# Uncertainty Quantification and Parameter Calibration for High-Dimensional Output Fields of Earth System Models

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## Objective

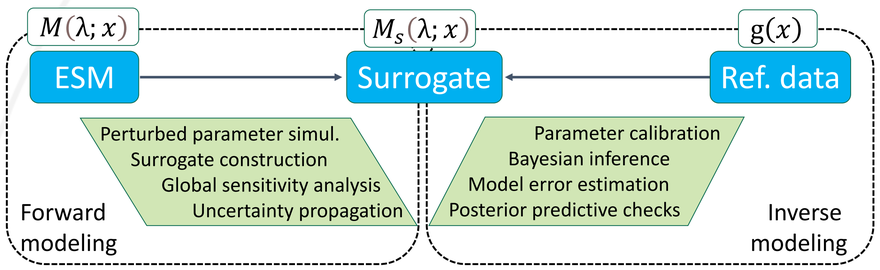
Develop workflows of surrogate construction for outputs of earth system models to enable uncertainty quantification (UQ)

Sample-intensive studies, such as UQ and parameter calibration, for earth system models require a construction of a **surrogate model** that approximates the ESM behavior across a range of conditions and input parameters.

ESM $M(\lambda; x)$ ≈ Surrogate $M_s(\lambda; x)$

- Model output Quantity of Interest (QoI)
- Uncertain input parameters
- Conditions, e.g. (Longitude, Latitude Altitude, Pressure, Time)

## UQ Workflow




**Major challenges:**

- **Large number of conditions / high-dimensional output fields**
  - ✓ Employ Karhunen-Loève decomposition to reduce dimensionality

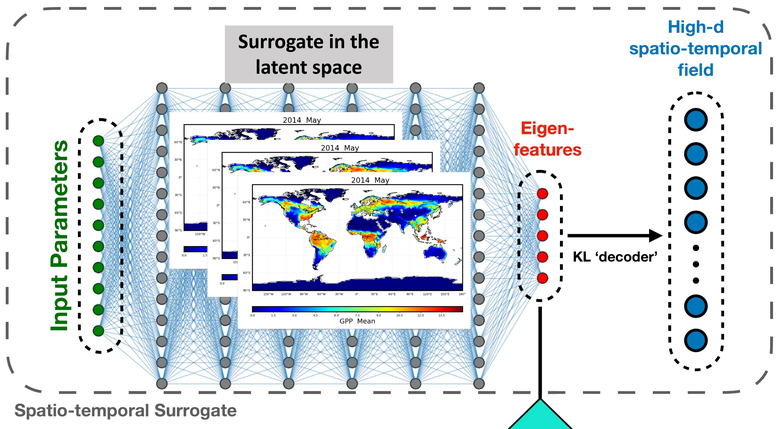
$$M(\lambda; x) \approx \bar{M}(\lambda; x) + \sum_{j=1}^{J} \xi_j(\lambda) \sqrt{\mu_j}\, \phi_j(x)$$

  - ✓ Construct surrogate in the latent eigen-space $\xi(\lambda) \approx \xi_s(\lambda)$

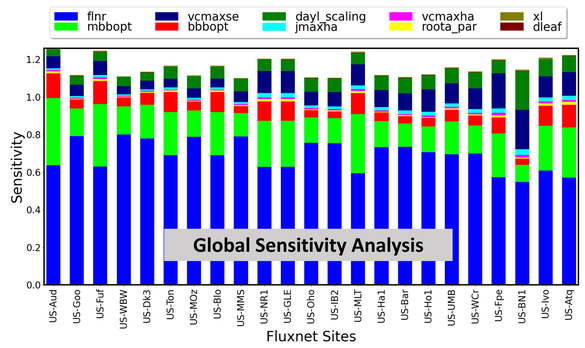
- **Large number of uncertain inputs / high-dimensional stochastic space**
  - ✓ Employ polynomial surrogates with compressed sensing to pick only relevant parameter combinations $\xi_s(\lambda) = \sum_{k=1}^{K} c_k \Psi_k(\lambda)$

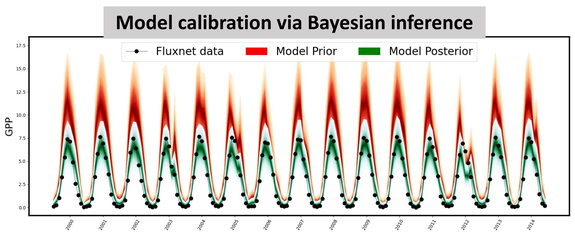
- **Expense of ESM / low number of training simulations**
  - ✓ No real remedy but cross-validation and hyperparameter optimization help.

