# A Novel Computational Framework for Optimal Experimental Design to Improve Climate Prediction

US CLIVAR Micro2Macro Workshop @University of Wyoming, Laramie

October 28-30, 2024

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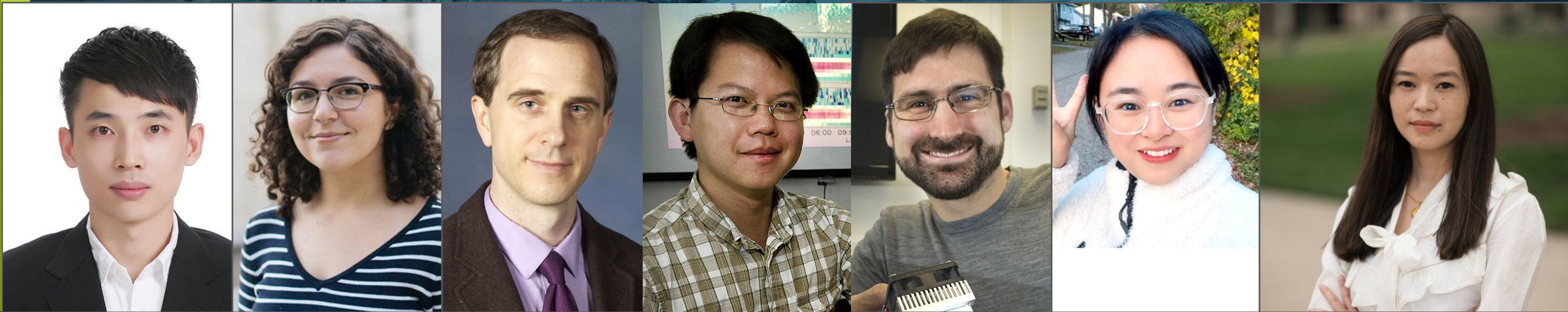
U.S. DEPARTMENT OF ENERGY



# A Novel Computational Framework for Optimal Experimental Design to Improve Climate Prediction

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## Computational Framework

Simulation (modeling)

Observation (e.g. , field campaign, lab experiments)

Theory

→ Improve Climate Predictability

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# What are the challenges? – Model observation integration

- Improvements in climate model predictability are hampered by **limited feedback between reducing model uncertainties and designing optimal observing systems**.

