Hit twice by the curse of dimensionality: spatio-temporal land model calibration using Karhunen-Loève expansions

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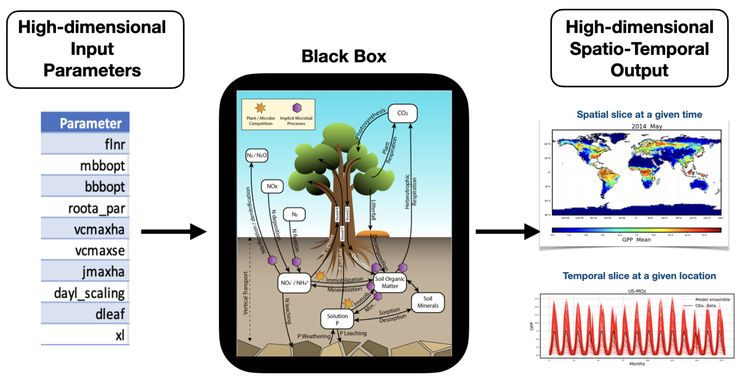
Email: ksargsy@sandia.gov

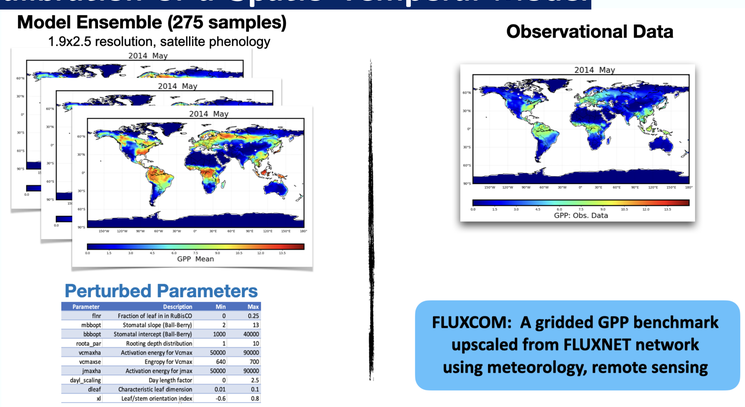
Khachik Sargsyan[1], Daniel Ricciuto[2], Cosmin Safta[1]

[1] Sandia National Laboratories, Livermore, CA, USA, [2] Oak Ridge National Laboratory, Oak Ridge, TN, USA

E3SM Land Model



Calibration of a Spatio-Temporal Model



Goal:
Calibrate model given observational data

$$f(\lambda; x, t) \approx g(x, t)$$

Need for a Surrogate Model

- Forward modeling: Global sensitivity analysis requires prohibitively many model evaluations
- Inverse modeling: Likelihood requires online evaluation of the model, e.g.

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

- Construct a surrogate, inexpensive approximation

$$f(\lambda; x, t) \approx f_s(\lambda; x, t)$$

using the perturbed ensemble of model simulations.

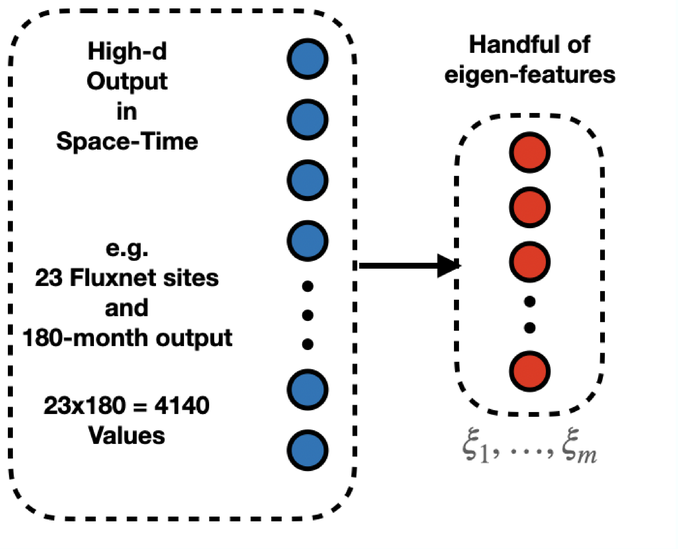
High-Dimensional Output

Karhunen-Loève (KL) Expansion:

