construction

$$y_i = f(x_i; \lambda + \delta_\alpha(\zeta)) + \epsilon_i = f_i(\tilde{\alpha}, \zeta) + \epsilon_i$$

- Likelihood $\mathcal{L}_g(\tilde{\alpha}) = p(y|\tilde{\alpha})$ challenging, but can compute moments

$$\mu_i(\tilde{\alpha}) = \mathbb{E}_\zeta[f_i(\tilde{\alpha}, \zeta)] \qquad \text{and} \qquad \sigma_i^2(\tilde{\alpha}) = \mathbb{V}_\zeta[f_i(\tilde{\alpha}, \zeta)] + s_i^2$$

GM Gauss-Marginal Approximate Likelihood:

$$\log \mathcal{L}_g(\tilde{\alpha}) \approx \sum_{i=1}^N \left[- \log \sigma_i(\tilde{\alpha}) - \frac{1}{2} \left(\frac{y_i - \mu_i(\tilde{\alpha})}{\sigma_i(\tilde{\alpha})} \right)^2 \right]$$

ABC Moment-matching / Approximate Bayesian Computation:

$$\log \mathcal{L}_g(\tilde{\alpha}) \approx \sum_{i=1}^N \left[-\frac{1}{2} \left(\frac{y_i - \mu_i(\tilde{\alpha})}{\epsilon_\mu} \right)^2 - \frac{1}{2} \left(\frac{\sigma_i(\tilde{\alpha}) - \gamma |y_i - \mu_i(\tilde{\alpha})|}{\epsilon_\sigma} \right)^2 \right]$$

- Non-intrusive spectral projection (NISP) with Polynomial Chaos

$$f_i(\tilde{\alpha}, \zeta) \overset{\text{NISP}}{\simeq} \sum_k f_{ik}(\tilde{\alpha}) \Psi_k(\zeta)$$

- ... provides easy access to mean and variance

$$\mu_i(\tilde{\alpha}) = f_{i0}(\tilde{\alpha}) \qquad \text{and} \qquad \sigma_i^2(\tilde{\alpha}) = \sum_{k \neq 0} f_{ik}^2(\tilde{\alpha}) ||\Psi_k||^2 + s_i^2$$

Model Error – Surrogate and Prediction

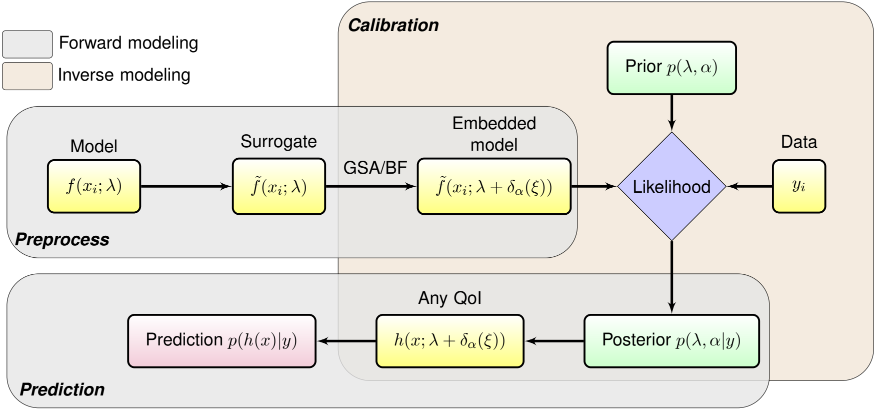
$$f_i(\lambda + \delta_\alpha(\zeta)) = f_i(\tilde{\alpha}, \zeta) \quad \overset{\text{NISP}}{\simeq} \quad \sum_k f_{ik}(\tilde{\alpha}) \Psi_k(\zeta)$$

- NISP is employed both for likelihood computation and for posterior/pushed-forward predictions in general
- In practice, $f_i(\cdot)$ is replaced by a pre-constructed polynomial surrogate
- Note: NISP with finite truncation is exact, if one truncates NISP at the same order as the surrogate of $f_i(\cdot)$
- Posterior predictive moments

$$\mu_i = \mathbb{E}_{\tilde{\alpha}} \left[\mu_i(\tilde{\alpha}) \right]$$

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

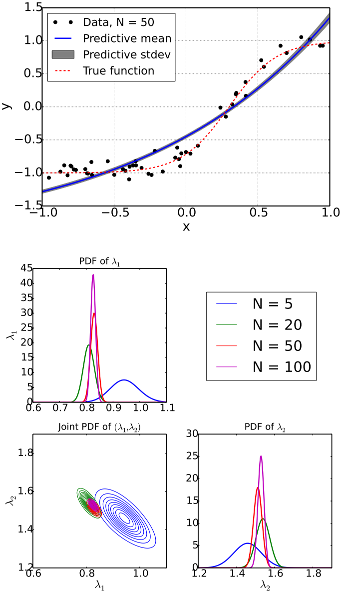
Model error embedding – workflow

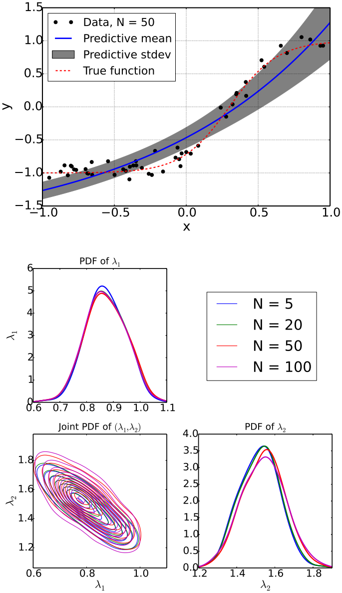


- Predictive uncertainty decomposition: Total Variance =

  Posterior uncertainty + Data noise + Model error + Surrogate error

.. back to toy example



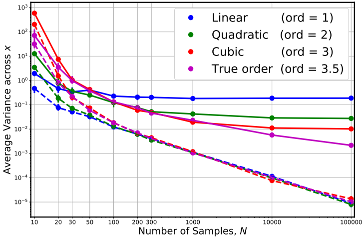


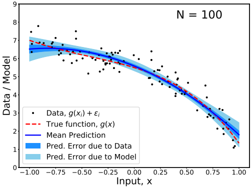
More data leads to ‘leftover’ model error