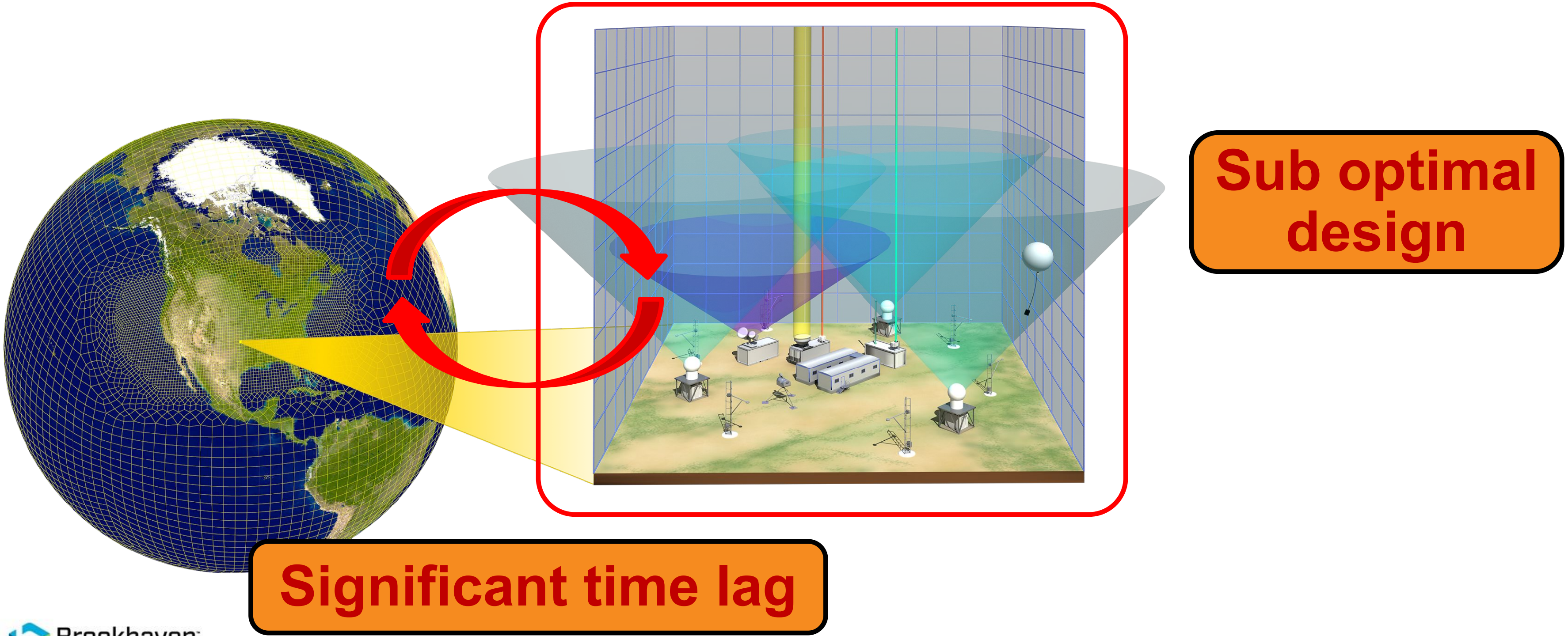


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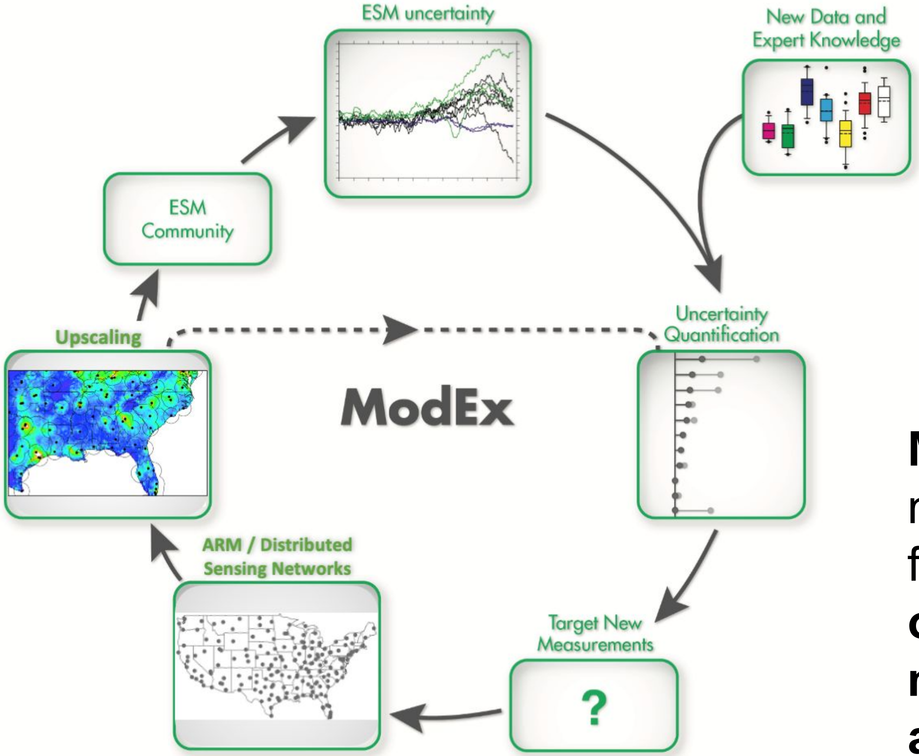
Image source: E3SM's Single-Column Model