- Optimal linear expansion in terms of eigenvalues of the covariance kernel.

$$f(\lambda; x, t) = \bar{f}(x, t) + \sum_{j=1}^{\infty} \xi_j(\lambda)\sqrt{\mu_j}\phi_j(x, t)$$

- Similar to principal components analysis, but in the continuous, (x, t) space.
- The analysis of spatio-temporal field $f(\lambda; x, t)$ reduces to a handful of eigen-features $\xi_j(\lambda)$
- KL expansion is an optimal linear auto-encoder



High-Dimensional Input

Option 1: Sparse Polynomial Chaos (PC) Surrogates for each $\xi_j(\lambda)$

$$\xi_i(\lambda) \approx \xi_i^{\mathrm{PC}}(\lambda) = \sum_{k=0}^{K} c_{ik}\Psi_k(\lambda)$$

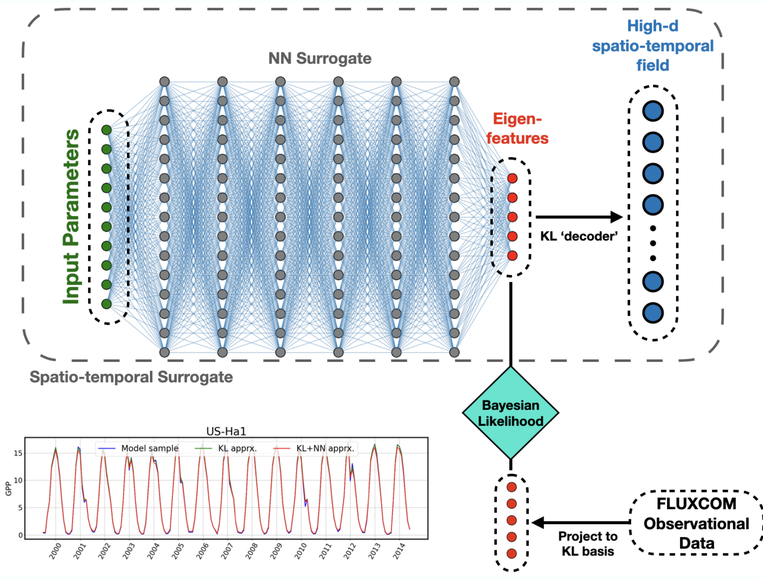
Option 2: Joint Neural Network (NN) Surrogate for all $\xi_j(\lambda)$'s

$$\boldsymbol{\xi}(\lambda) \approx \boldsymbol{\xi}^{\mathrm{NN}}(\lambda)$$

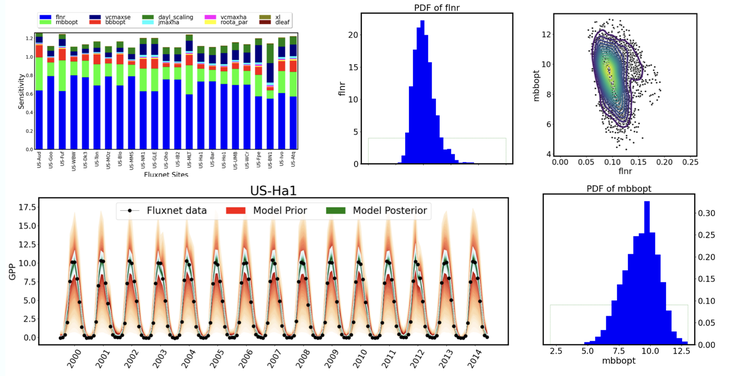
Surrogate-enabled Bayesian Calibration

Joint spatio-temporal surrogate

$$f(\lambda; x, t) = \bar{f}(x, t) + \sum_{j=1}^{m} \xi_j^{\mathrm{NN}}(\lambda)\sqrt{\mu_j}\phi_j(x, t)$$



Results and Summary



- High-dimensional spatio-temporal output well-represented with a few KL eigen-features with a fraction of ELM cost
- 4140 spatio-temporal cells down to 5 eigen-features with 1% loss of accuracy only
- Global sensitivity analysis using the KL+NN surrogate
- Bayesian calibration performed in the eigen-space

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