Bayesian Inference for Structural Error Quantification

Khachik Sargsyan, Xun Huan, Habib Najm

Sandia National Laboratories

Livermore, CA

SIAM CS&E
Spokane, WA
Feb 25 - Mar 1, 2019

Acknowledgements

T. Casey, B. Debusschere, C. Safta, — SNL, CA
M. Eldred, G. Geraci — SNL, NM

R. Ghanem — USC
Y. Marzouk, C. Feng — MIT
D. Ricciuto, P. Thornton – ORNL
J. Bender – LLNL

This work was supported by:

- DOE, Advanced Scientific Computing Research (ASCR), SciDAC
- DOE, Basic Energy Sciences (BES)
- DOE, Biological and Environmental Research (BER)
- DOD, DARPA Enabling Quantification of Uncertainty in Physical Systems (EQUiPS) program

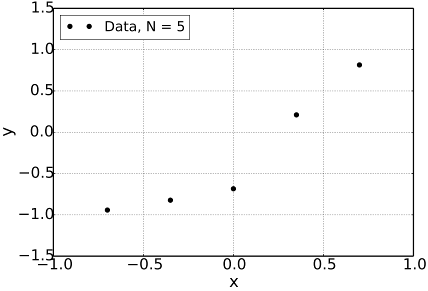
Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

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

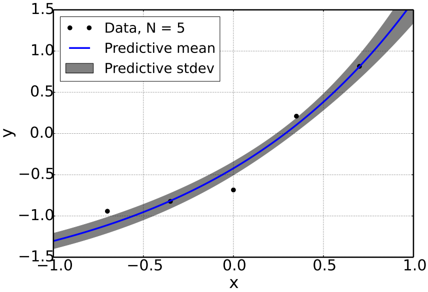
Ignoring model error leads to overconfident and biased predictions



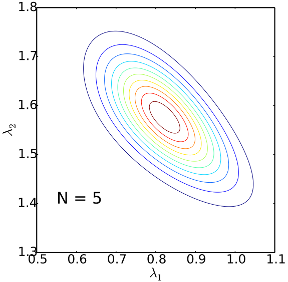
Model-data fit

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

Ignoring model error leads to overconfident and biased predictions



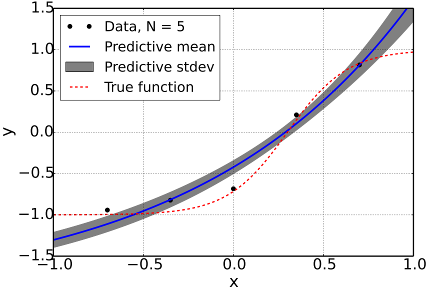
Model-data fit



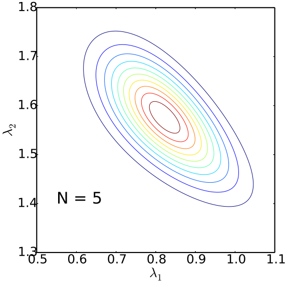
Posterior on parameters

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

Ignoring model error leads to overconfident and biased predictions



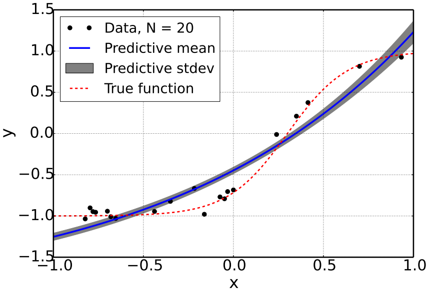
Model-data fit



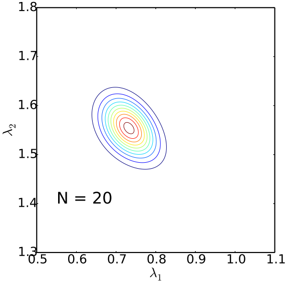
Posterior on parameters

- Given noisy data, calibrate an exponential model: $g(x) \approx f(x;\lambda)$
- Employ Bayesian inference to obtain posterior PDFs on λ
- True model – dashed-red – is *structurally* different from fit model $f(x,\lambda)$