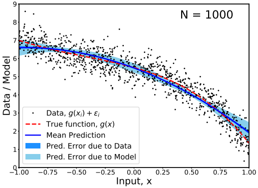
Calibrating a quadratic $f(x) = \lambda_0 + \lambda_1 x + \lambda_2 x^2$
w.r.t. ‘truth’ $g(x) = 6 + x^2 - 0.5(x+1)^{3.5}$ measured with noise $\sigma = 0.1$.

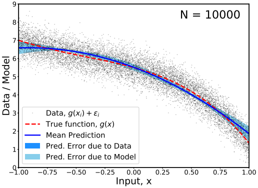
Summary of features:

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

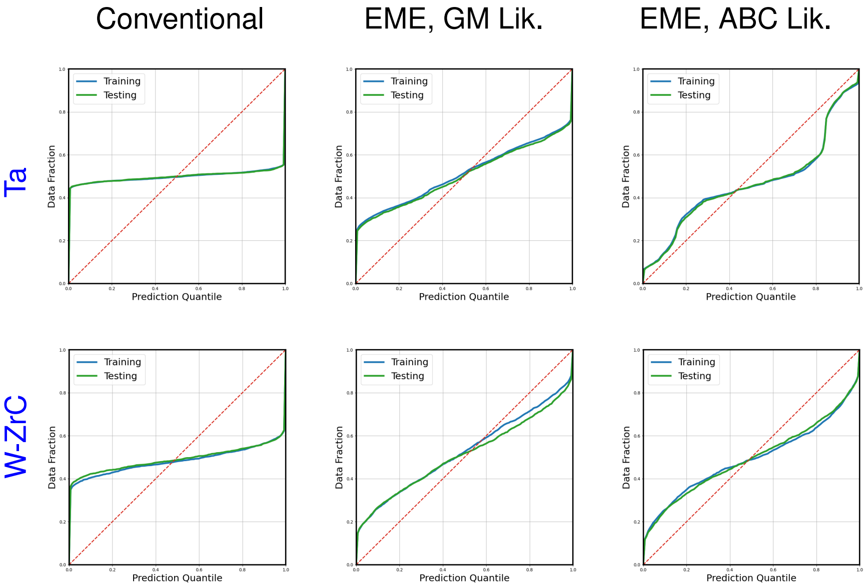








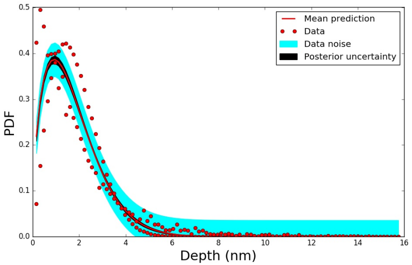
App.: Interatomic Potential Modeling



App.: Fusion Science

- Evolution of implanted gas in tungsten plasma-facing component
- Assess the uncertainties in helium flux
- Account for variability due to the two different data sources

Without EME



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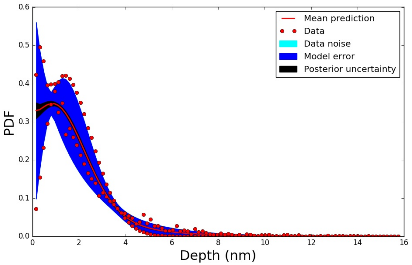


[O. Cekmer, K. Sargsyan, S. Blondel, H. Najm, D. Bernholdt,, B.D. Wirth, “Uncertainty quantification for incident helium flux in plasma-exposed tungsten”, *Int. J. Uncertainty Quantification*, 8(5), 2018]

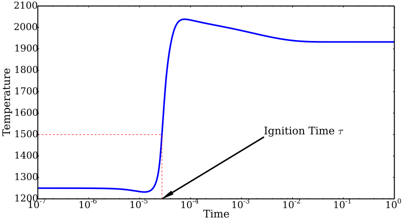
App.: Chemical Kinetics

- Two-step global reaction model calibrated against shock tube experimental data
- Operating conditions: pressure P, initial temperature T_0 & equivalence ratio ϕ

$$C_{12}H_{26} + \frac{25}{2}O_2 \xrightarrow{k_1} 12CO + 13H_2O$$

$$CO + \frac{1}{2}O_2 \underset{k_{2b}}{\overset{k_{2f}}{\rightleftharpoons}} CO_2.$$

$$k_1 = Ae^{\left(-\frac{E}{RT}\right)}[C_{12}H_{26}]^{0.25}[O_2]^{1.25}$$



- Data: log(ignition time)
- Embedding
  $(\ln A, E) = \sum_k \boldsymbol{\alpha}_k \Psi_k(\boldsymbol{\xi})$

[K. Sargsyan, X. Huan, H. Najm. "Embedded Model Error Representation for Bayesian Model Calibration", arXiv:1801.06768, in press, *Int. J. Uncert. Quant.*, 9(4), 2019]

