# Stochastic Surrogates and Quantification of Model Errors in Earth System Models

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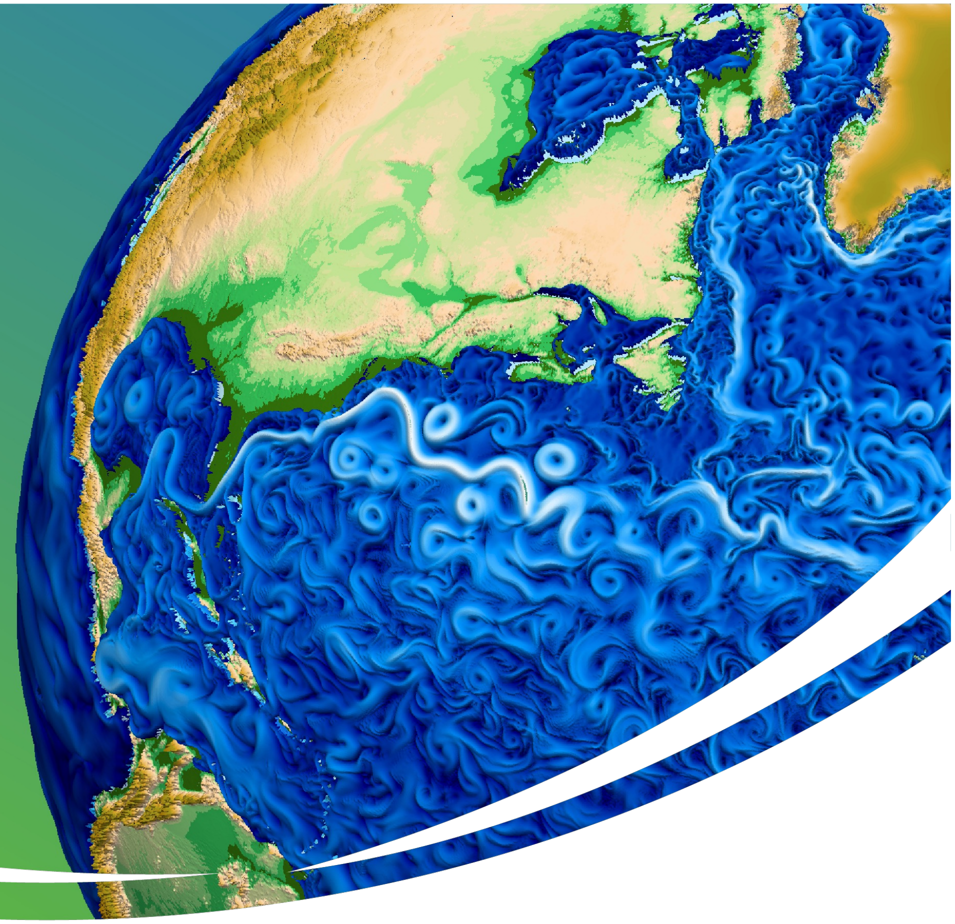
Daniel Ricciuto (ORNL)



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E3SM Energy Exascale Earth System Model

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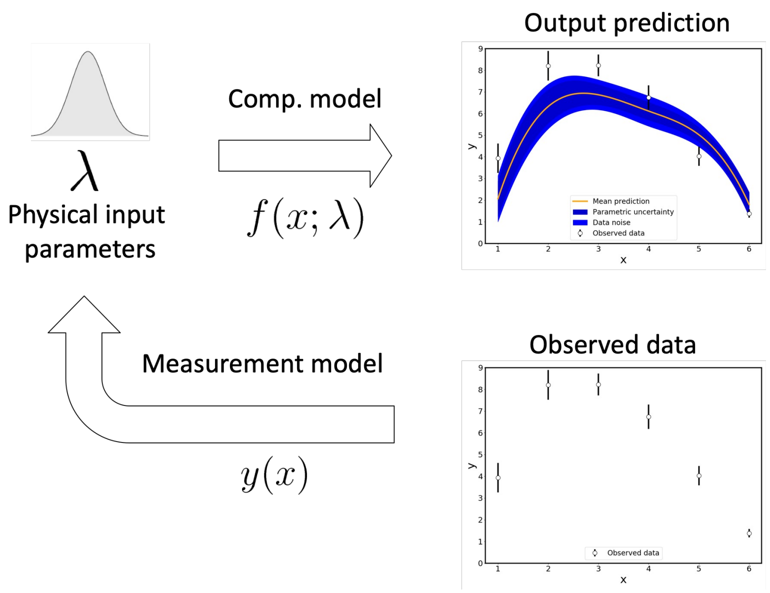
# Overview

- Focusing on uncertainty budget and attribution for computational models
- … on the example of E3SM land model (ELM)

- Two major non-trivial elements / advances
  - Stochastic surrogate (forward UQ)
  - Embedded model error (inverse UQ)

# Uncertainty Budget in Computational Models




**Forward UQ**
**(Uncertainty propagation, Global sensitivity analysis)**

- Parametric Uncertainty
- Surrogate Error
- Intrinsic Variability

**Inverse UQ**
**(Parameter estimation, Model calibration, validation, Model selection)**

- Posterior Uncertainty
- Model Form Error

# Polynomial Chaos -- the main tool for uncertainty quantification

- Represent a random variable $X$ as a polynomial expansion with respect to standard random variables $\xi$:

$$X \simeq \sum_{k=0}^{p} x_k \, \psi_k(\xi)$$

Convergent for finite-variance r.v. $X$.

- Describes the *random variable* $X$ with a vector of *deterministic* coefficients, *PC modes* $(x_0, x_1, \ldots, x_p)$.
- Theory is solid: in the limit of infinite order and dimensions; but in practice these are modeling choices.
- Enables functional analysis methods for forward UQ.
- PC first introduced by [Wiener, 1938]; revitalized in [Ghanem&Spanos, 1991].

# Forward UQ: parametric uncertainty and surrogate

Input $\lambda = \sum_k \lambda_k \Psi_k(\xi)$ $y = f(\lambda)$ Output $y = \sum_k y_k \Psi_k(\xi)$

- Cast input parameters as uncertain random variables:
  - e.g. the simplest version, first order Legendre-Uniform PC
  - … or first order Gauss-Hermite PC

$$\lambda = \lambda_0 + \lambda_1 \xi$$

- Then effectively PC of output is a *surrogate* model $f(\lambda) \approx \sum_k y_k \Psi_k(\lambda)$
- Regression (supervised ML) helps find coefficients $y_k$
  - … given training set or perturbed parameter ensemble $\{\lambda^{(i)}, f(\lambda^{(i)}\}_{i=1}^N$

