AGU Fall Meeting 2019
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Calibration and Propagation of Model Structural Error for E3SM Land Model

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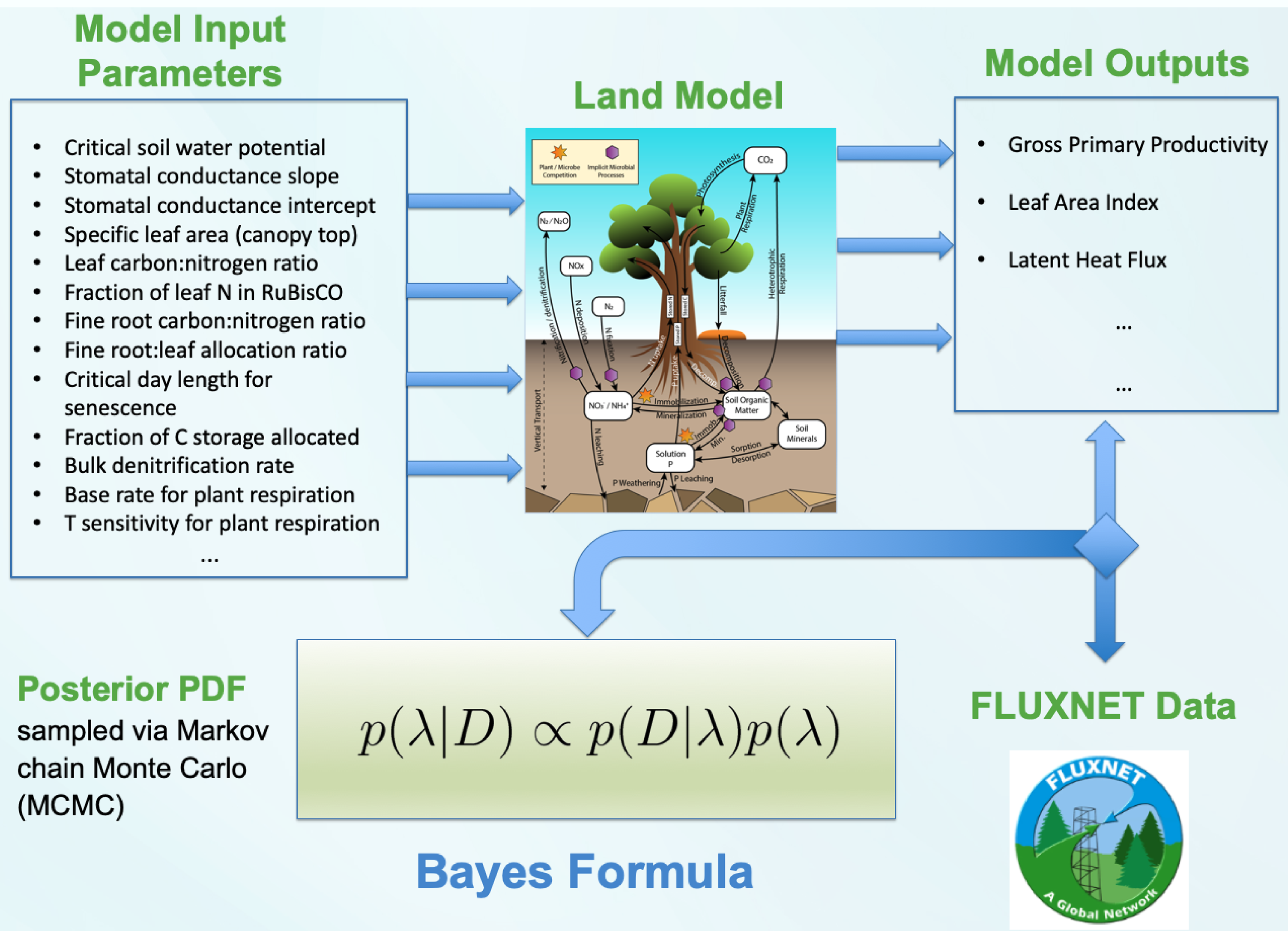
Bayesian Calibration of a Black-Box Land Model



Expense Mitigated by Surrogate Construction

Key Challenge

Likelihood requires online evaluation of model at candidate values

$$p(D|\lambda) \propto \exp\left(-\frac{1}{2}||D - f(\lambda)||^2\right)$$

Surrogate Construction

Construct a surrogate, inexpensive approximation

$$f(\lambda) \approx f_s(\lambda)$$

using a few 'training' simulations.