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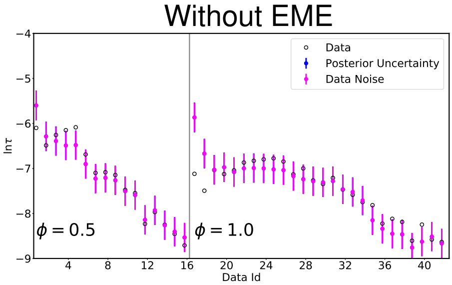
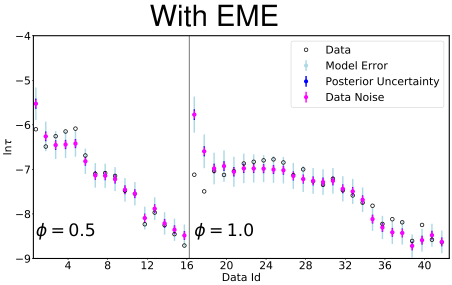
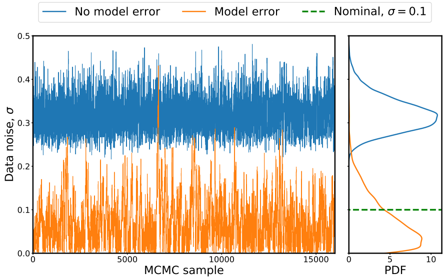


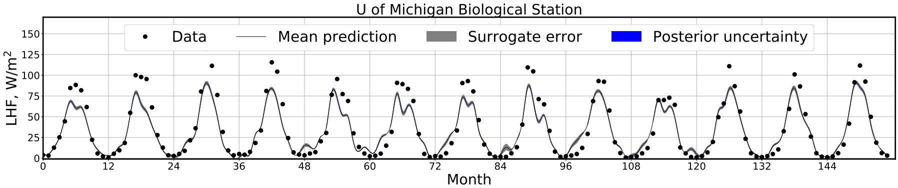


- Model error disambiguated from data error
- Data error correctly captured
- Meaningful extrapolative predictions



App.: E3SM Land Model (ELM)

- US Department of Energy (DOE) Earth system model, *e3sm.org*
- Land, atmosphere, ocean, ice, human system components
- High-resolution, employ DOE leadership-class computing facilities



- Conventional calibration without model error

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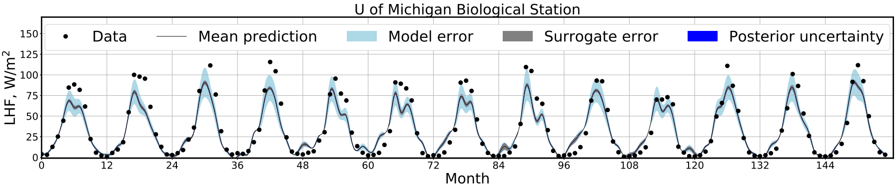

- Predictive variance decomposition with model-error component
- ... with predictive uncertainty that captures model error

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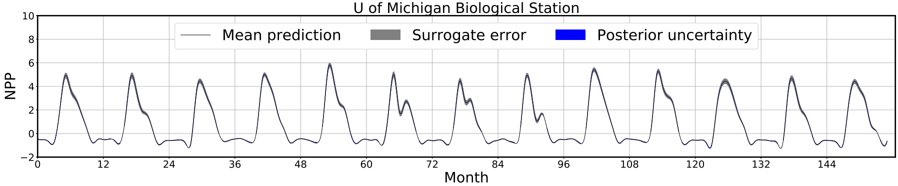

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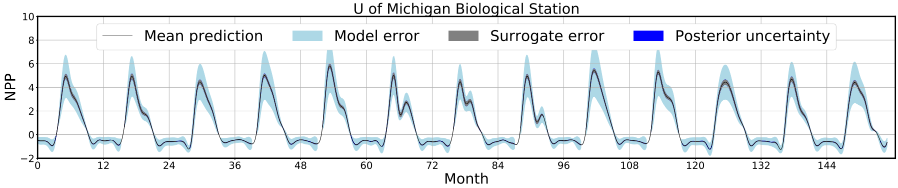

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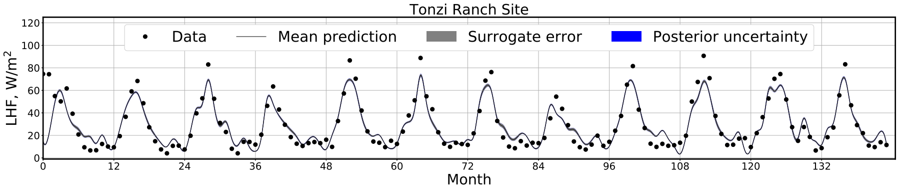

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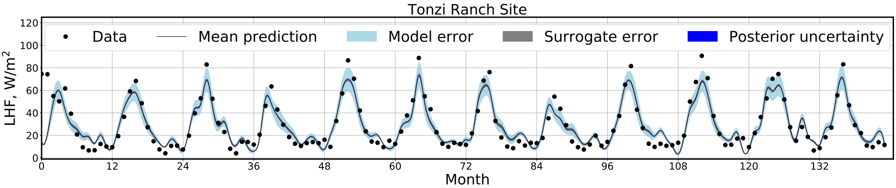