Ignoring model error leads to overconfident and biased predictions



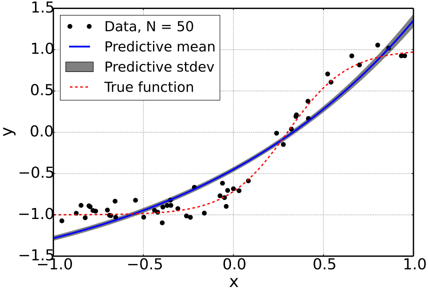
Model-data fit



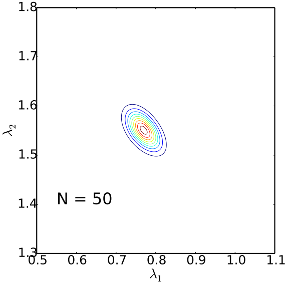
Posterior on parameters

- Given noisy data, calibrate an exponential model: $g(x) \approx f(x; \lambda)$
- Employ Bayesian inference to obtain posterior PDFs on λ
- True model – dashed-red – is *structurally* different from fit model $f(x, \lambda)$
- Higher data amount reduces posterior and predictive uncertainty
  - Increasingly sure about predictions based on the *wrong* model

Ignoring model error leads to overconfident and biased predictions



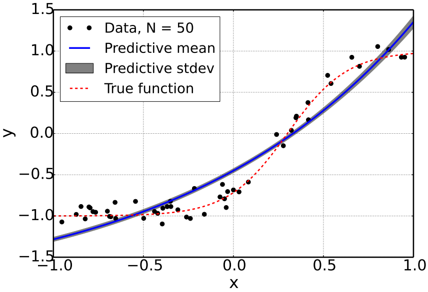
Model-data fit



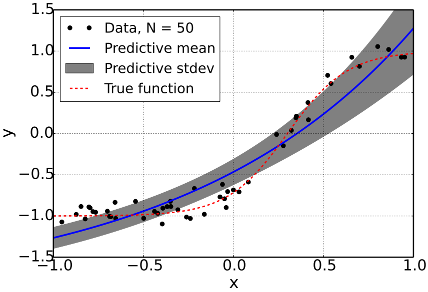
Posterior on parameters

- Given noisy data, calibrate an exponential model: $g(x) \approx f(x;\lambda)$
- Employ Bayesian inference to obtain posterior PDFs on λ
- True model – dashed-red – is *structurally* different from fit model $f(x,\lambda)$
- Higher data amount reduces posterior and predictive uncertainty
    - Increasingly sure about predictions based on the *wrong* model

Ignoring model error leads to overconfident and biased predictions



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?

- Outside:

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

  - 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.

- Inside:

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

  - 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

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

- Gauss-Marginal Approximate Likelihood compares data y_i and model predictions:

$$\mathcal{L}_g(\tilde{\alpha}) \approx \frac{1}{(2\pi)^{N/2}} \prod_{i=1}^N \frac{1}{\sigma_i(\tilde{\alpha})} \exp\left(-\frac{1}{2}\left(\frac{y_i - \mu_i(\tilde{\alpha})}{\sigma_i(\tilde{\alpha})}\right)^2\right)$$

- 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

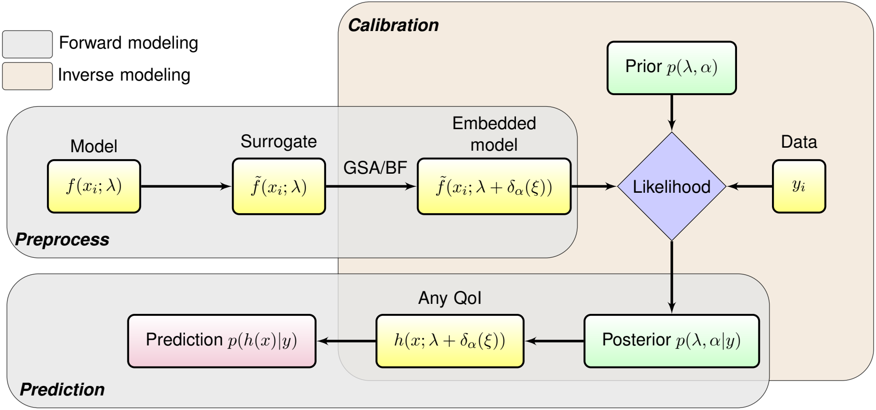
$$f_i(\lambda + \delta_\alpha(\zeta)) = f_i(\tilde{\alpha}, \zeta) \quad \overset{\text{NISP}}{\simeq} \quad \sum_k f_{ik}(\tilde{\alpha})\Psi_k(\zeta)$$