# Forward UQ: parametric uncertainty and surrogate

Parametric Uncertainty

Surrogate Error

Relatively routine

Deterministic model

$$y = f(\lambda)$$

Intrinsic Variability

This work: stochastic surrogate via PC

Stochastic model

Key challenge: no control over the stochastic seed $\omega$

$$y = f(\lambda, \omega)$$

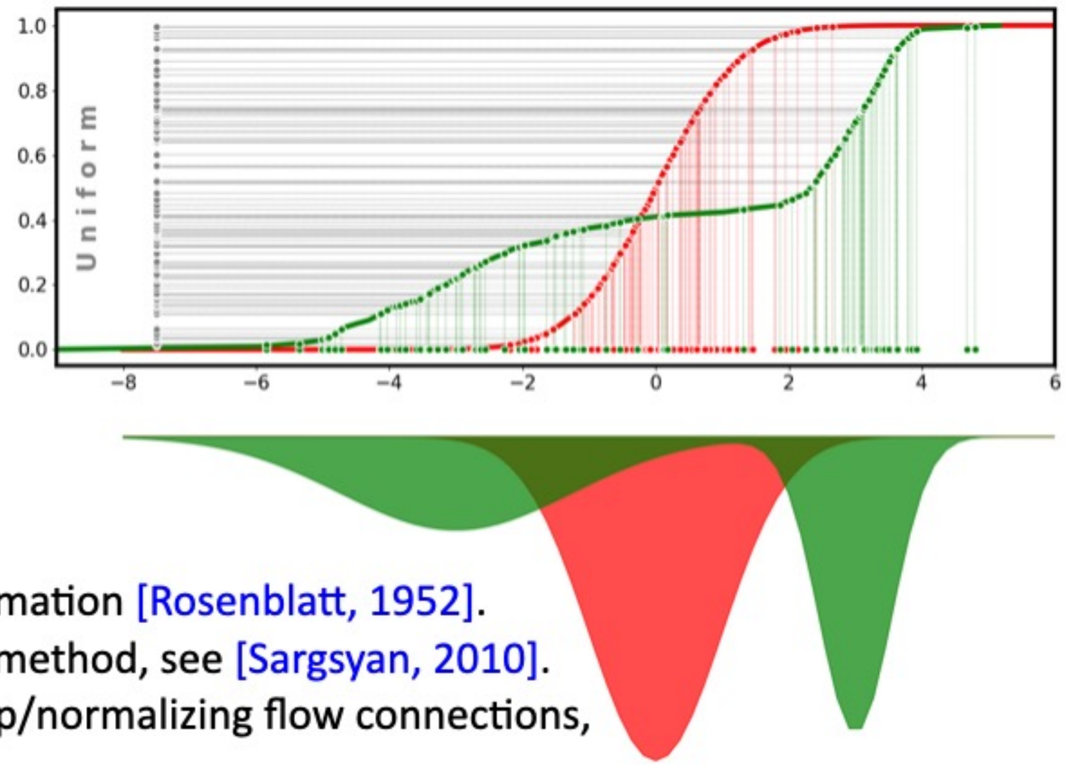
We will employ cumulative distribution function theorem to extract the map.

F(X) is Uniform[0,1] if F is CDF of X.

# Rosenblatt transformation allows unsupervised PC construction

$$X(\xi) \simeq \sum_{k=0}^{p} x_k \, \psi_k(\xi)$$

**General R.V.** **Normal**




- With the $X \leftrightarrow \xi$ map in place, the PC construction becomes a regression/projection (supervised learning) problem

- In >1 dim: Rosenblatt transformation [Rosenblatt, 1952].
- For kernel density estimation method, see [Sargsyan, 2010].
- For more recent transport map/normalizing flow connections, see [Baptista, 2024].

# Joint parametric-stochastic PC surrogate

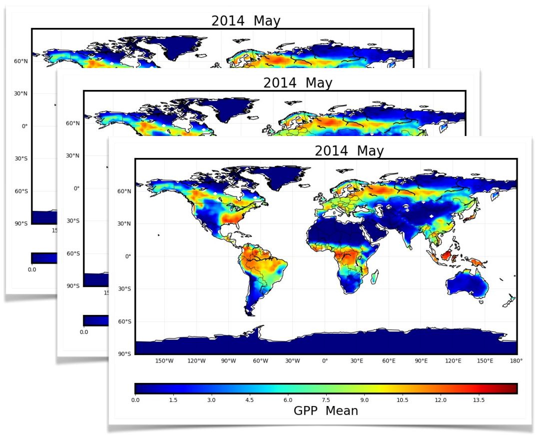
- With simple scaling of parameters and Rosenblatt map, we can cast joint PC construction as a regression problem.
- Training set sample both parametric space (perturbed parameter) and the stochastic space (random seed).
- Relies on Kernel Density Estimate for CDF evaluation *[Mueller et al, 2025].*
- Resulting joint PC expansion has additional dimensions responsible for intrinsic variability.

$$f(\lambda, \omega) \approx \sum_k c_k \Psi_k(\xi, \zeta)$$

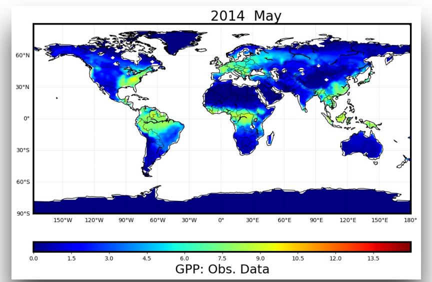
parametric stochastic

# Energy Exascale Earth System Model (E3SM)

- US Dept of Energy (DOE) sponsored Earth system model, *e3sm.org*
- Land, atmosphere, ocean, ice, human system components
- High-resolution, employ DOE leadership-class computing facilities

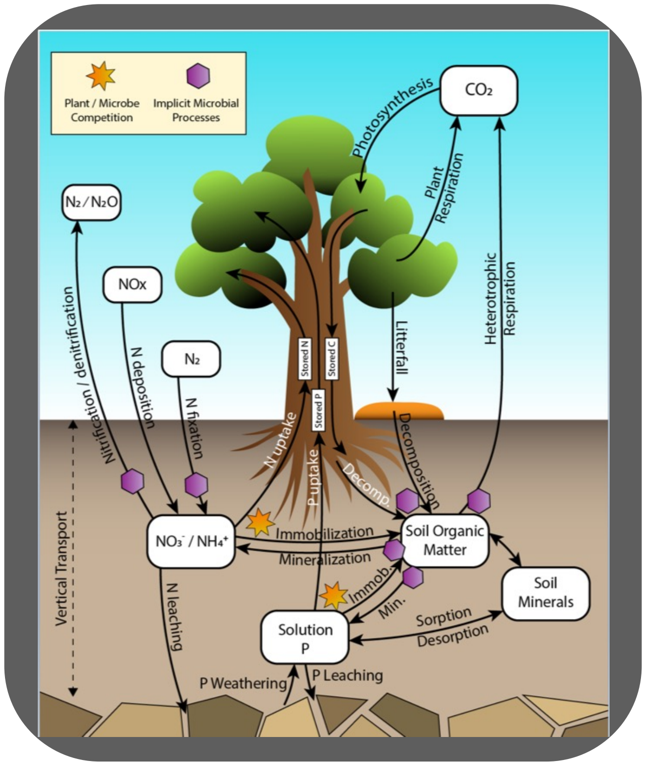



Model (Parameter-Perturbed) Ensemble



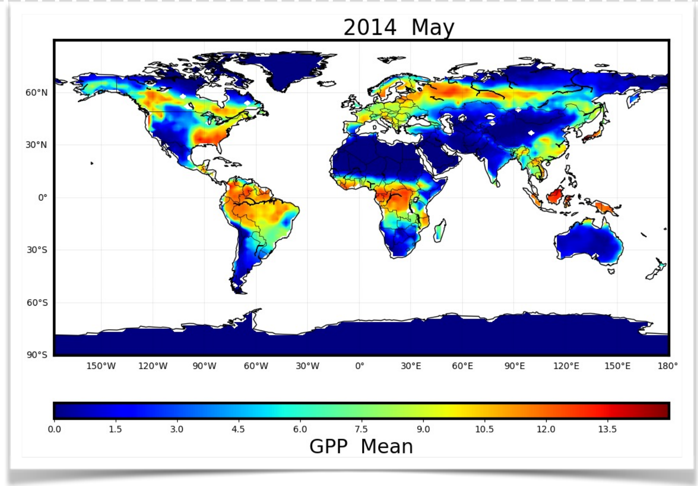

Observational Data

# E3SM Land Model (ELM)

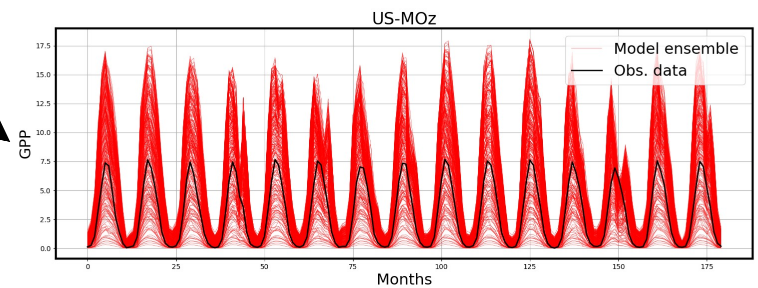



Quantity of Interest:
Gross primary productivity (GPP)…

… resolved in space, …




… and in time.

