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Bayesian Framework for Structural Uncertainty Estimation of Land Models

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Goal: Model Error Quantification

Develop statistical framework for model error representation, quantification and propagation for physical models.

- Represent and estimate the error associated with
  - Simplifying assumptions, parameterizations
  - Mathematical formulation, theoretical framework
  - Numerical discretization
- Inverse modeling context $\quad y_i = f(x_i;\lambda) + \epsilon_i$
- Given data, calibrate for λ, accounting for model error
- Model error is deviation from 'truth'

Truth $g(x) \neq f(x;\lambda)$ Model

Embedded Model Error Representation

x are operating conditions, design parameters, various QoIs
λ are model parameters to be inferred/calibrated

- Default: Ignore model errors:

$$g(x) = f(x;\lambda) + \epsilon$$

  - Biased or overconfident physical parameters
  - Wrong model predictions

- Conventional: Correct for model errors:

$$g(x) = f(x;\lambda) + \delta(x) + \epsilon$$

  - Physical parameters are ok
  - Wrong model predictions (data-specific corrections)
  - Model and data errors mixed up

- What we do: Correct *inside* the model:

$$g(x) = f(x;\lambda + \delta(x)) + \epsilon$$

  - Embedded model error
  - Preserves model structure and physical constraints
  - Disambiguates model and data errors
  - Allows meaningful extrapolation

Bayesian Estimation of Model Error

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

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

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

- To estimate the likelihood $L_y(\tilde{\alpha}) = p(y|\tilde{\alpha}) = p(y|\lambda,\alpha)$, one needs uncertainty propagation through $f(x_i;\underbrace{\lambda+\delta_\alpha}_{\text{stochastic}})$

Forward Prediction with Polynomial Chaos

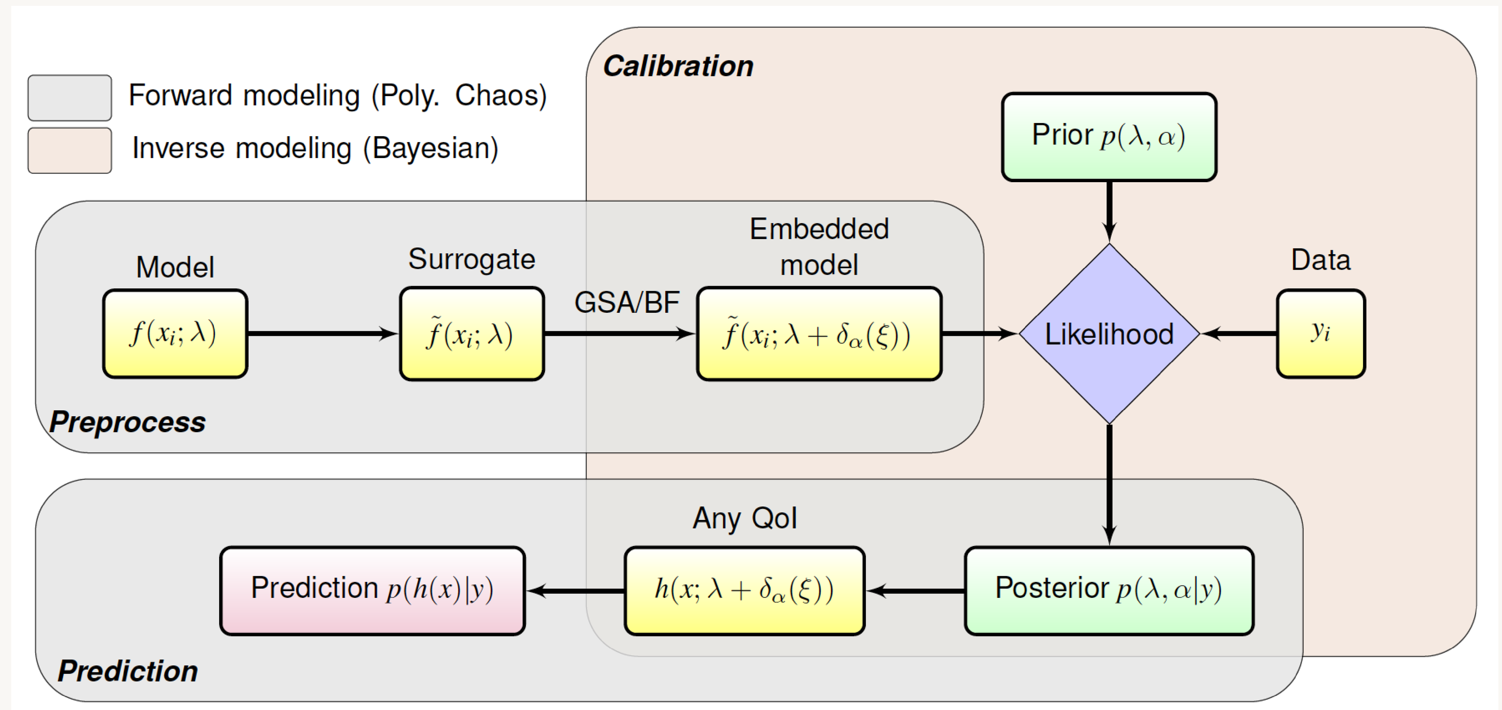
$$f(x;\lambda+\delta_\alpha) = f\left(x;\textstyle\sum_k \alpha_k \Psi_k(\xi)\right) \stackrel{NISP}{=} \textstyle\sum_k f_k(x;\alpha)\Psi_k(\xi)$$