- 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

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

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

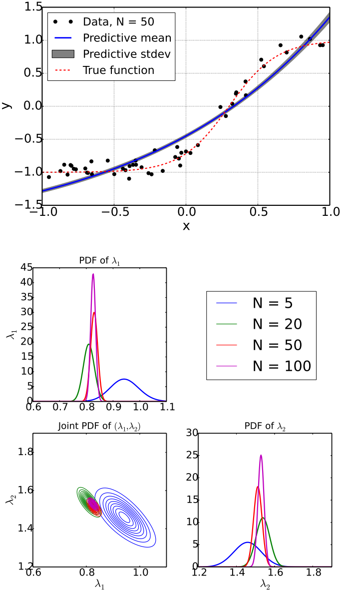
Model error embedding – workflow

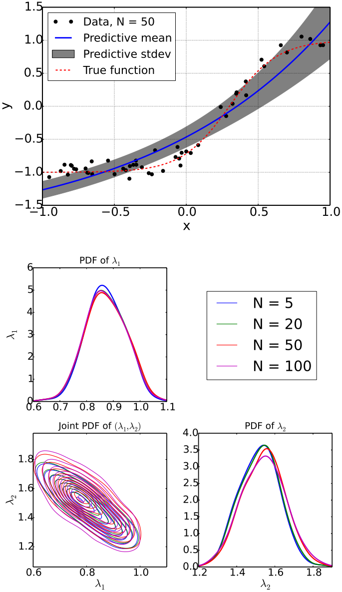


- Predictive uncertainty decomposition: Total Variance =

  Posterior uncertainty + Data noise + Model error + Surrogate error

.. back to toy example



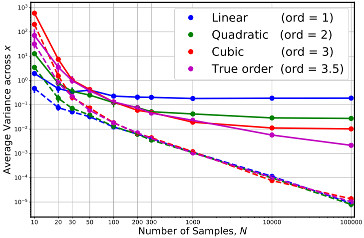


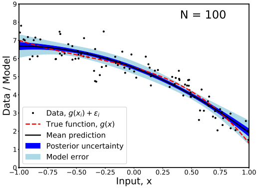
More data leads to ‘leftover’ model error

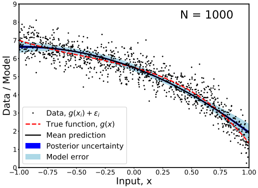
Calibrating a quadratic $f(x) = \lambda_0 + \lambda_1 x + \lambda_2 x^2$
w.r.t. ‘truth’ $g(x) = 6 + x^2 - 0.5(x+1)^{3.5}$ measured with noise $\sigma = 0.1$.

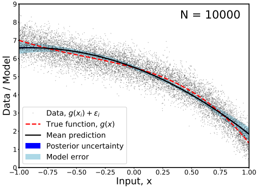
Summary of features:

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









Ignition time in chemical kinetics

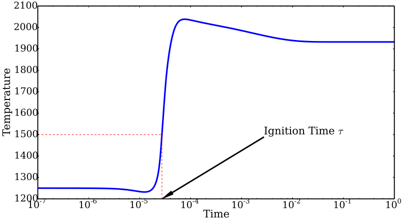
- Two-step global reaction model calibrated against shock tube experimental data
- Operating conditions: pressure P, initial temperature T_0 & equivalence ratio ϕ

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

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

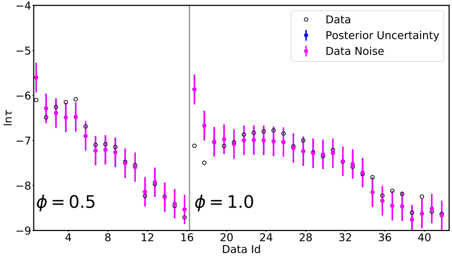
$$k_1 = Ae^{\left(-\frac{E}{RT}\right)}[C_{12}H_{26}]^{0.25}[O_2]^{1.25}$$

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

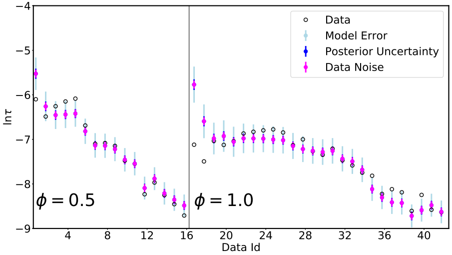


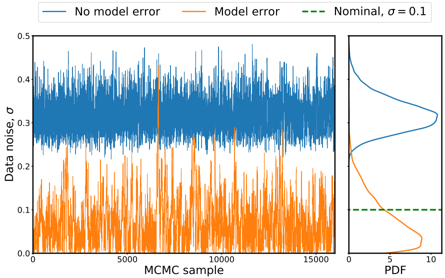
Ignition time in chemical kinetics

Without model error



With model error

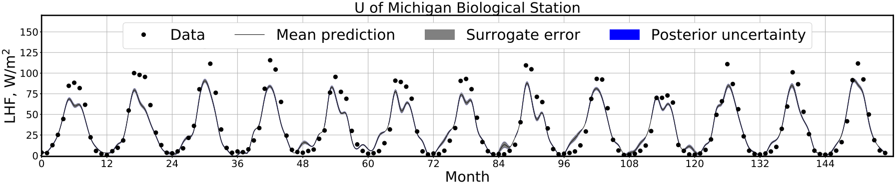




- Model error disambiguated from data error
- Data error correctly captured
- Meaningful extrapolative predictions