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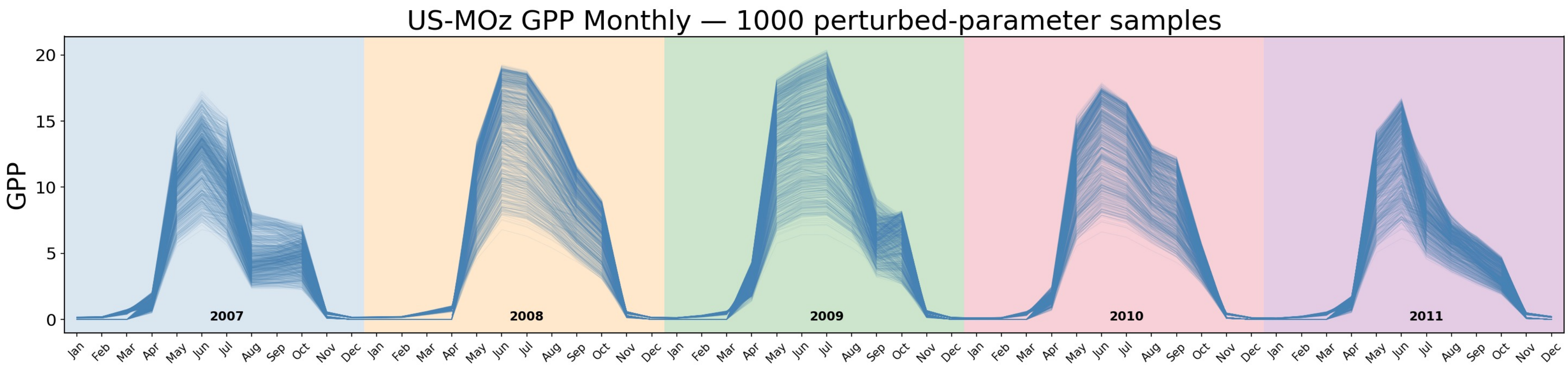
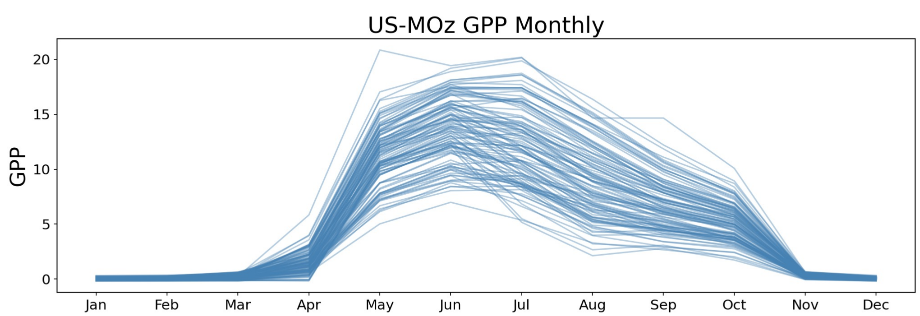
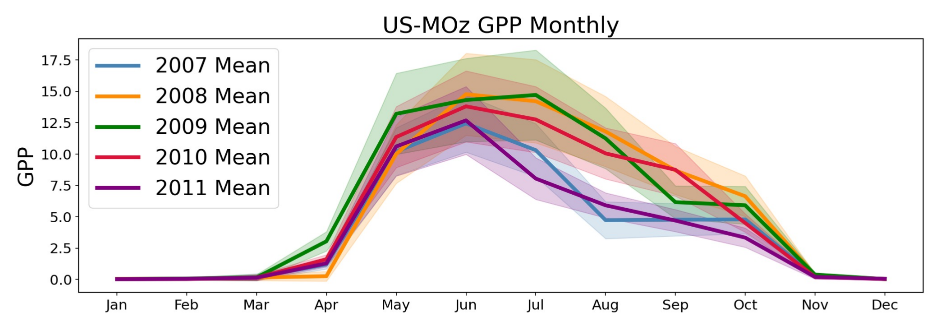
# Interannual variability as an 'intrinsic' variability



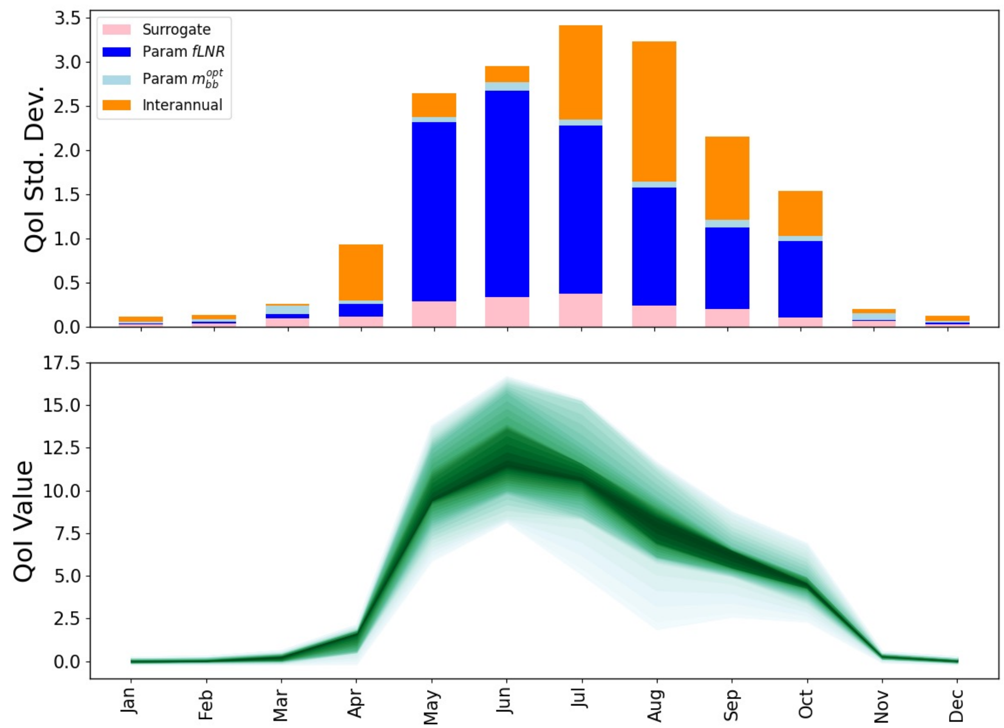



# Interannual variability as an ‘intrinsic’ variability

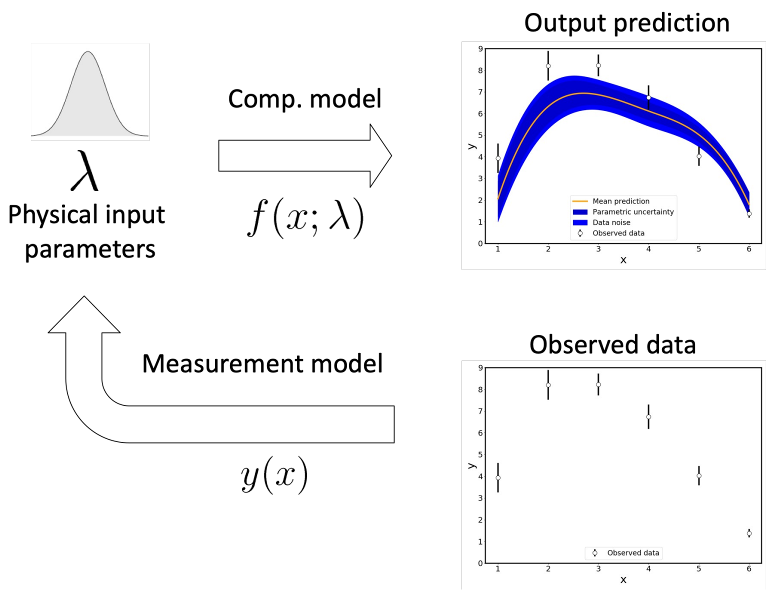
$$f(\lambda,\omega) \approx \sum_k c_k \Psi_k(\xi,\zeta)$$

parametric → $\xi$, stochastic → $\zeta$

- PC expansion allows ‘free’ global sensitivity analysis (GSA) due to orthogonality of the bases
- GSA or variance decomposition can be augmented, empirically, with MSE of the surrogate for another error component



# Uncertainty Budget in Computational Models




**Forward UQ**
**(Uncertainty propagation, Global sensitivity analysis)**

- Parametric Uncertainty
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**Inverse UQ**
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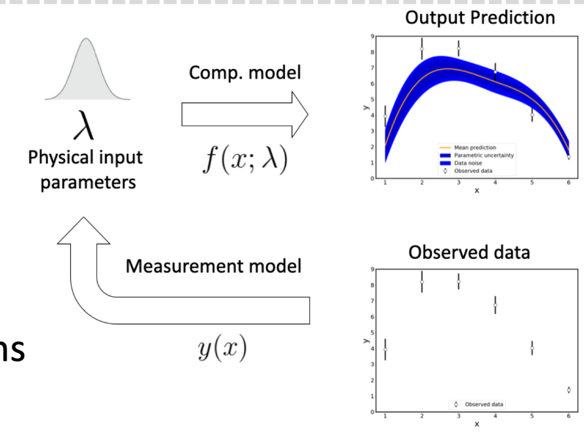
# Inverse Modeling Setup

- Compare observational/measurement data with the model
- Tune model parameters (and sometimes model form) to fit the data




- Bayesian methods are best suited for probabilistic inverse problems
  - Meaningful aggregation of various sources of uncertainty
  - Rigorous mathematical footing

- Collected data $\{(x_i, y_i)\}_{i=1}^N$
- Data model $y_i = f(x_i; \lambda) + \epsilon_i$

## Bayes formula

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

[Tarantola, 2005]

# How to Correct for Model Error

*External:* Conventional *statistical* Gaussian Process correction *[Kennedy, O'Hagan, 2001]*

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

Challenges when it comes to *physical* models.