# Solutions– Model observation integration

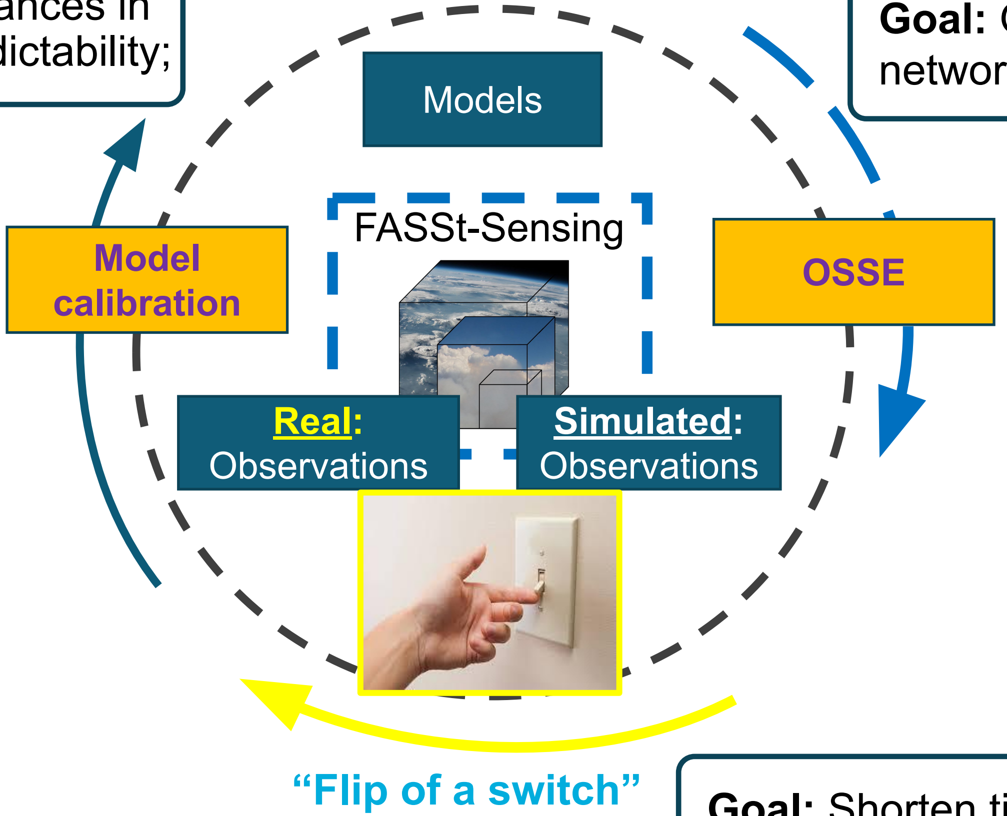



**ModEx** is a concept to enable this model-observation coupling but is often not fully realized because **models and observing systems often have a mismatch in scales (spatial/temporal) and focus.**

# Model-Observing System Co-Design

**Goal:** Lead to advances in climate model predictability;

**Goal:** Optimize observational network design;




**Goal:** Shorten timelines between observation and discovery.

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# Earth System Model Framework

**Input**

**Parameters**
**Initial & boundary conditions**

**Numerical model**

**Dynamical core**
(Navier-Stokes equations)

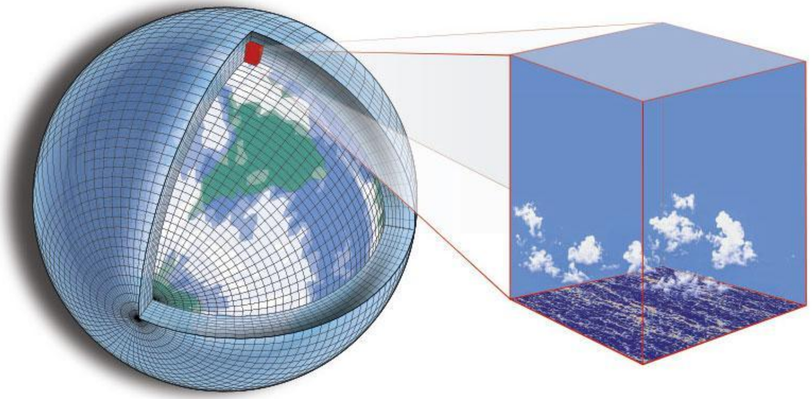
**Parameterization**
(subgrid physical & chemical processes)

**Output**

**Model output assessment**

## What are the sources of uncertainty in the earth system model?

**Parametric uncertainty**



**Model structural uncertainty**

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# Uncertainty Quantification Framework

**UQ** is a field of study that deals with assessing, analyzing, and managing uncertainty in various mathematical models and simulations.