E3SM Land Model (ELM)

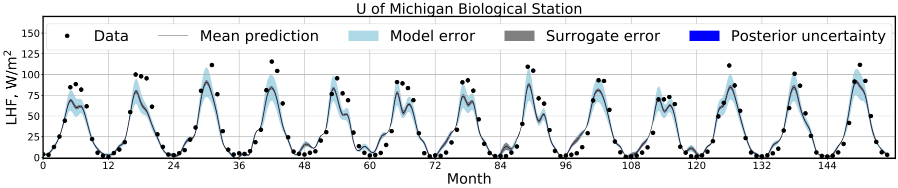
- US Department of Energy (DOE) sponsored Earth system model
- Land, atmosphere, ocean, ice, human system components
- High-resolution, employ DOE leadership-class computing facilities



- Conventional calibration without model error

E3SM Land Model (ELM)

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

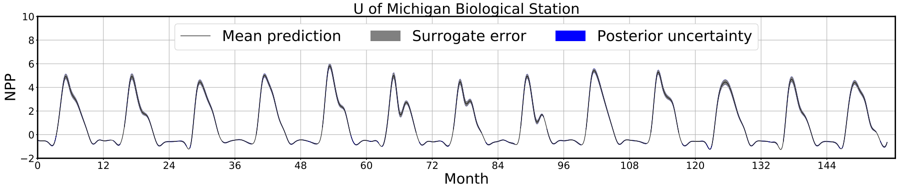


- Predictive variance decomposition with model-error component
- ... with predictive uncertainty that captures model error

E3SM Land Model (ELM)

E3SM Energy Exascale Earth System Model

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

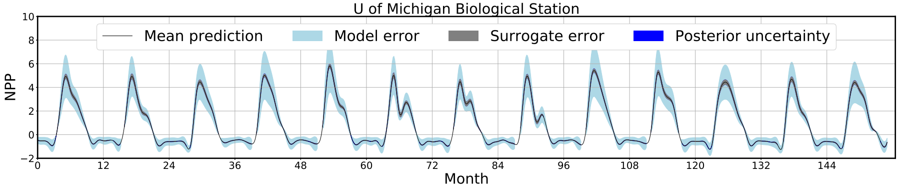


- Predictive variance decomposition with model-error component
- Allows meaningful prediction of other QoIs
(e.g. no data/observable)

E3SM Land Model (ELM)

E3SM Energy Exascale Earth System Model

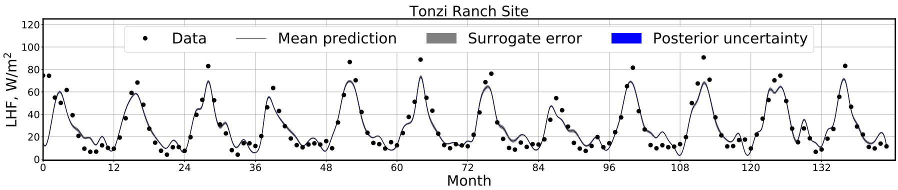
- US Department of Energy (DOE) sponsored Earth system model
- Land, atmosphere, ocean, ice, human system components
- High-resolution, employ DOE leadership-class computing facilities



- Predictive variance decomposition with model-error component
- Allows meaningful prediction of other QoIs
  (e.g. no data/observable)
- ... with predictive uncertainty that captures model error

E3SM Land Model (ELM)

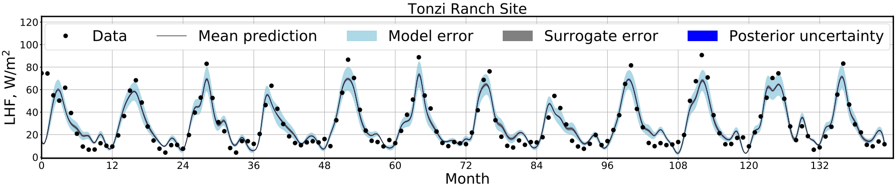
- US Department of Energy (DOE) sponsored Earth system model
- Land, atmosphere, ocean, ice, human system components
- High-resolution, employ DOE leadership-class computing facilities