---

*Embedded Intrusive:* Model-specific corrections: changing the model/code

$$g(x_i) = \tilde{f}(\lambda; x_i; \delta_\alpha(x_i)) + \epsilon_i$$

---

*Embedded Non-Intrusive:* Model-agnostic: cast deterministic model parameter as a random variable *[Sargsyan, 2019]*

$$g(x_i) = f(\lambda + \delta_\alpha(x_i), x_i) + \epsilon_i$$

# PC Expansions Help Propagate Embedded Errors

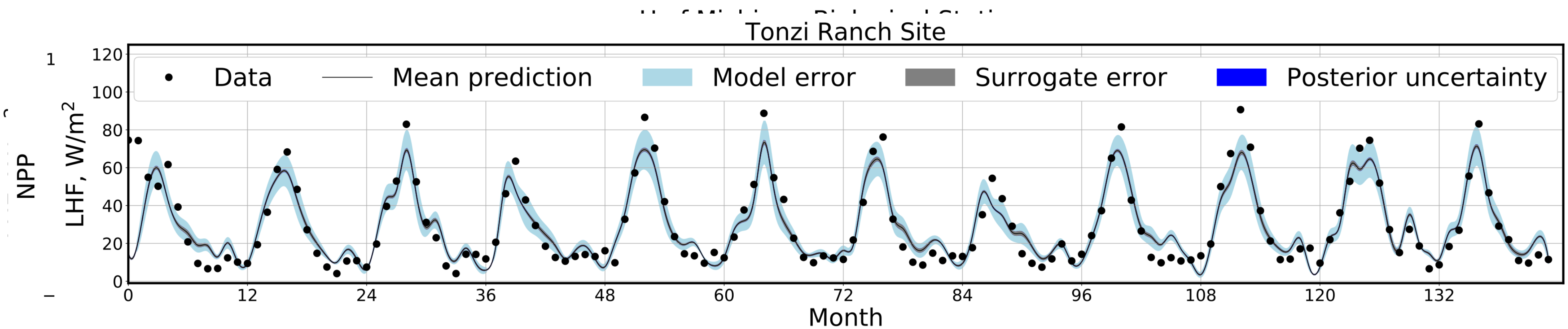
- Allows meaningful extrapolation
- Respects physics
- Disambiguates model and data errors
- Predictive uncertainty attribution

$$g(x_i) = f(\lambda + \delta_\alpha(x_i), x_i) + \epsilon_i$$

- Infer physical parameters $\lambda$ and model-error parameters $\alpha$ together
- In practice, cast the parameters as a PC expansion $\lambda = \sum_k \alpha_k \Psi_k(\xi)$
- Propagate (forward UQ) PC $f\left(\sum_k \alpha_k \Psi_k(\xi), x_i\right) \approx \sum_k f_k(\alpha)\Psi_k(x_i)$
- Build approximate likelihood functions based on data model $g(x_i) = \sum_k f_k(\alpha)\Psi_k(x_i) + \epsilon_i$
  (e.g. match moments, or Gaussian iid approximation)

*[Sargsyan et al, 2019; Kuppa et al, 2026]*

# Embedded Model Error captures residual discrepancies better



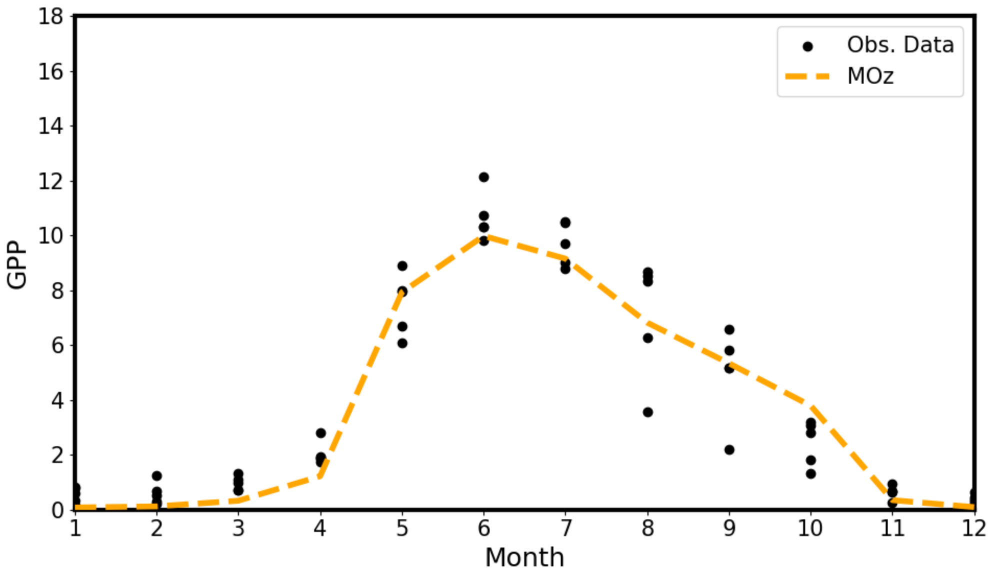

Predictive uncertainty attributed to model error

Allows (dangerous!) extrapolation to other sites

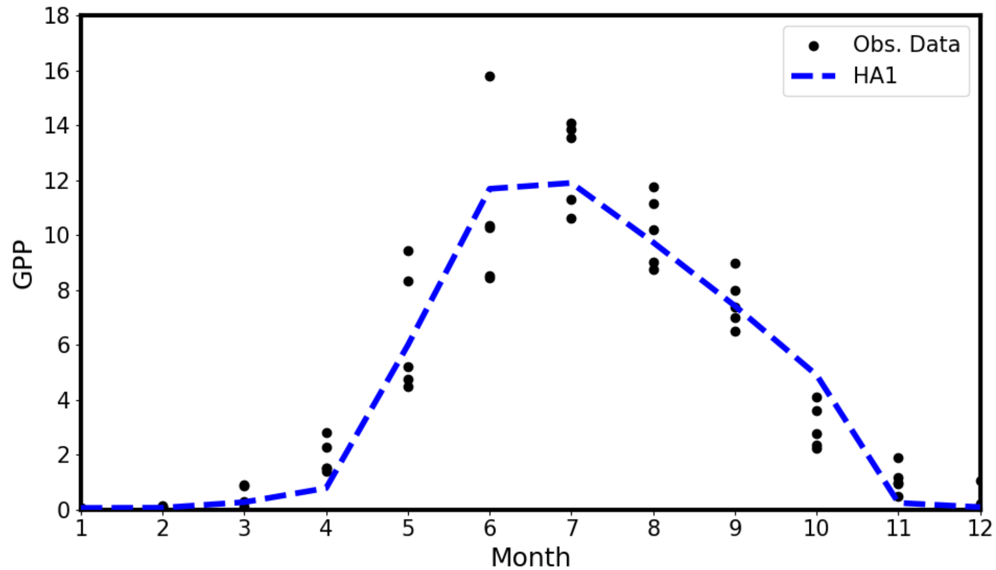
Allows meaningful prediction of other QoIs (e.g. NPP with no data)