- Non-intrusive spectral projection (NISP) employed for
  - Likelihood computation and posterior predictions
  - Easy access to first two moments:

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

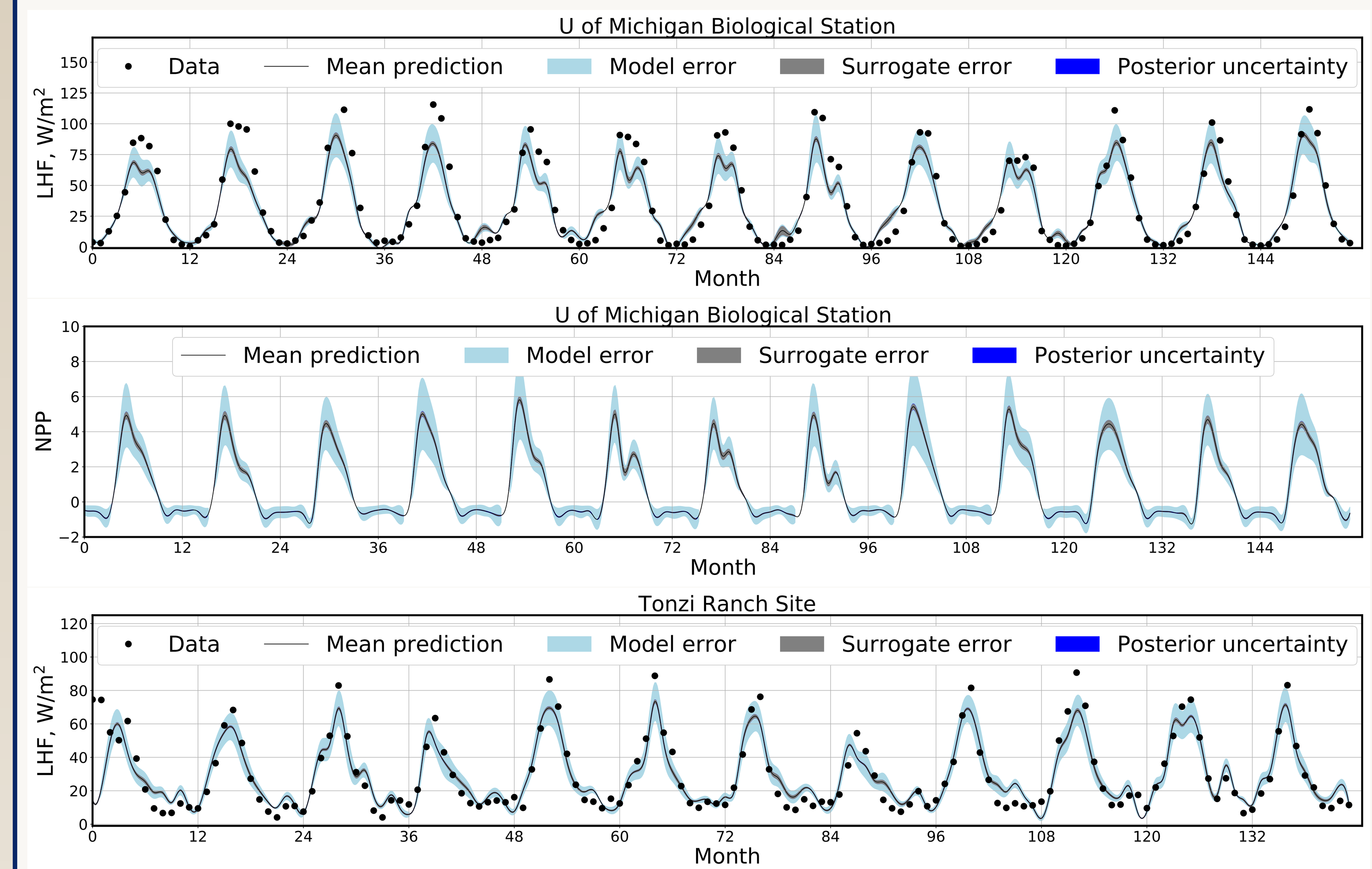
- Predictive mean $\quad \mathbb{E}[y(x)] = \mathbb{E}_\alpha[\mu(x;\alpha)]$
- Decomposition of predictive variance