Automated financial trading

Self-driving car

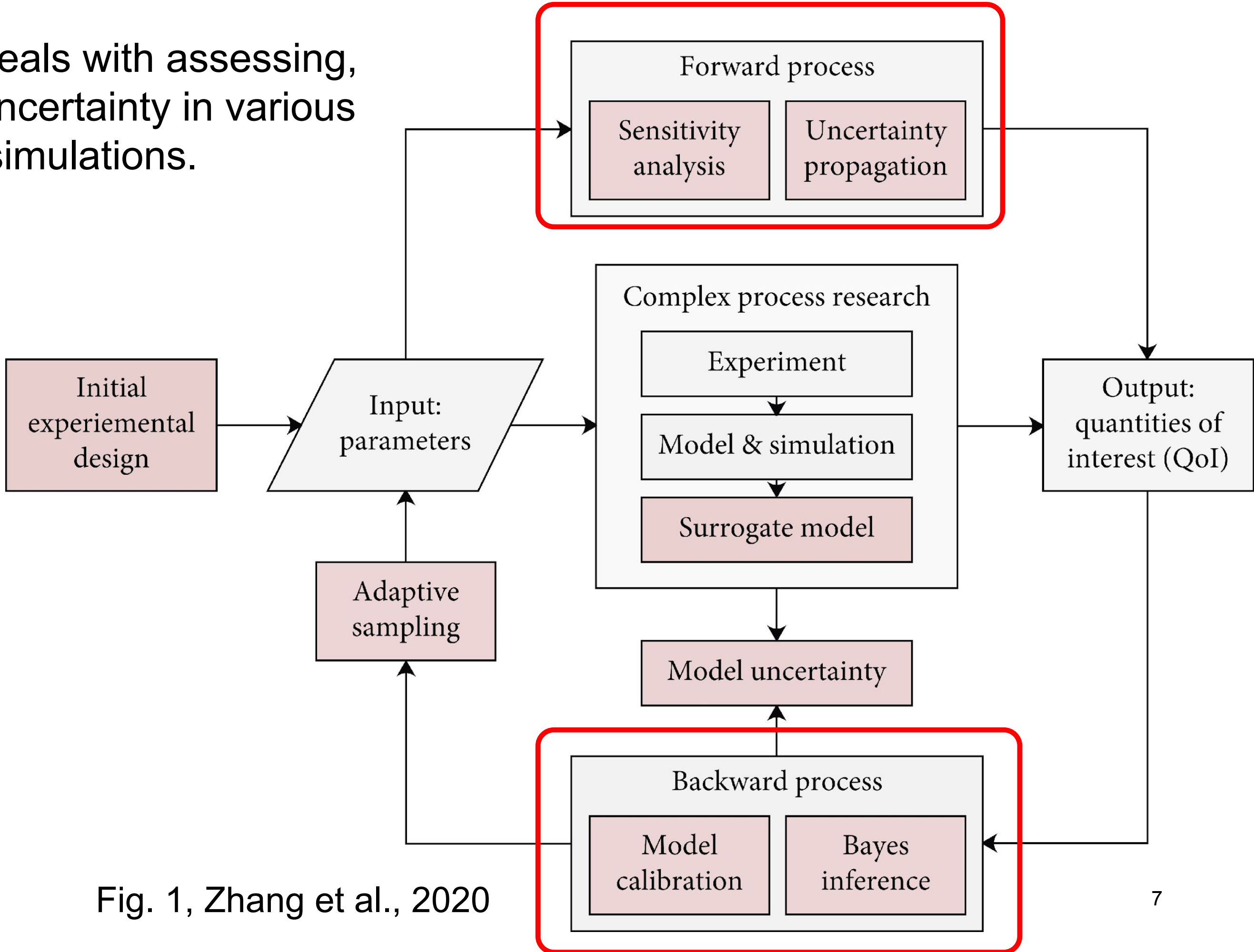