- Predictive variance decomposition with model-error component
- Allows (a more dangerous) extrapolation to other sites

E3SM Land Model (ELM)

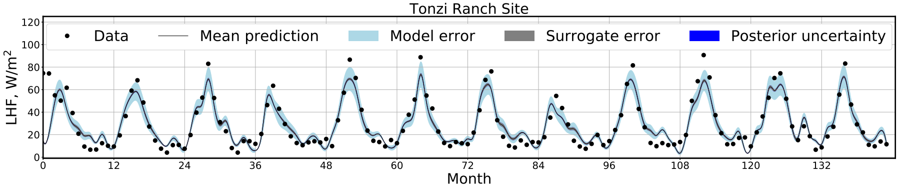
- US Department of Energy (DOE) sponsored Earth system model
- Land, atmosphere, ocean, ice, human system components
- High-resolution, employ DOE leadership-class computing facilities



- Predictive variance decomposition with model-error component
- Allows (a more dangerous) extrapolation to other sites
- ... with predictive uncertainty that captures model error

E3SM Land Model (ELM)

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



Summary

- Embedded, *non-intrusive* model error quantification
- PC-based representation and propagation
- Bayesian framework for simultaneous estimation of model inputs and model error parameters
- All developments done within UQTk, lightweight C++/Python library out of SNL-CA
  www.sandia.gov/uqtoolkit
- Challenges:
  - High-d inference problem
  - Identifiability
  - Extrapolation/generalization
  - Where/how to embed
  - Likelihood degeneracy
  - Priors
- Opportunities:
  - Intrusive, domain-knowledge based corrections
  - Field (x-dependent) correction
  - Handling discrete inputs, relation to BMA

Literature

Thank you!

M. Kennedy and A. O'Hagan, "Bayesian Calibration of Computer Models", *Journal of the Royal Statistical Society*, Series B. 63, 425-464, 2001.

D. Higdon, M. Kennedy, J. C. Cavendish, J. A. Cafeo, and R. D. Ryne. "Combining Field Data and Computer Simulations for Calibration and Prediction", *SIAM Journal on Scientific Computing*, 26(2):448-466, 2004.

M. Bayarri, J. Berger, R. Paulo, J. Sacks, J. Cafeo, J. Cavendish, C. Lin, and J. Tu. "A Framework for Validation of Computer Models", *Technometrics*, 49(2):138-154, 2007.

V. R. Joseph and S. N. Melkote. "Statistical Adjustments to Engineering Models", *Journal of Quality Technology, 41(4):362*, 2009.

T. A. Oliver, G. Terejanu, C. S. Simmons, and R. D. Moser, "Validating Predictions of Unobserved Quantities", *Computer Methods in Applied Mechanics and Engineering*, 283:1310-1335, 2015.

J. Brynjarsdottir and A. O'Hagan. "Learning about Physical Parameters: The Importance of Model Discrepancy". *Inverse Problems*, 30, 2014.

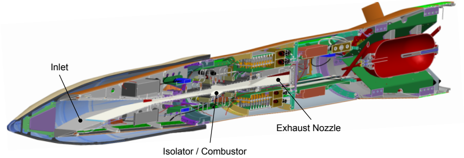
K. Sargsyan, H. Najm, R. Ghanem, "On the Statistical Calibration of Physical Models", *Int. J. Chem. Kinetics*, 47(4), 246-276, 2015.

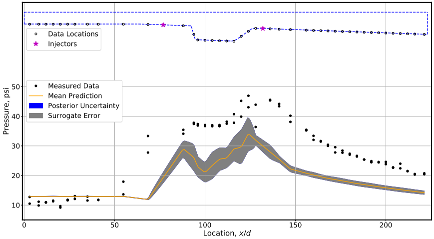
K. Sargsyan, X. Huan, H. Najm. "Embedded Model Error Representation for Bayesian Model Calibration", arXiv:1801.06768, in press, *Int. J. Uncert. Quant.*, 2019.