## Case Study 1: E3SM Land Model Biogeochemistry




- ~5000 spatio-temporal cells down to ~10 eigenfeatures with 1% loss of accuracy
- The overall spatio-temporal surrogate has a fraction of ELM cost

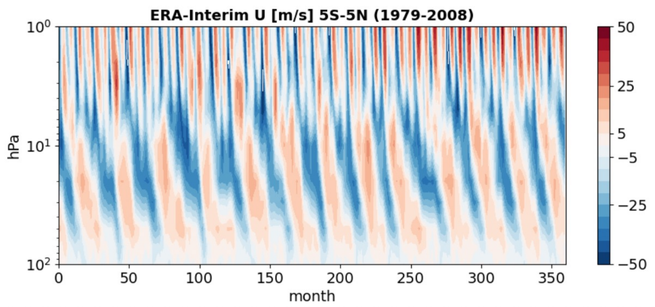


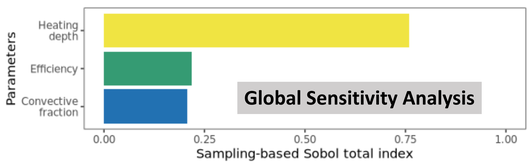



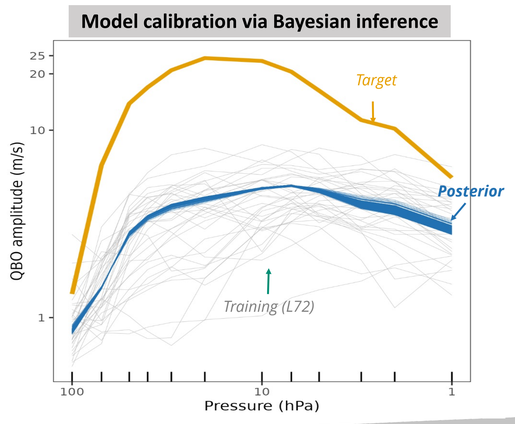

## Case Study 2: E3SM Quasi-Biennial Oscillation (QBO)

SciDAC Project: Improving the Quasi-biennial oscillation through **surrogate-accelerated parameter optimization** and vertical grid modification

Alternating zonal wind in the equatorial stratosphere with a period ~28 months and peak amplitude ~25 m/s at ~20 hPa



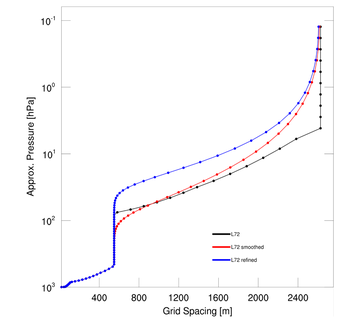

**UQ challenge**:

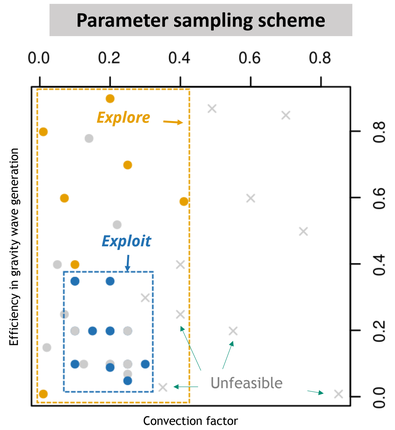
- Expense (and occasional failure) of model simulations
- Low signal-to-ratio noise

**Modeling challenge**:

- Current vertical grid (L72) does not respond to changes in key parameters driving the resolved and parametrized gravity waves.
- Default grid underpredicts amplitude by 3x.

Currently investigating a new grid design (L80): in-progress simulations show a better resolution of the QBO phenomenon

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