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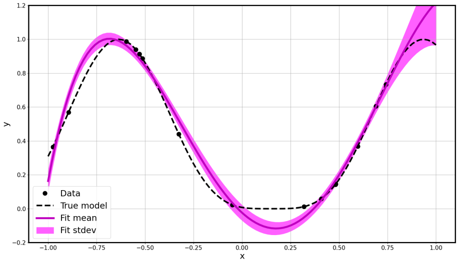
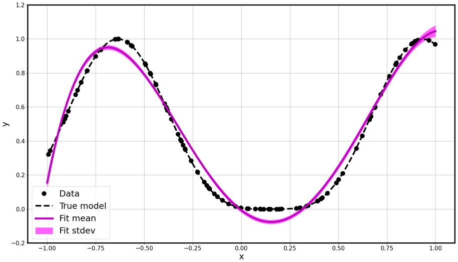
Connection to Variational Inference

Embedded Model Error	Variational Inference
Casting physical parameters λ as random variable	Casting (NN) weights w in a variational family
Infer (λ_0, λ_1)	Infer (μ, σ)
Bayesian/MCMC	Optimization/SGD
Uses ABC/Moment matching in the output	Uses Kullback-Leibler (KL) divergence in the input
PC-based propagation	Functional VI: KL in the output

EME uncertainty is well-calibrated compared to LSQ or VI

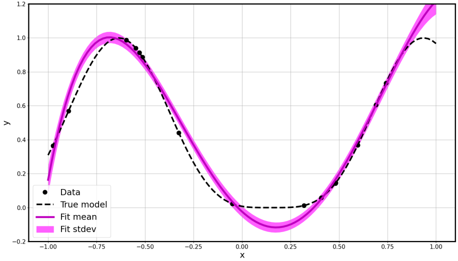
LSQ

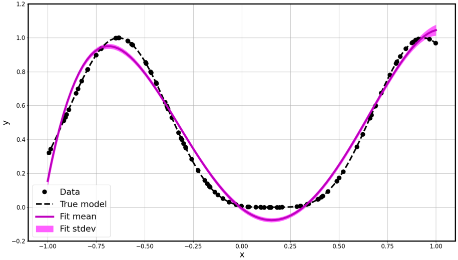




EME uncertainty is well-calibrated compared to LSQ or VI

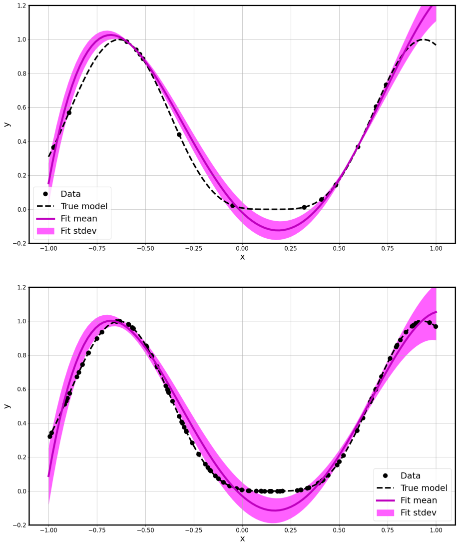
VI



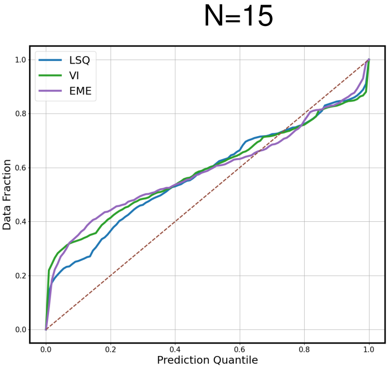


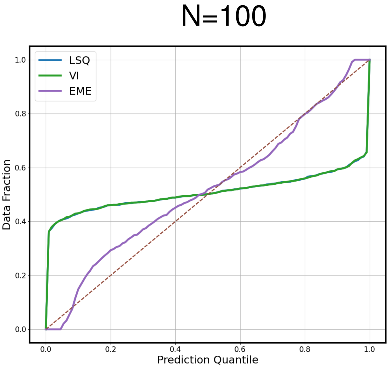
EME uncertainty is well-calibrated compared to LSQ or VI

EME



EME uncertainty is well-calibrated compared to LSQ or VI





Summary

- Embedded, but *non-intrusive* model error quantification
- PC-based representation and propagation
- Simultaneous estimation of model inputs and model error
- Predictive uncertainty attribution due to model error

- Challenges:
  - Higher-d inference problem
  - Identifiability
  - Prior selection
  - Where/how to embed
  - Likelihood degeneracy
  - Extrapolation/generalization

- Opportunities:
  - Field (x-dependent) correction
  - Intrusive, domain-knowledge corrections
  - Non-physical models: parallel to VI
  - Handling discrete/categorical inputs: parallel to BMA

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Thank you!

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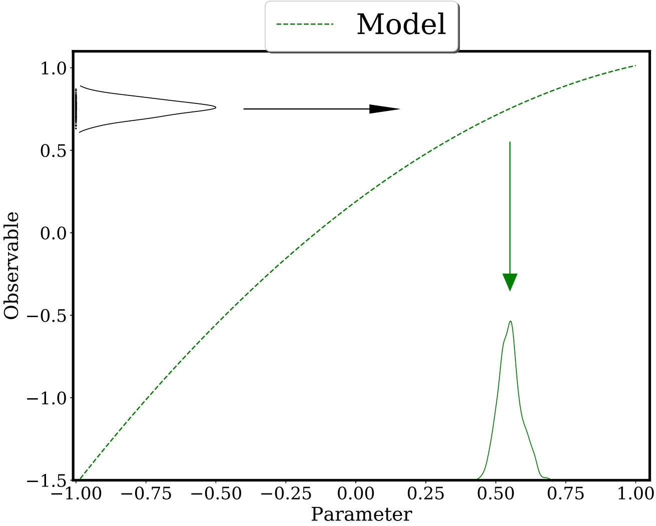
Additional Material

Data informs model parameters:

but what if the model is only an approximation?