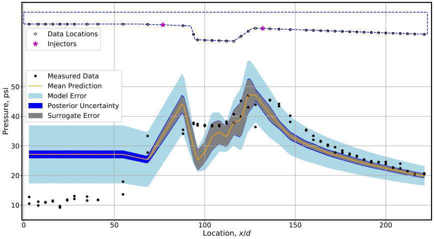
Additional Material

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

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:

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

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

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

moderr/data2d-eps-conver

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

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

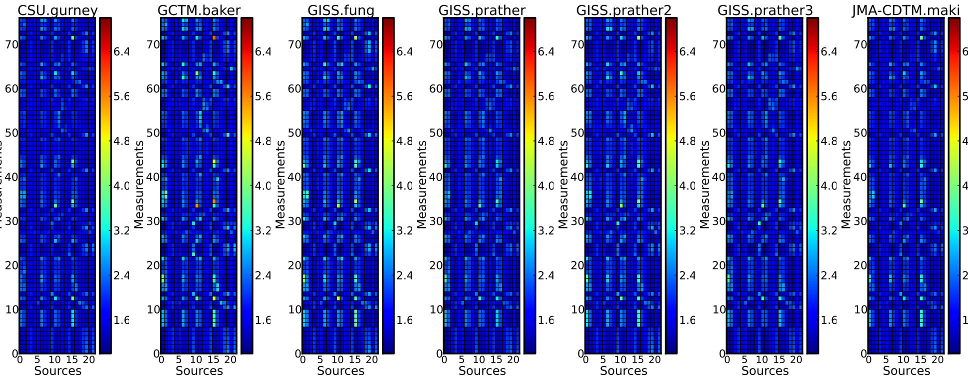
[Gurney *et al.*, Tellus B, 2003]

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

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

- 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

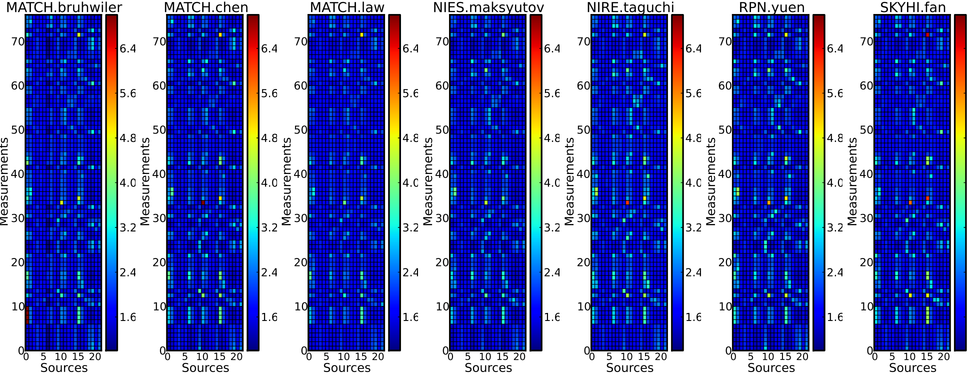
Consider 14 different response models $\mathbf{R}$



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

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

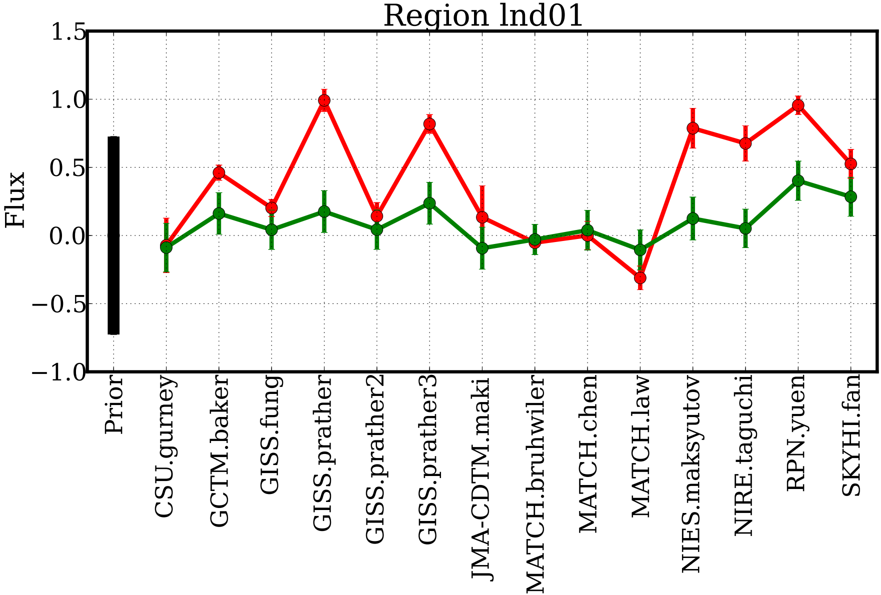
Consider 14 different response models $\mathbf{R}$