Conventional calibration without model error

# Multiple Sites Joint Calibration

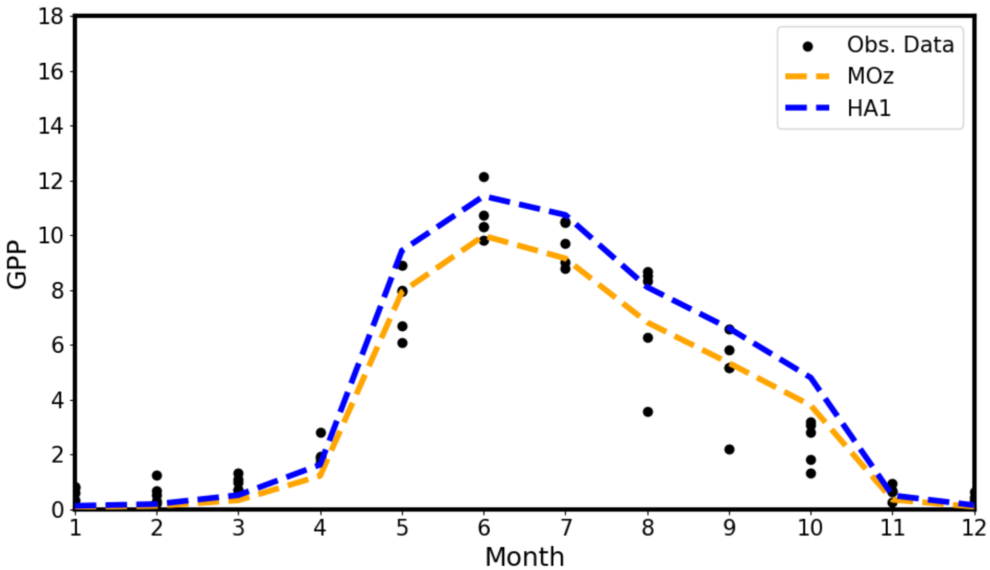



US – MOz




US – Ha1

# Multiple Sites Joint Calibration

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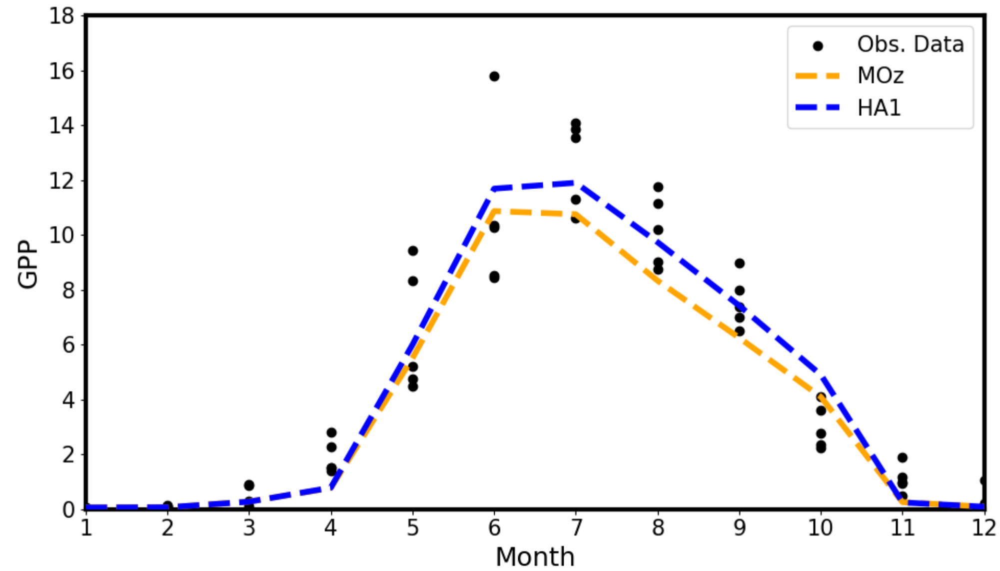


US – Ha1

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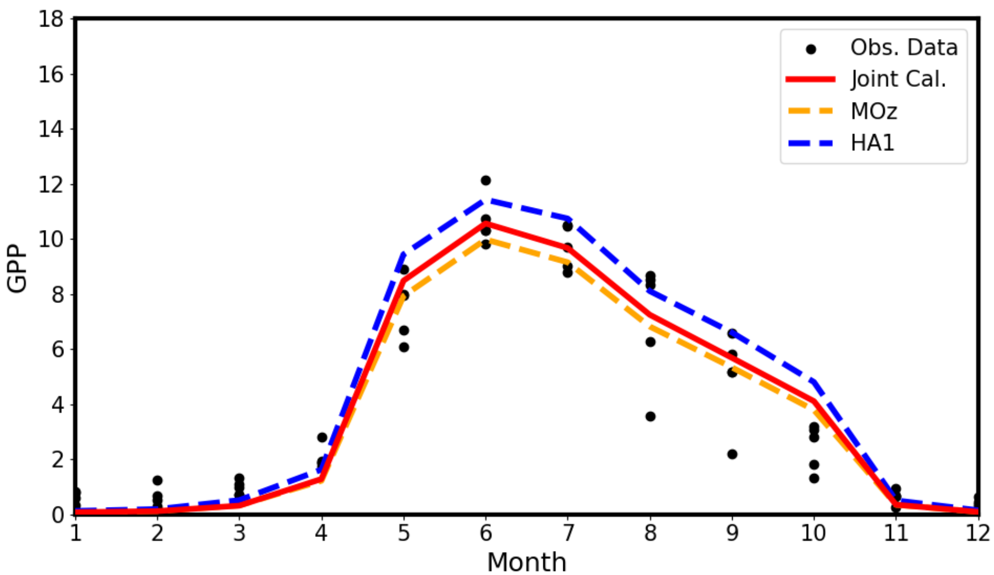
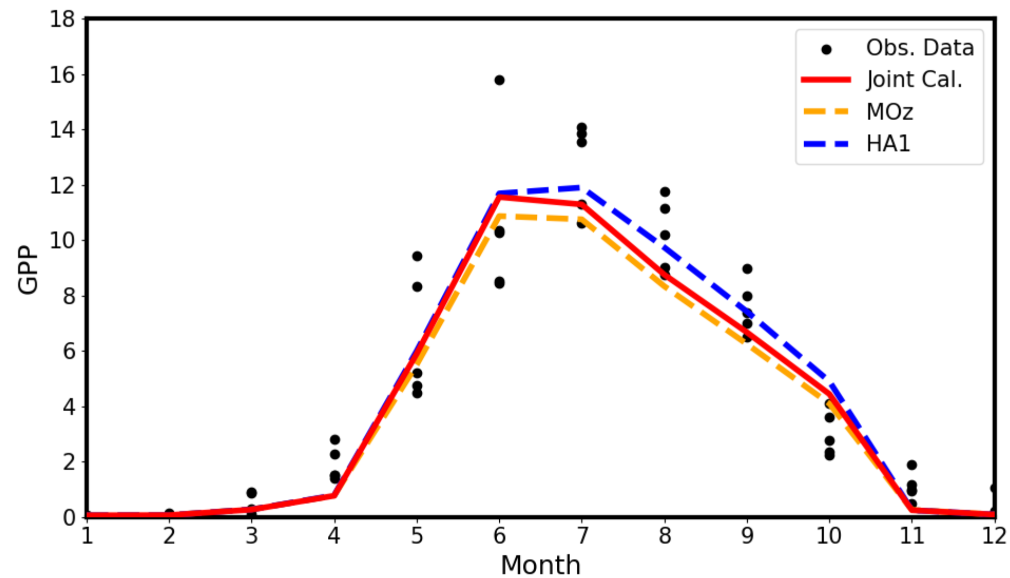