Side Effect: Global Sensitivity Analysis

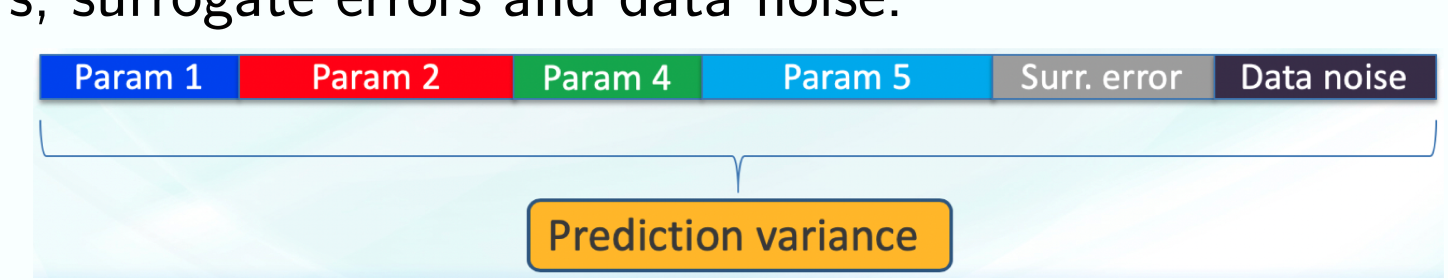
We employ Polynomial Chaos surrogates

$$f_s(\lambda) = \sum_k c_k \Psi_k(\lambda)$$

enabling variance decomposition (global sensitivity analysis) and uncertainty propagation.

This is business-as-usual

Predictive uncertainty is decomposed due to model parameters, surrogate errors and data noise.



What About Model Structural Error?

Uncertainty decomposition of model prediction needs to account for model error – often the dominant component of the uncertainty.

Elephant in the room!

Error associated with

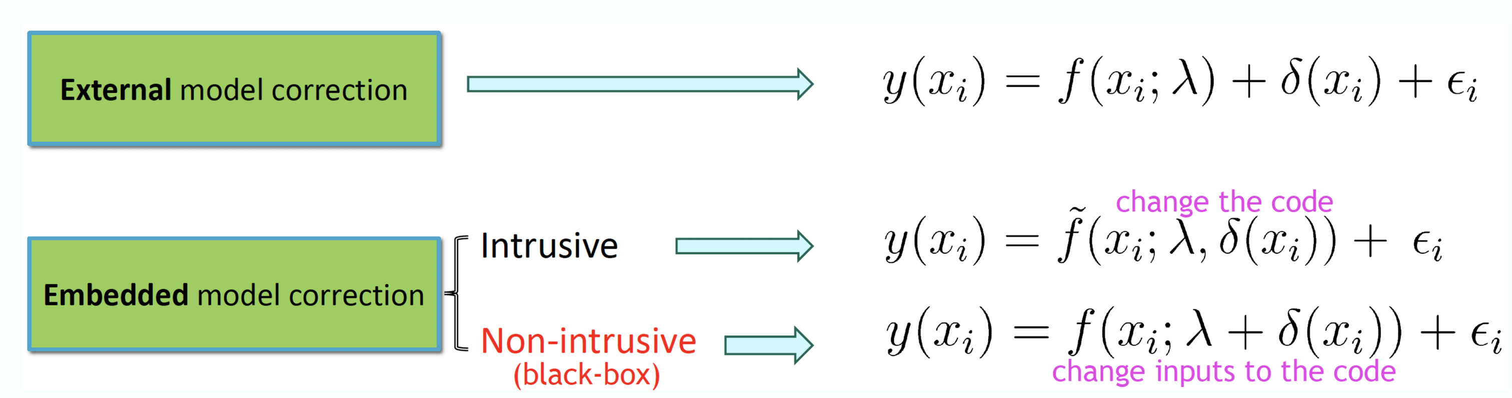
- Simplifying assumptions, parameterizations
- Mathematical formulation, theoretical framework.