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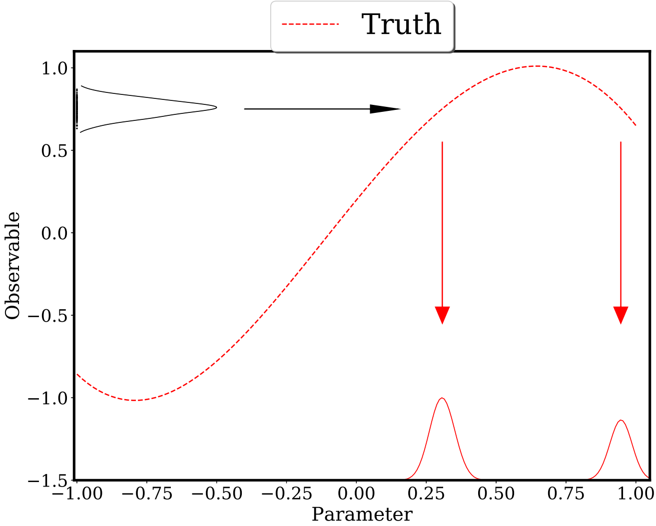

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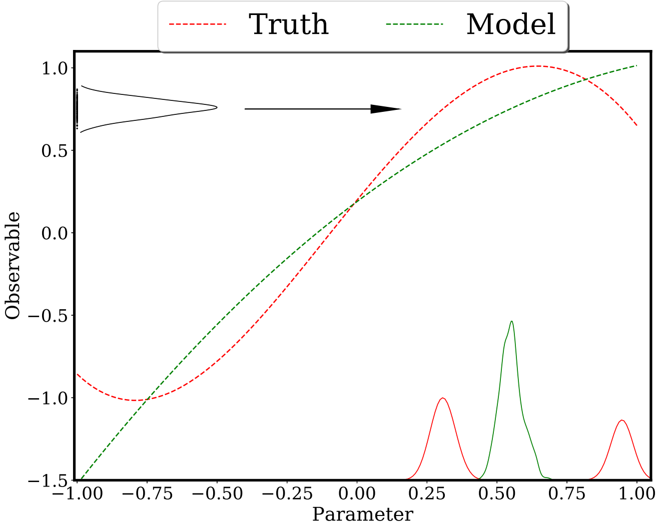

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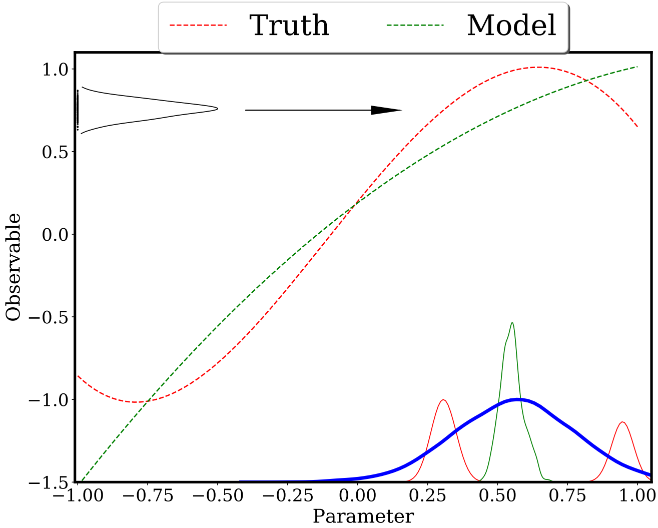
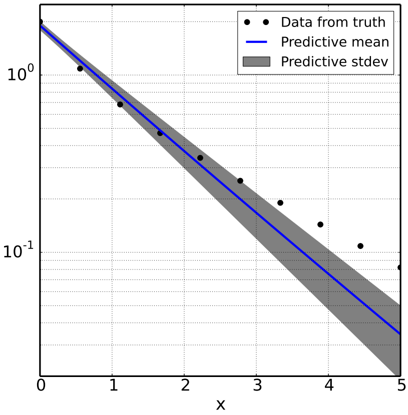


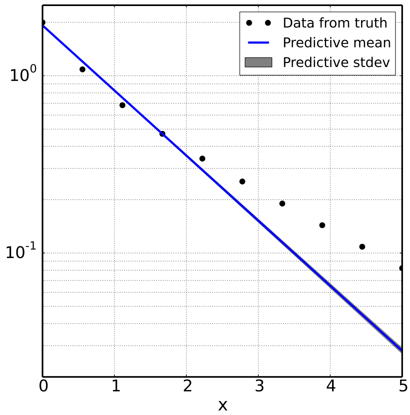
Predictions account for model error

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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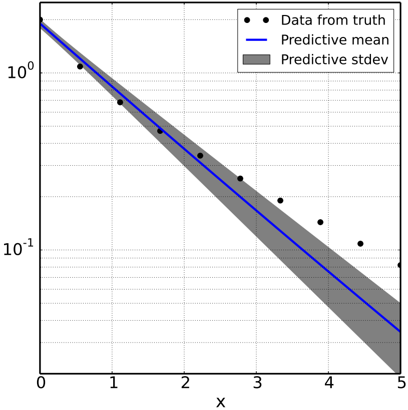
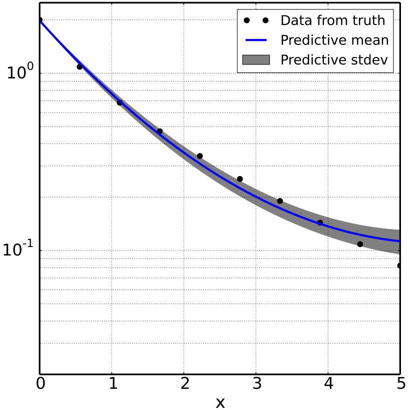