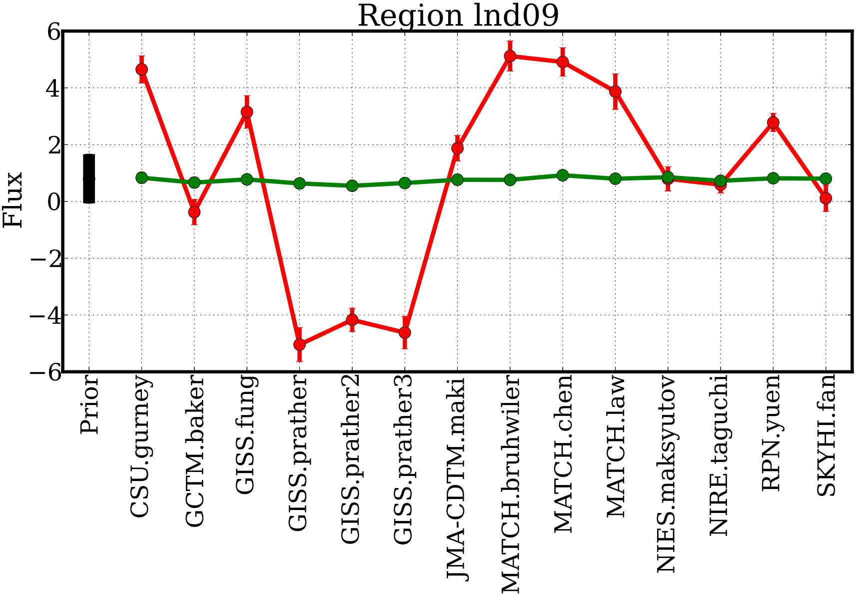
Infer fluxes $\mathbf{s}$, given measurements $\mathbf{d}$ to satisfy $\mathbf{d} \approx \mathbf{R}\mathbf{s}$

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

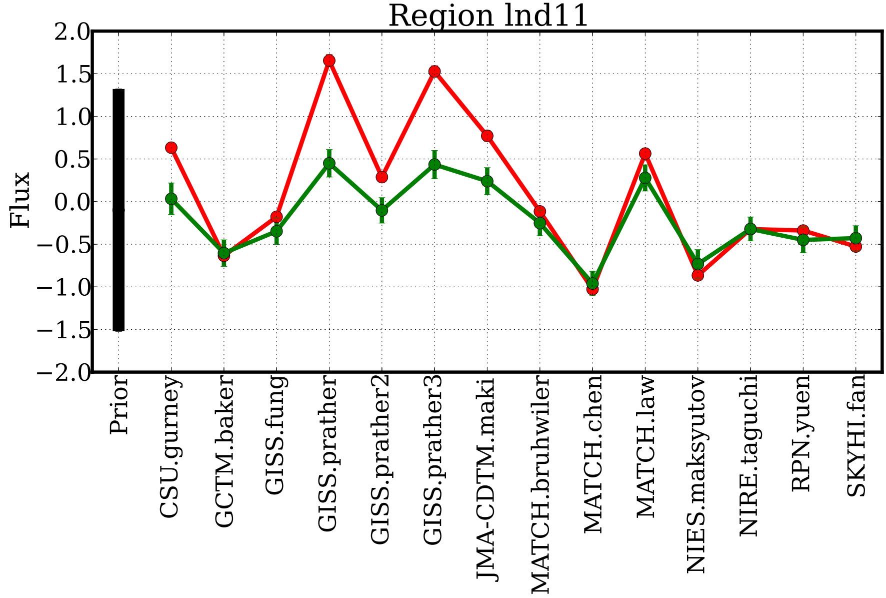
Inferred fluxes show less variability across models



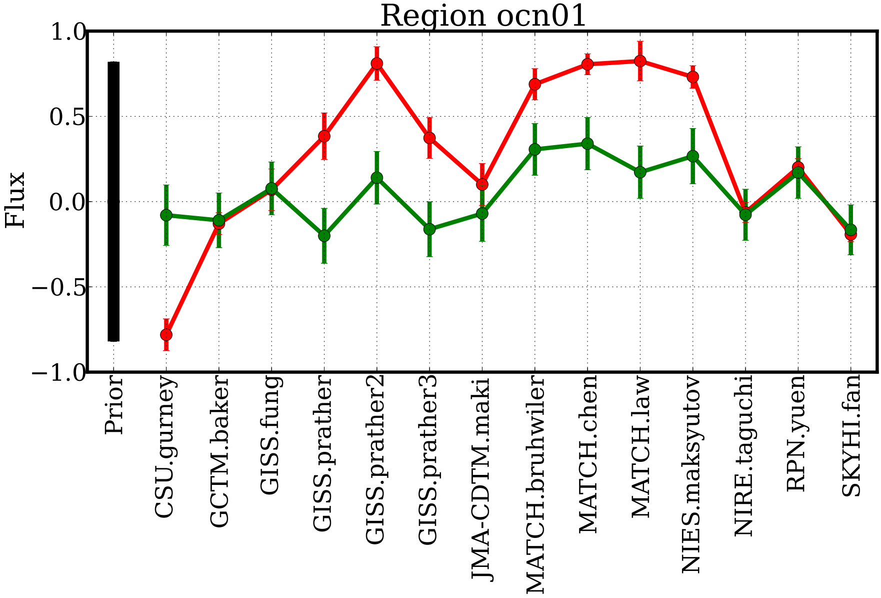
Inferred fluxes show less variability across models