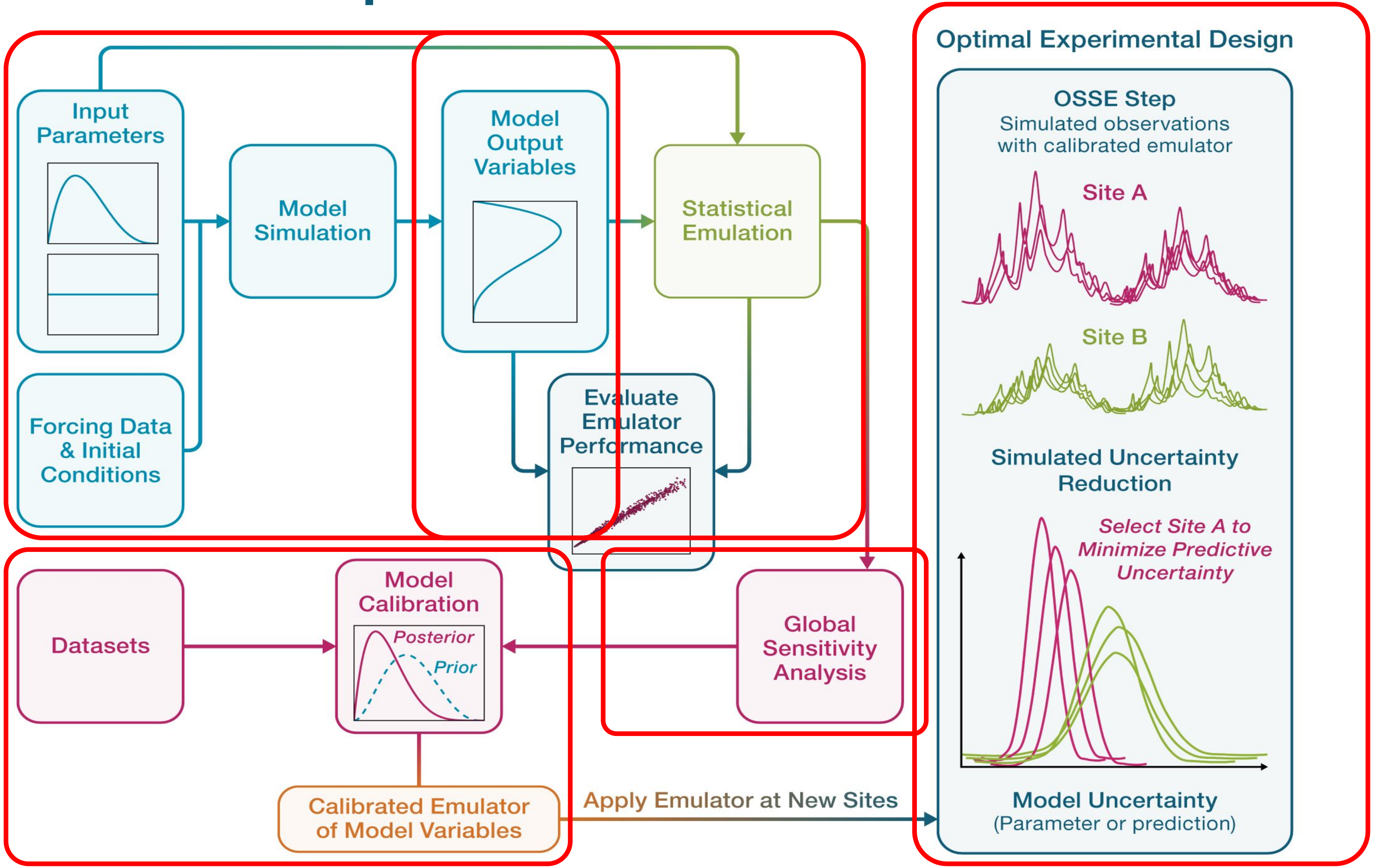
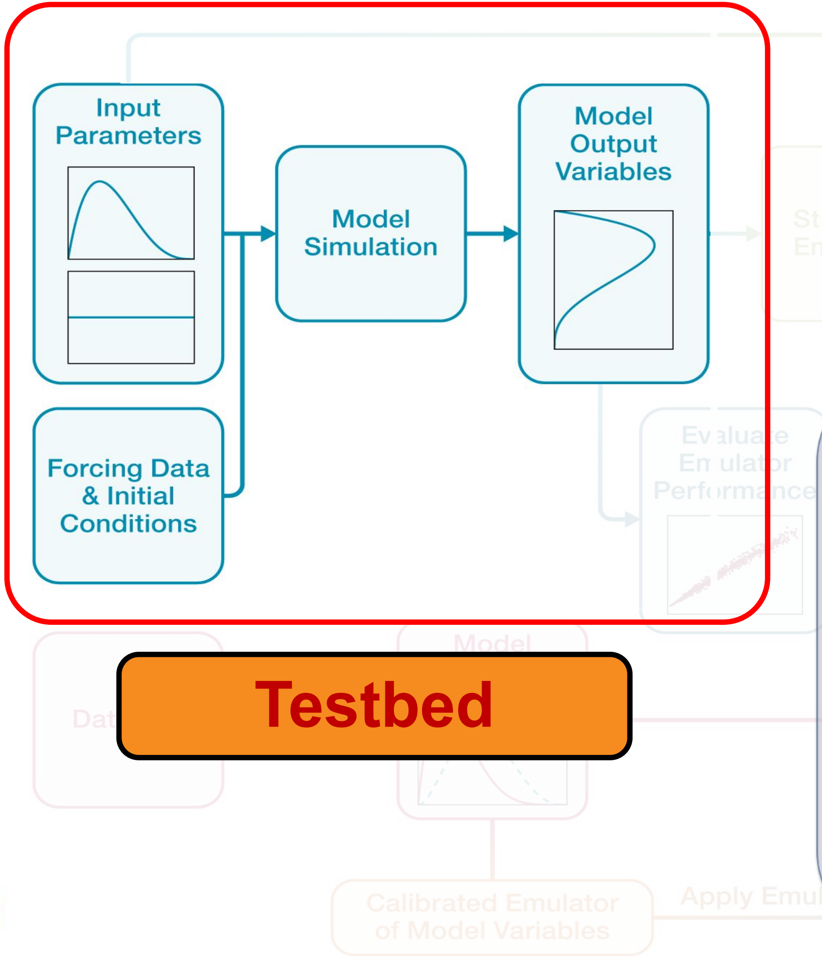