Quadratic-exponential $f_2(x, \lambda) = e^{\lambda_1 + \lambda_2 x + \lambda_3 x^2}$



Chemistry problem – ABC

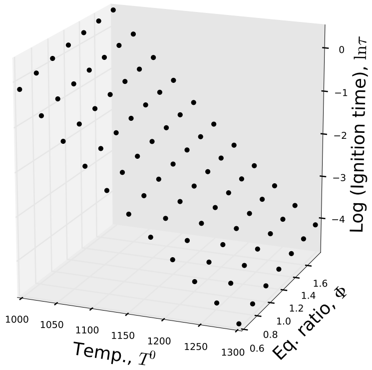
- Homogeneous ignition, methane-air mixture
- Single-step global reaction model calibrated against a detailed chemical kinetic model

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

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

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

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

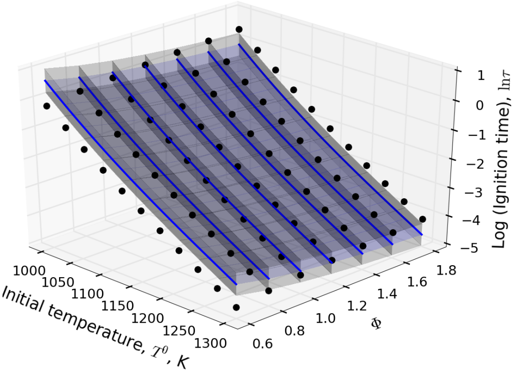


Quality of Uncertain Calibrated Model Predictions

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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”On the Statistical Calibration of Physical Models”
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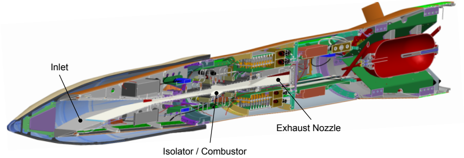
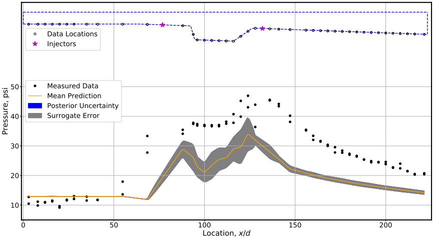
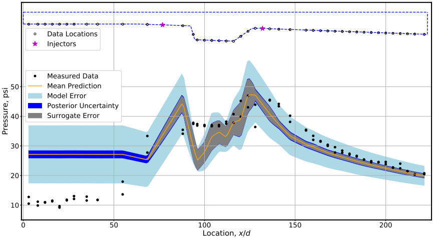
LES: Turbulent Combustion in Scramjet Engine

- HIFiRE (Hypersonic International Flight Research and Experimentation) scramjet
- Pressure data from NASA Langley Research Center
- Highly complex LES model







- Augmenting model error leads to more ‘physical’ likelihood

TransCom3 Experiment of CO_2 Flux Inversion

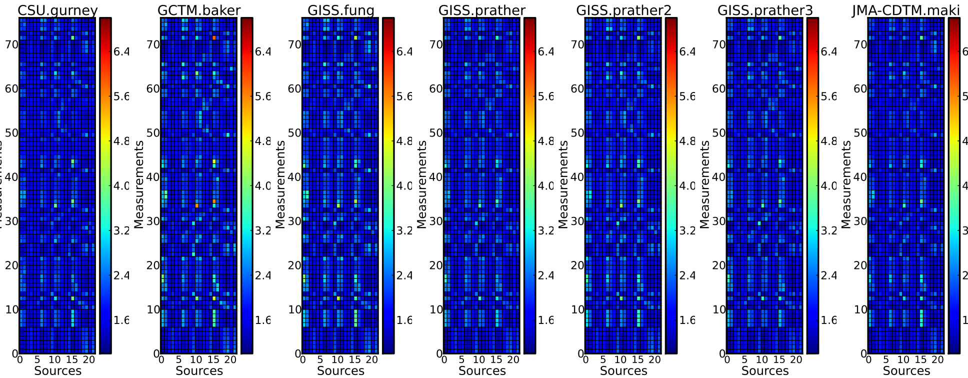
[Gurney *et al.*, Tellus B, 2003]

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

$$\mathbf{d} = \mathbf{R}\mathbf{s} + \boldsymbol{\epsilon}_{\mathbf{d}}$$

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

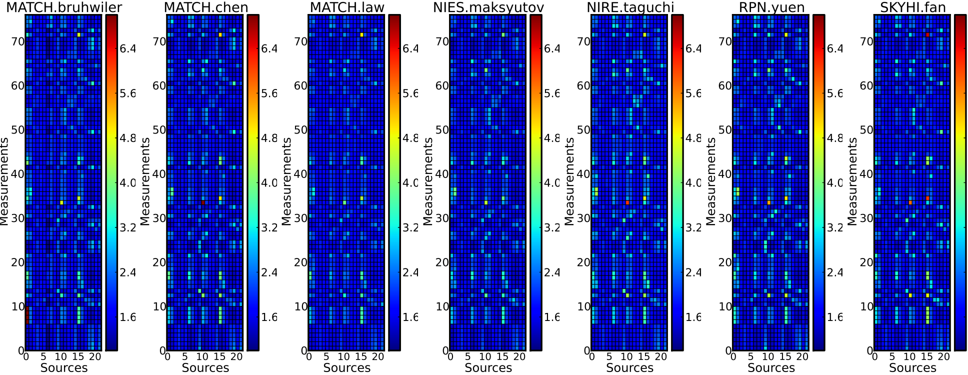
Consider 14 different response models $\mathbf{R}$