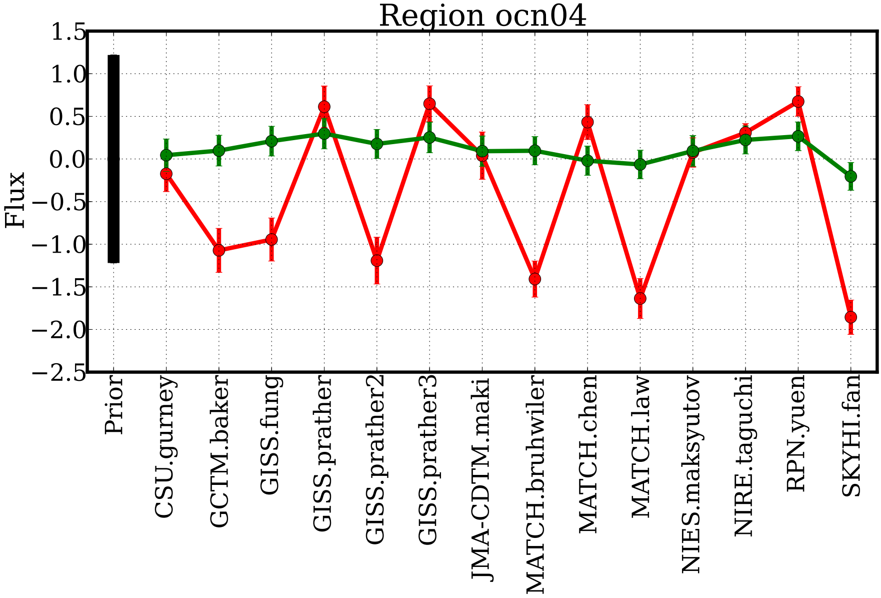
Inferred fluxes show less variability across models



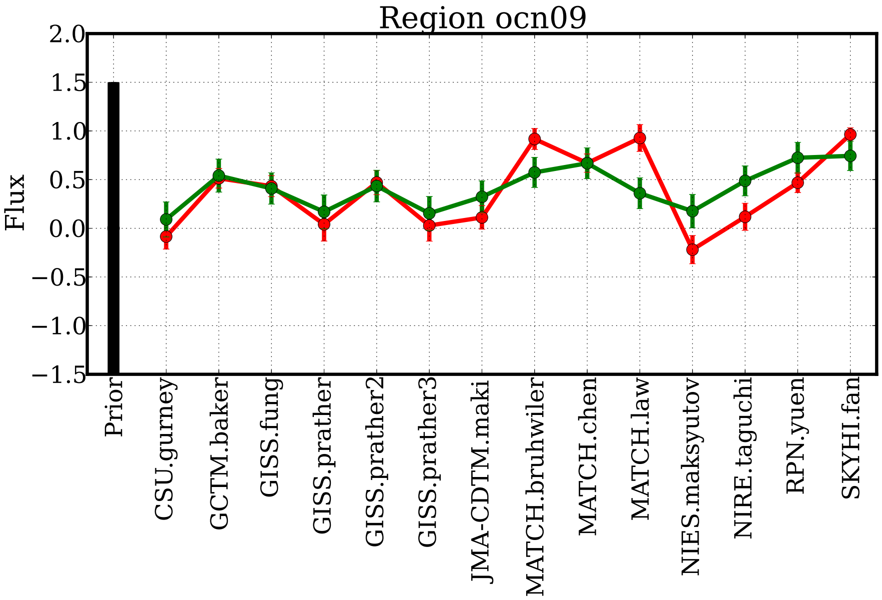
Inferred fluxes show less variability across models



Inferred fluxes show less variability across models



Inferred fluxes show less variability across models



Inferred fluxes show less variability across models