Scientific discovery and model development: "is it worth resolving details, or just parameterize empirically?"

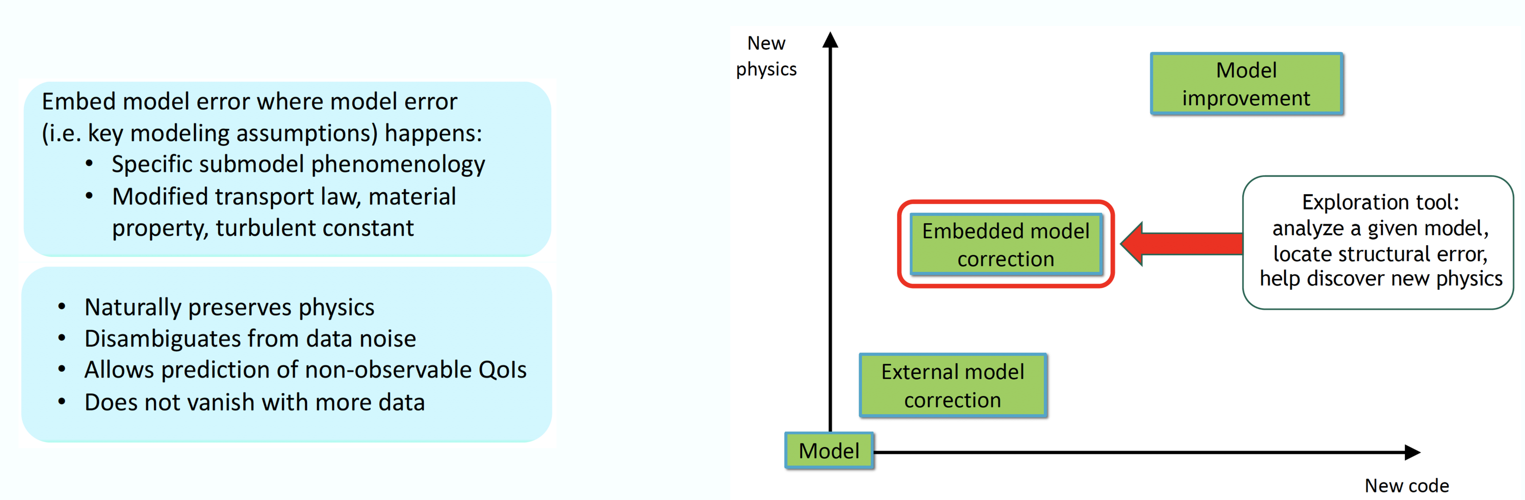
Optimal resource allocation: "do I improve my model (e.g. high-res), or run more simulations?"

Embedded Model Structural Error

How to account for model error

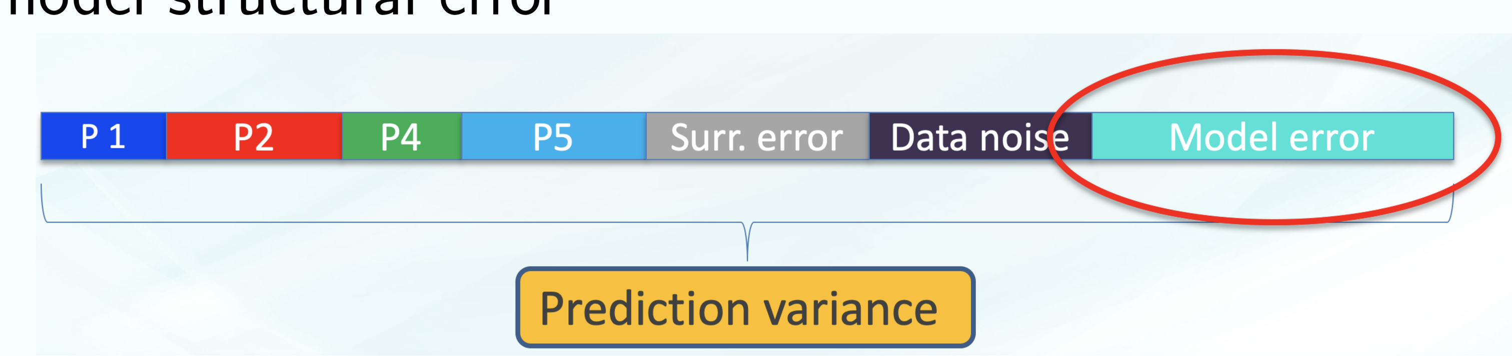


Embedded but non-intrusive!