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

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



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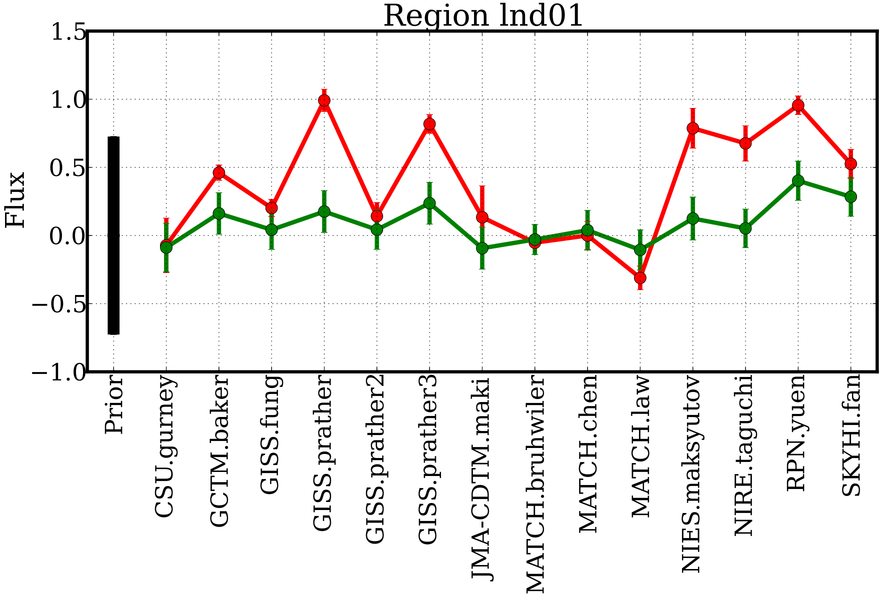
Inferred fluxes show less variability across models



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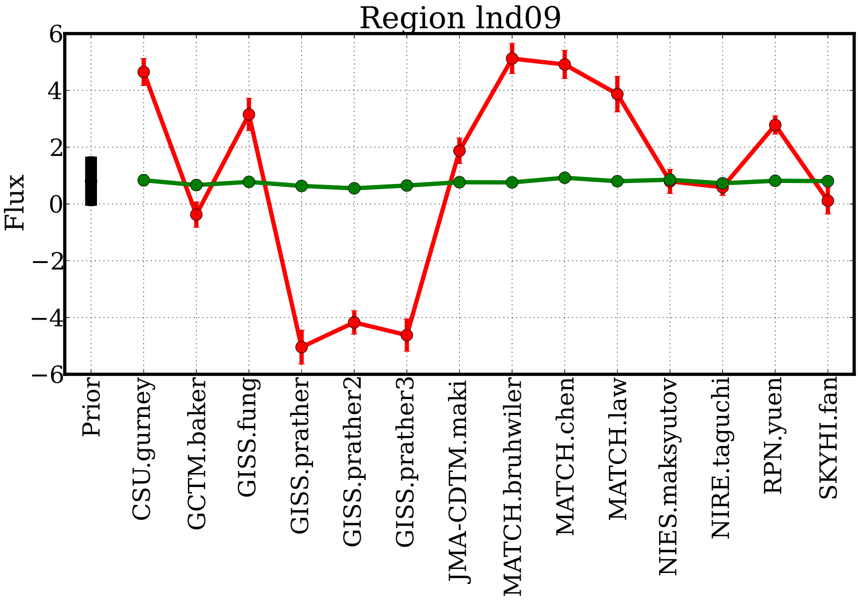

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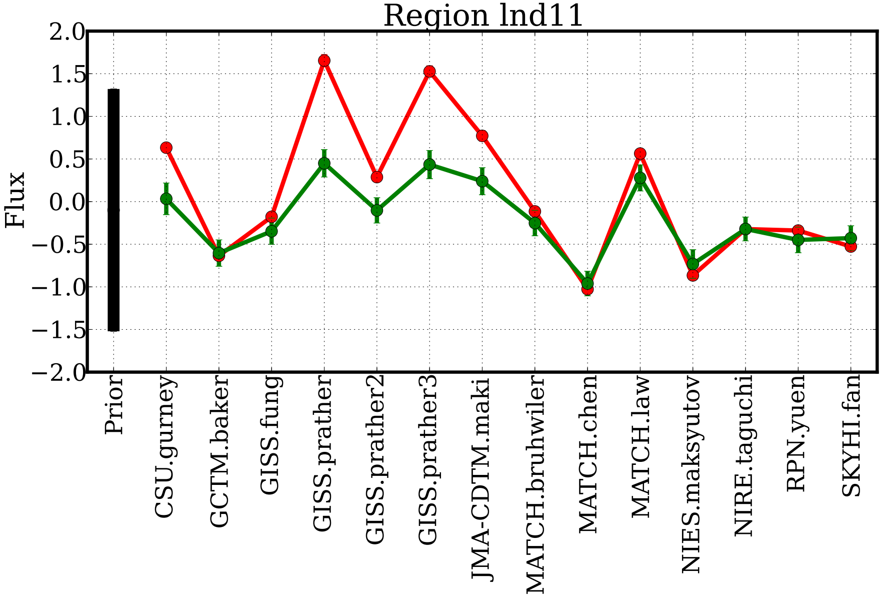