US – MOz




US – Ha1

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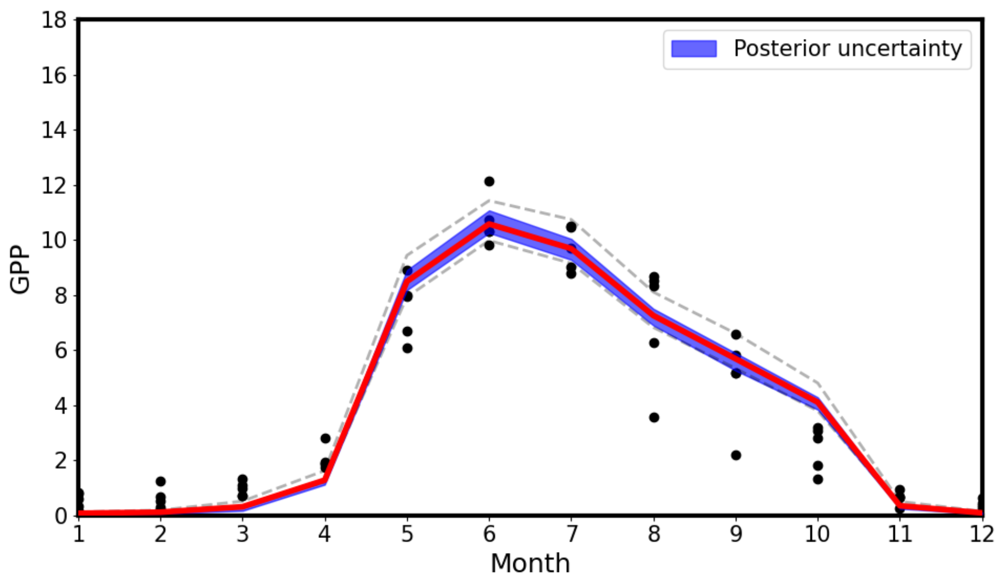
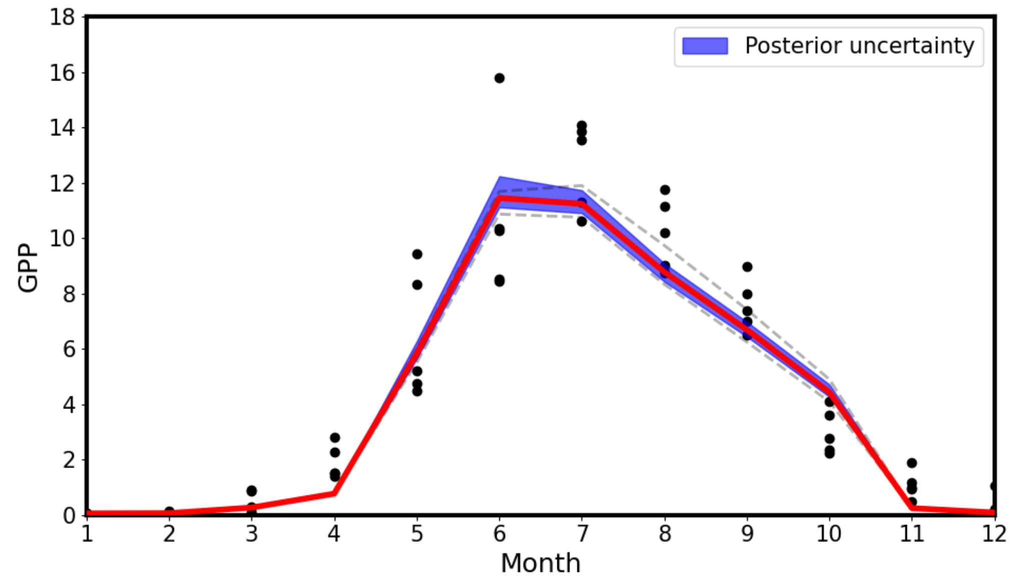
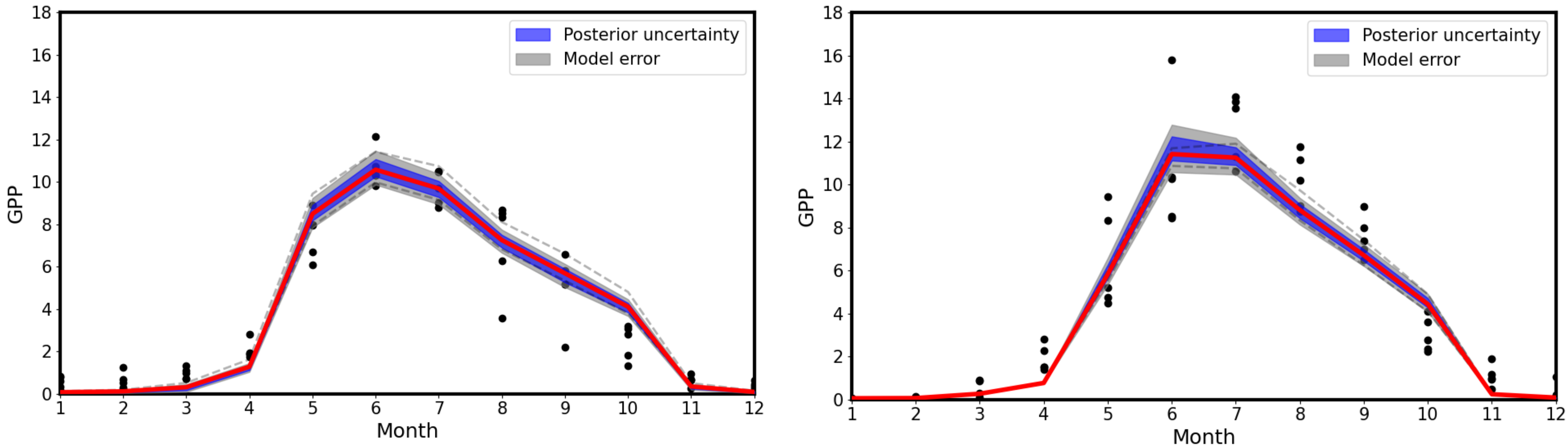



- Posterior uncertainty quantifies the impact of data quality and quantity

# Multiple Sites Joint Calibration




- Posterior uncertainty quantifies the impact of data quality and quantity
- Model error quantifies the impact of the assumption that ELM parameters are constant across sites

# Summary

- PC based uncertainty attribution of computational models
- Focusing on two non-standard components:
  - Intrinsic variability via stochastic surrogate (forward UQ)
  - Model form error via embedded model error inference (inverse UQ)
- Demonstrations on E3SM Land Model (ELM)
- Both stochastic surrogate construction and embedded model error are implemented in PyTUQ, *github.com/sandialabs/pytuq*

# Cited Literature

**Classics**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**Forward UQ (stochastic/surrogate)**


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**Inverse UQ (embedded model error)**


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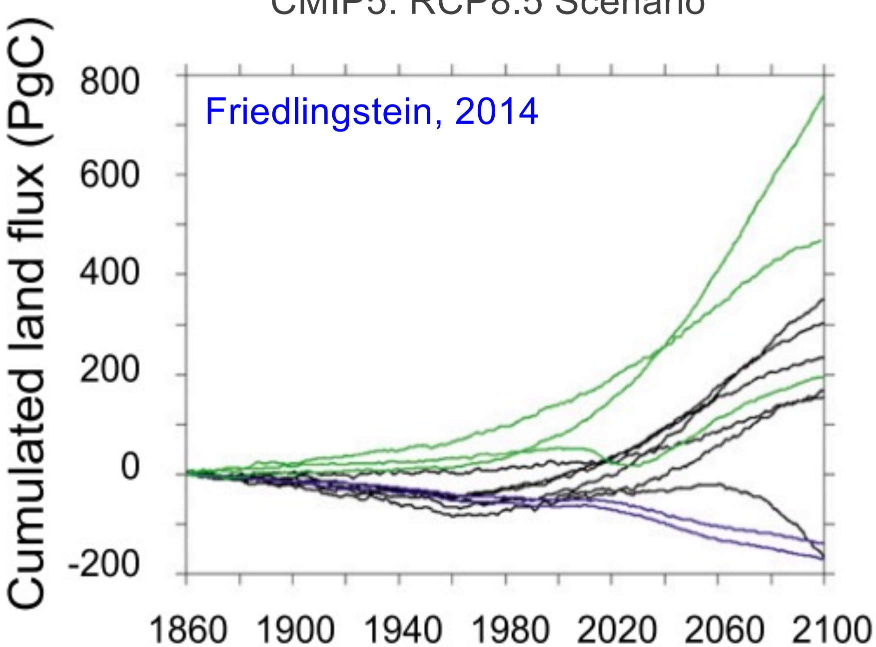
- K. Sargsyan, X. Huan, H. Najm. “Embedded Model Error Representation for Bayesian Model Calibration”, *Int. J. Uncertainty Quantification*, 9:4, (2019).
- M. Kuppa , K. Sargsyan, M. Panesi, and H. Najm “Model Error Embedding with Orthogonal Gaussian Processes”, *SIAM/ASA Journal of Uncertainty Quantification*, in review (2026).
- N. Iyengar, D. Ricciuto, K. Sargsyan, “Uncertainty Quantification and Calibration of the E3SM Land Model using an Embedded Model Error Approach”, to be submitted (2026).