Simultaneous Bayesian inference of model parameters and structural error

Posterior predictive uncertainty decomposition accounts for model structural error



General Embedding UQ Workflow

Polynomial chaos representation as embedded model error correction

$$f\left(x;\lambda+\overbrace{\sum_k \alpha_k\Psi_k(\xi)}^{\text{PC}}\right) \overset{\text{NISP}}{\simeq} \sum_k f_k(x;\overset{\text{physical}}{\lambda},\overset{\text{model-error}}{\alpha})\Psi_k(\xi) \to \mu(x;\lambda,\alpha),\ \sigma^2(x;\lambda,\alpha)$$

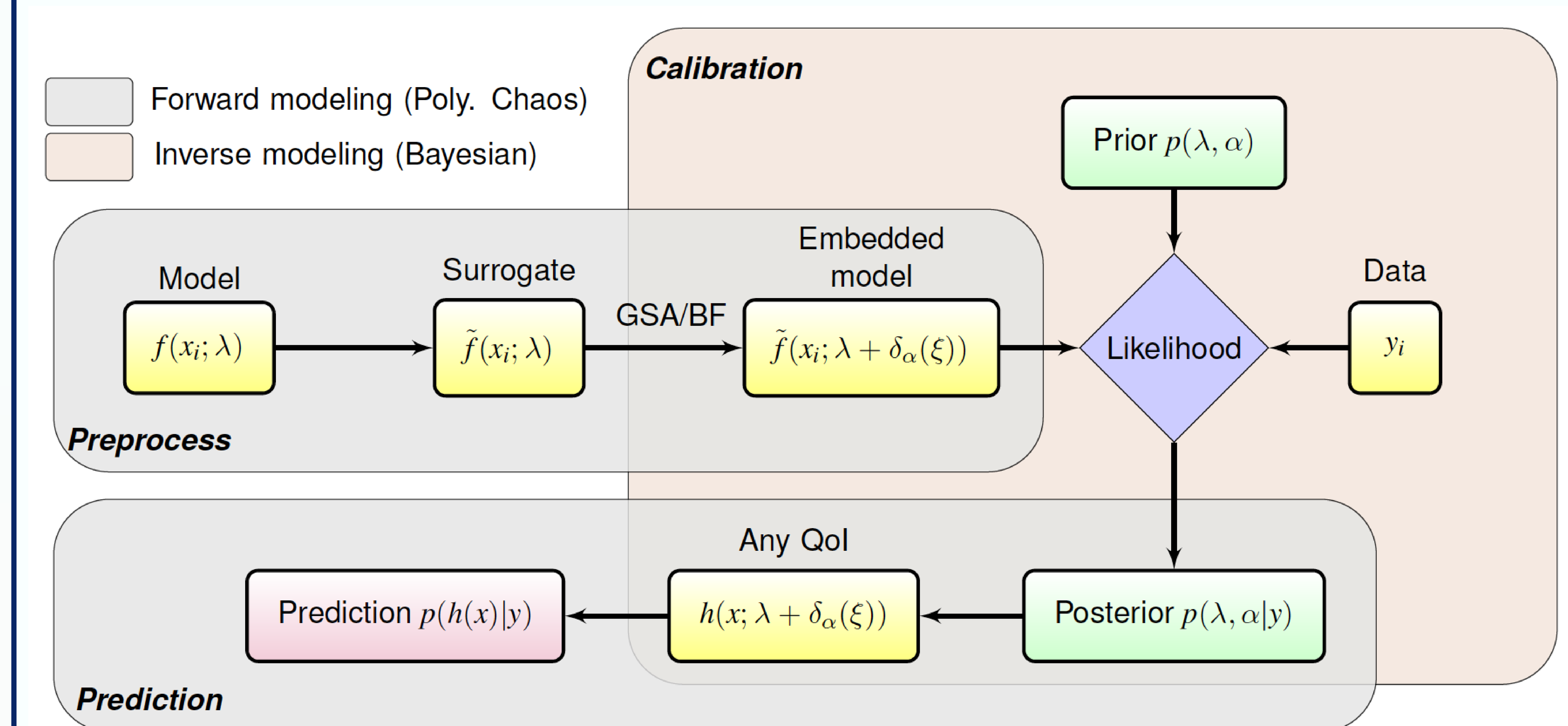
Technical ingredients

- Non-intrusive spectral projection (NISP) for uncertainty propagation
- Simultaneous Bayesian inference of λ and α via Markov chain Monte Carlo
- Prediction of full set of QoIs with variance decomposition of predictive uncertainty

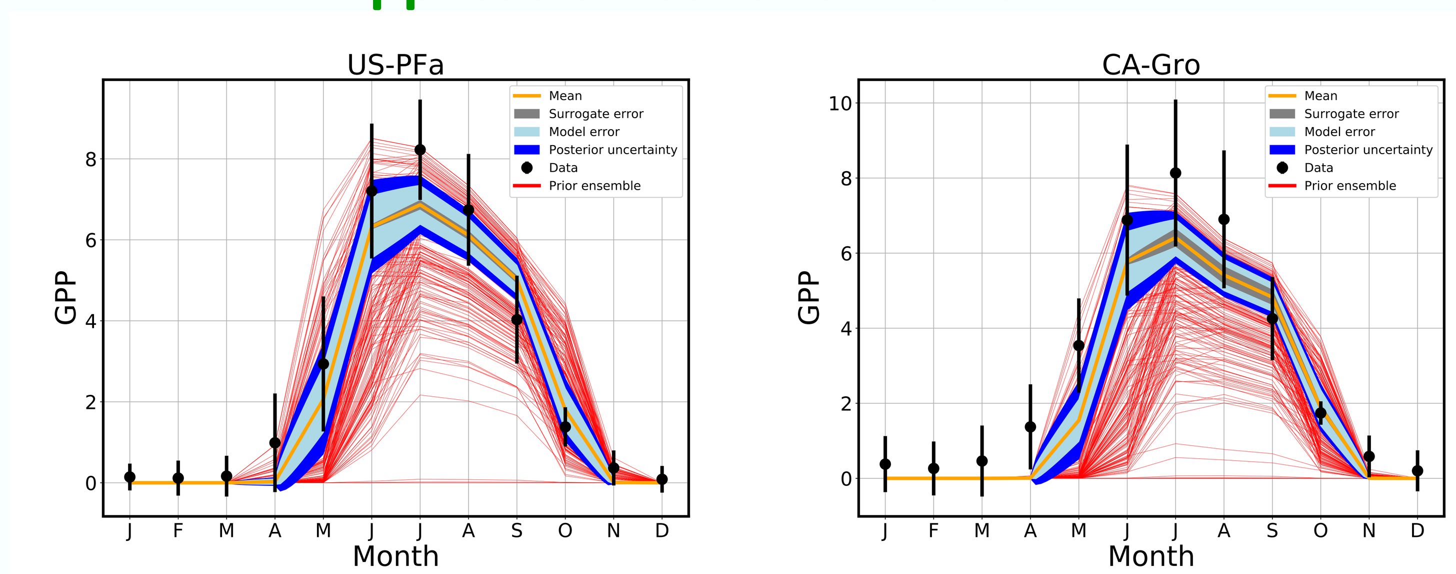
$$\mu(x) = \mathbb{E}_{\lambda,\alpha}[\mu(x;\lambda,\alpha)]$$

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

- Automated workflow is implemented in UQ Toolkit (`www.sandia.gov/uqtoolkit`)



Application to land model



Reference: K. Sargsyan, X. Huan, H. Najm, Embedded model error representation for Bayesian model calibration, International Journal for Uncertainty Quantification, 9(4), pp. 365-394. Also on arXiv:1801.06768.

This research was supported as part of
- the Energy Exascale Earth System Model (E3SM) project, funded by the U.S. Department of Energy, Office of Science, Office of Biological and Environmental Research (BER).
- the U.S. Department of Energy, Office of Science, Scientific Discovery through Advanced Computing (SciDAC) program through the FASTMath Institute.

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