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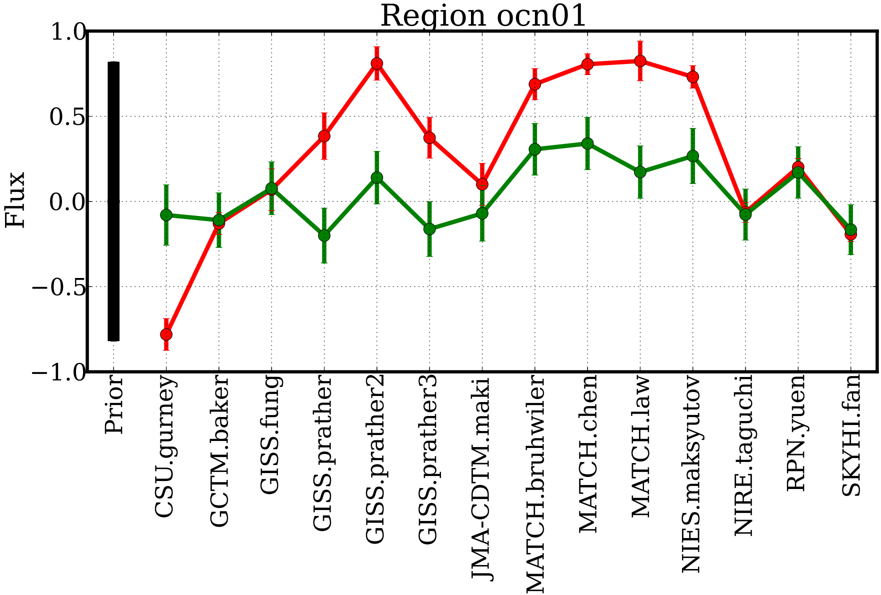

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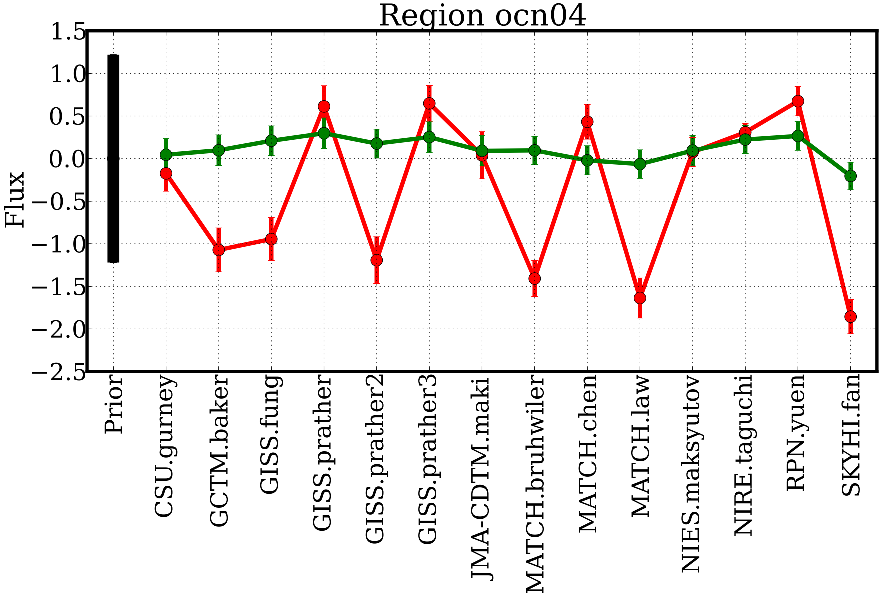

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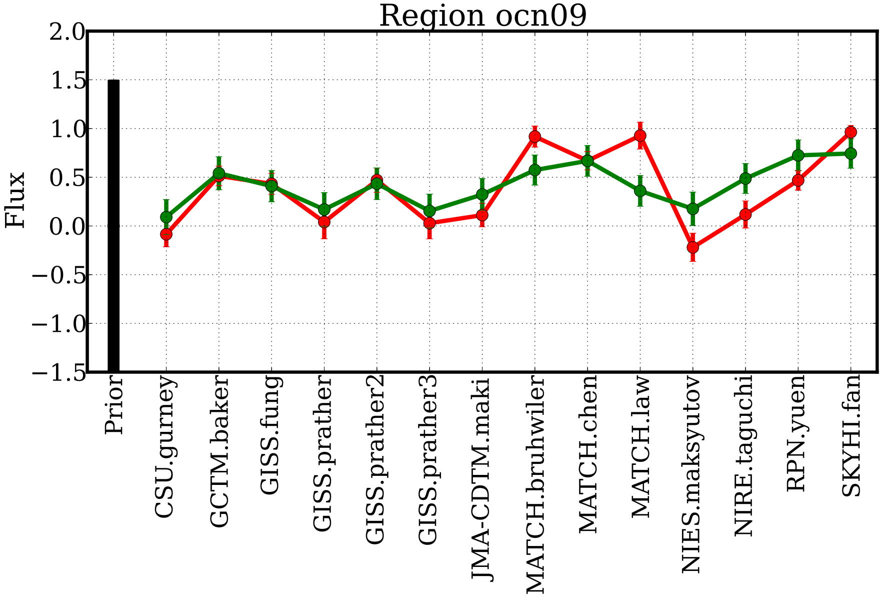

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