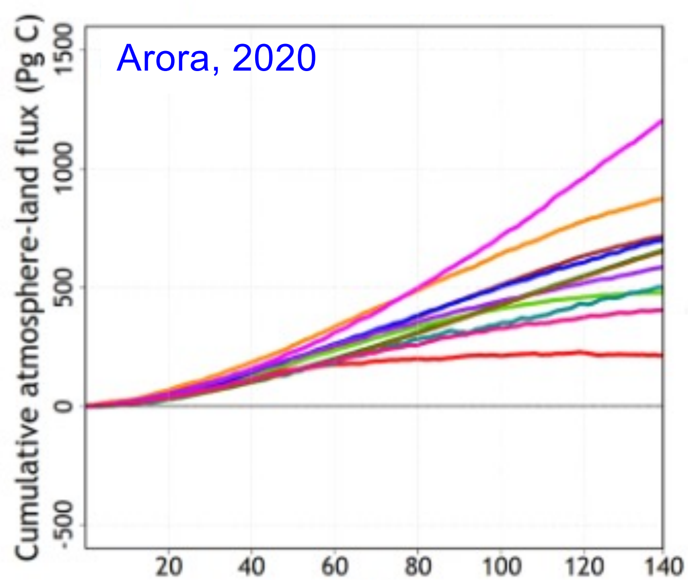
# Trunk

# Motivation: Uncertainties in Carbon Flux

CMIP5: RCP8.5 Scenario

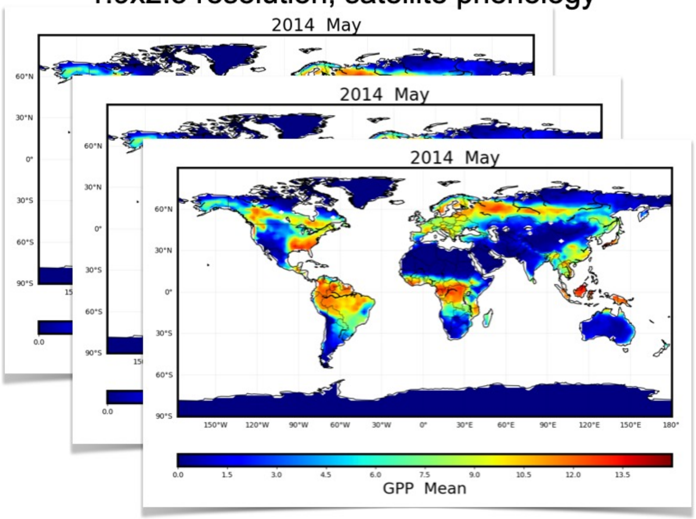



CMIP6: 1%/yr $CO_2$ incr. Scenario



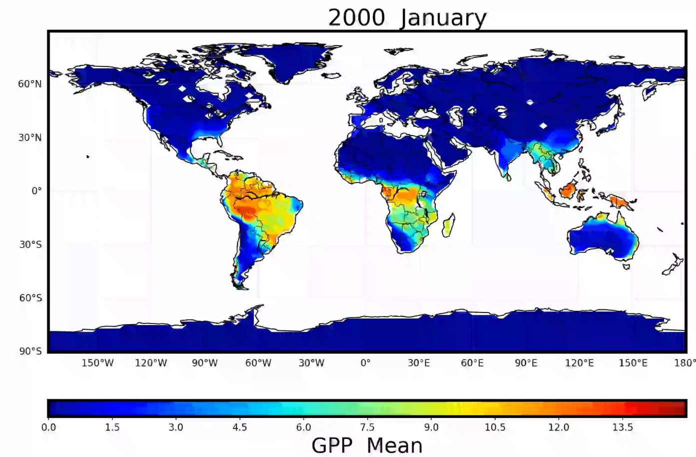
# Model Ensemble (275 samples)

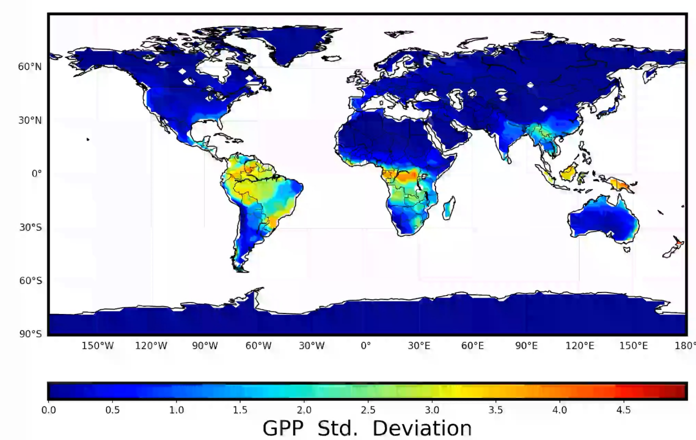
1.9x2.5 resolution, satellite phenology




## Perturbed Parameters

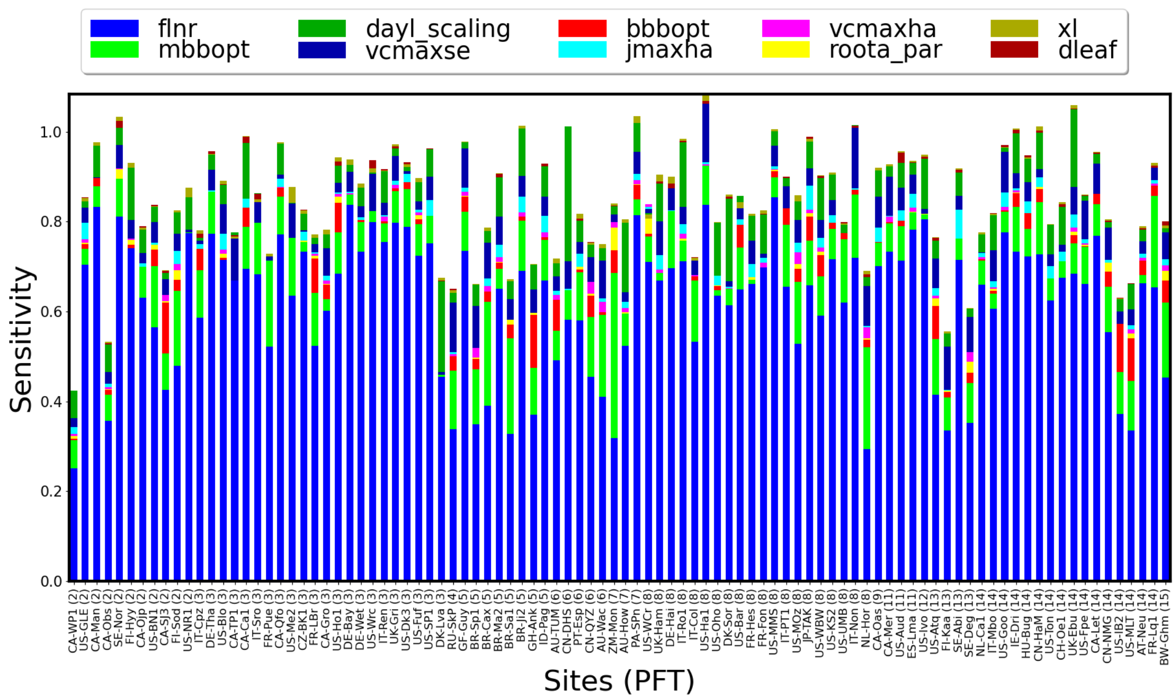
| Parameter | Description | Min | Max |
|---|---|---|---|
| flnr | Fraction of leaf in in RuBisCO | 0 | 0.25 |
| mbbopt | Stomatal slope (Ball-Berry) | 2 | 13 |
| bbbopt | Stomatal intercept (Ball-Berry) | 1000 | 40000 |
| roota_par | Rooting depth distribution | 1 | 10 |
| vcmaxha | Activation energy for Vcmax | 50000 | 90000 |
| vcmaxse | Engropy for Vcmax | 640 | 700 |
| jmaxha | Activation energy for jmax | 50000 | 90000 |
| dayl_scaling | Day length factor | 0 | 2.5 |
| dleaf | Characteristic leaf dimension | 0.01 | 0.1 |
| xl | Leaf/stem orientation index | -0.6 | 0.8 |