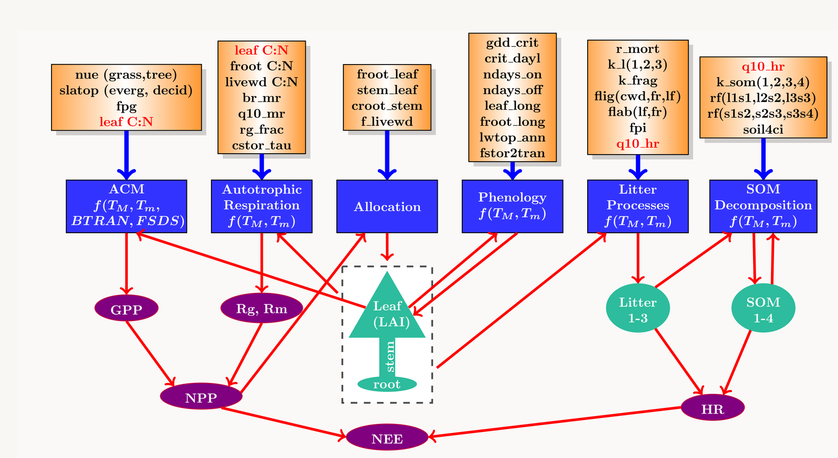
$$\mathbb{V}[y(x)] = \underbrace{\mathbb{E}_\alpha[\sigma^2(x;\alpha)]}_{\text{Model error}} + \underbrace{\mathbb{V}_\alpha[\mu(x;\alpha)] + \sigma_d^2}_{\text{Poserior/Data error}}$$



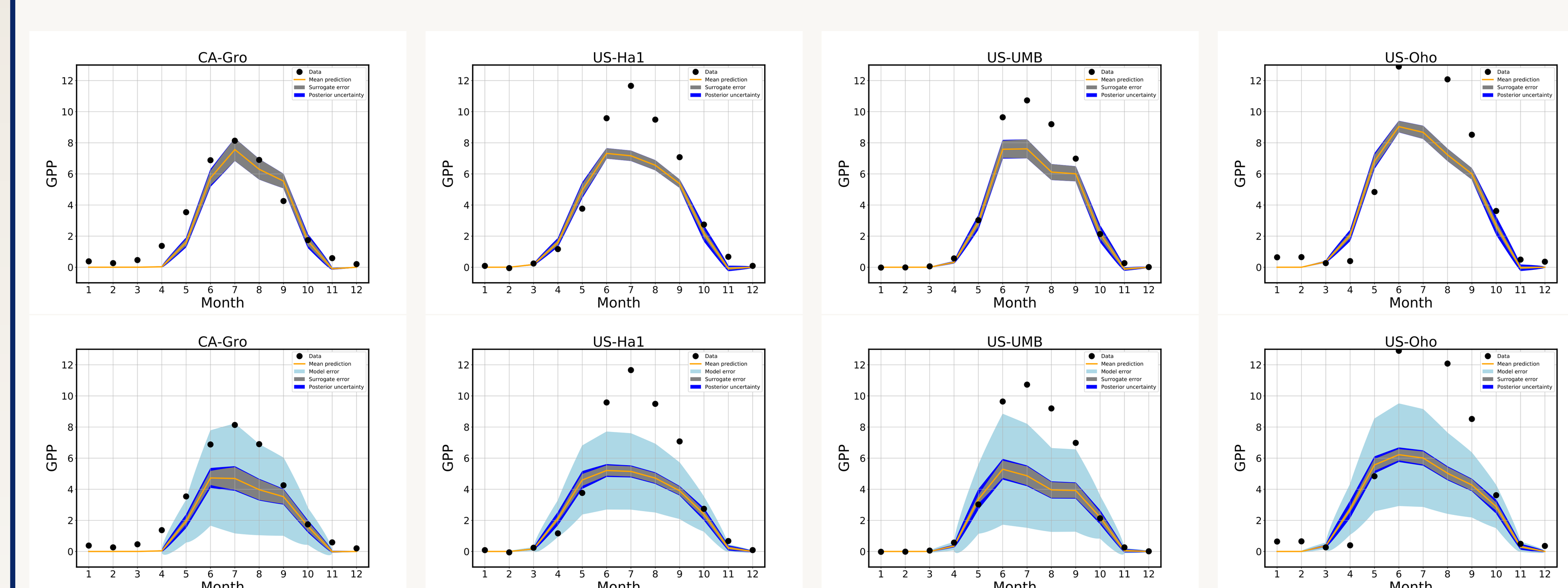
Application: E3SM Land Model

- US Dep-t of Energy (DOE) Earth system model
- Land, atmosphere, ocean, ice, human system components; high-resolution
- Employ DOE leadership computing facilities





- **ELM-LF** is a lower-fidelity, python version of ELM.
- Calibration with select FLUXNET sites data.
- Model error is the dominant uncertainty component: removes biases and overfitting.



Reference: K. Sargsyan, X. Huan, H. Najm, Embedded model error representation for Bayesian model calibration, arXiv preprint arXiv:1801.06768, 2018.

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