E3SM
Energy Exascale
Earth System Model

# Sensitivity at 96 FLUXNET sites: RuBisCO leaf fraction (fLNR) is the most impactful param.

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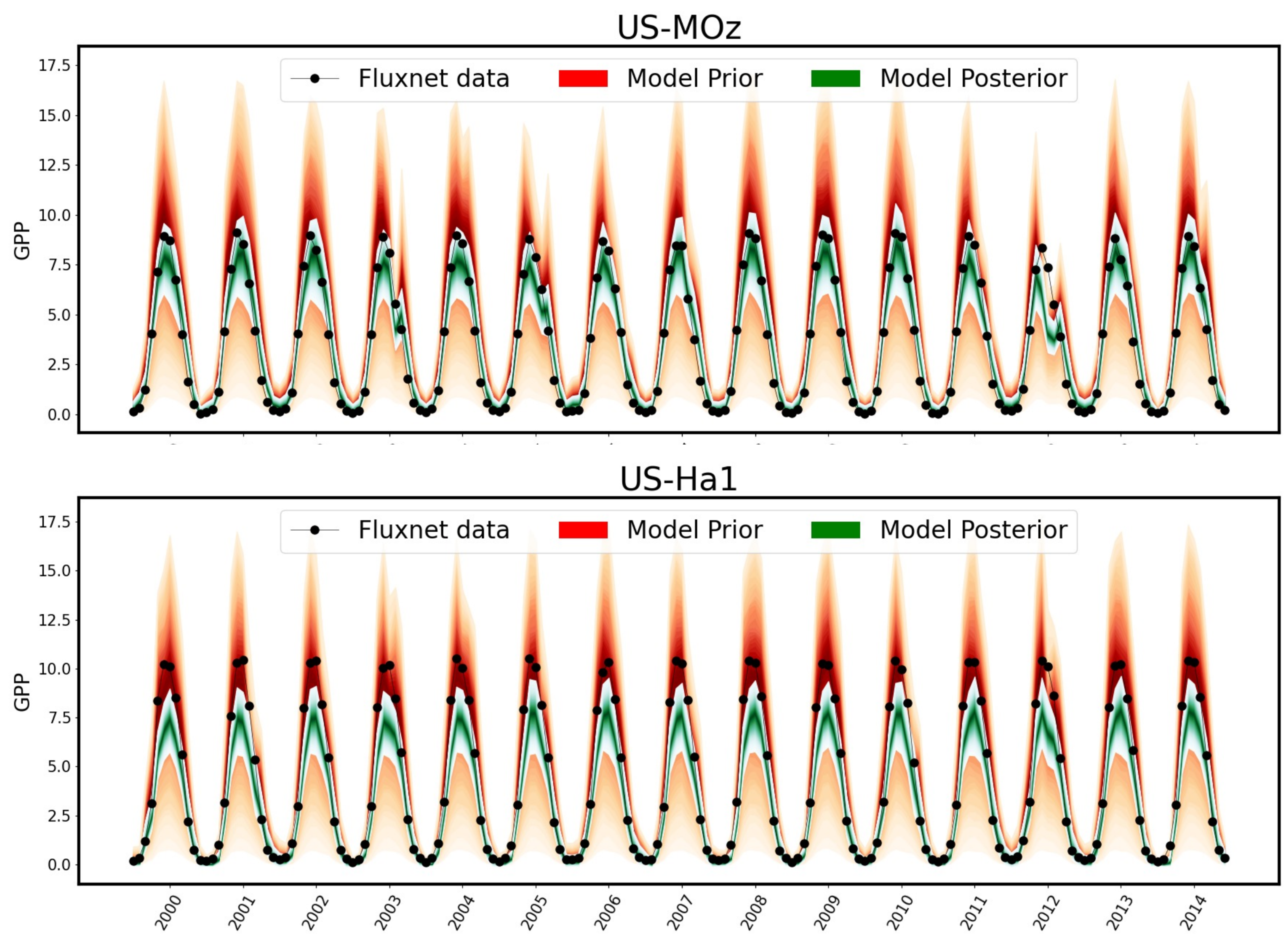
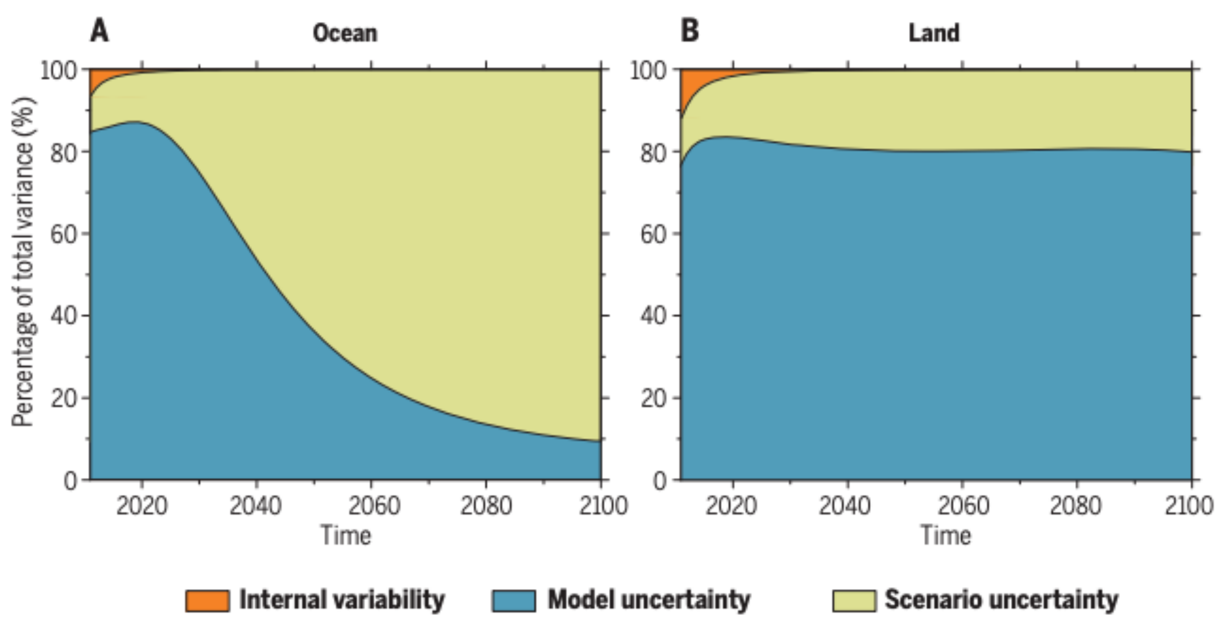
Time evolution of GPP at select FLUXNET sites



# Motivation: Model Uncertainty dominates for Land Model

**Fig. 4. Ocean and land carbon cycle uncertainty.** The percentage of total variance attributed to internal variability, model uncertainty, and scenario uncertainty in projections of cumulative global carbon uptake from 2006 to 2100 differs widely between (**A**) ocean and (**B**) land. The ocean carbon cycle is dominated by scenario uncertainty by the middle of the century, but uncertainty in the land carbon cycle is mostly from model structure. Data are from 12 ESMs using four different scenarios (94).




Bonan and Doney,
Climate, ecosystems, and planetary futures: The challenge to predict life in Earth system models. Science, 2018

# Polynomial Chaos intro

- Our traditional tool for uncertainty representation and propagation
- Random variables represented as polynomial expansion of standard random variables, such as gaussian or uniform

$$\xi = \sum_{k=1}^{K} c_k \, \psi_k(\eta)$$

- Convenient for uncertainty propagation

$$f(\xi) = \sum_{k=0}^{K} f_k \, \psi_k(\eta)$$

- Moment estimation
- Global Sensitivity Analysis (a.k.a. Sobol indices or variance-based decomposition)

# Global Sensitivity Analysis (Parameter importance via variance decomposition)