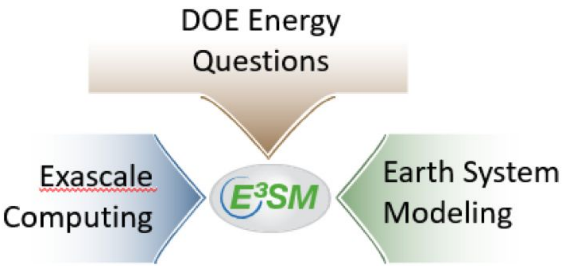

Fig. 1, Zhang et al., 2020

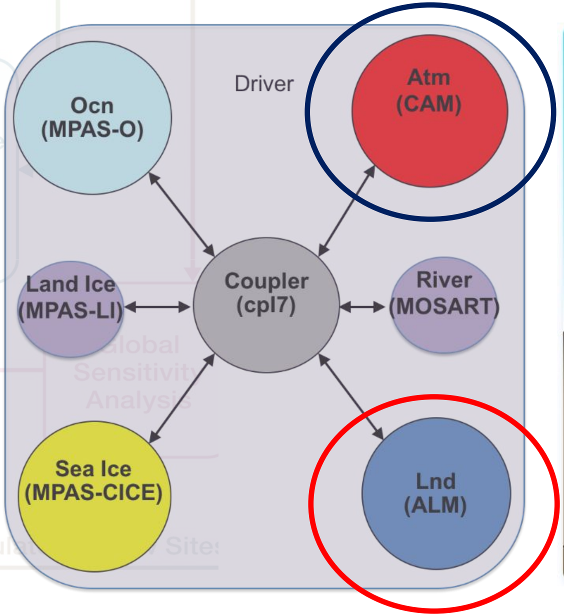
# Computational Framework

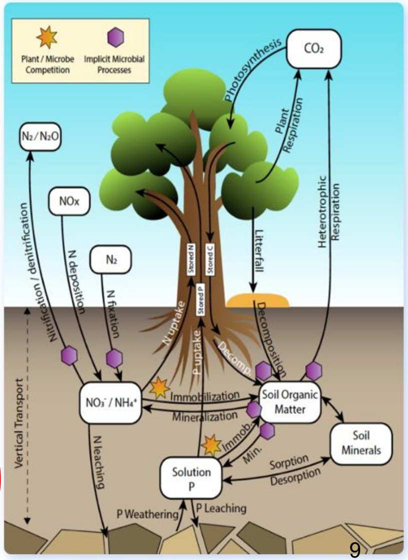


# Model-E3SM Land Model



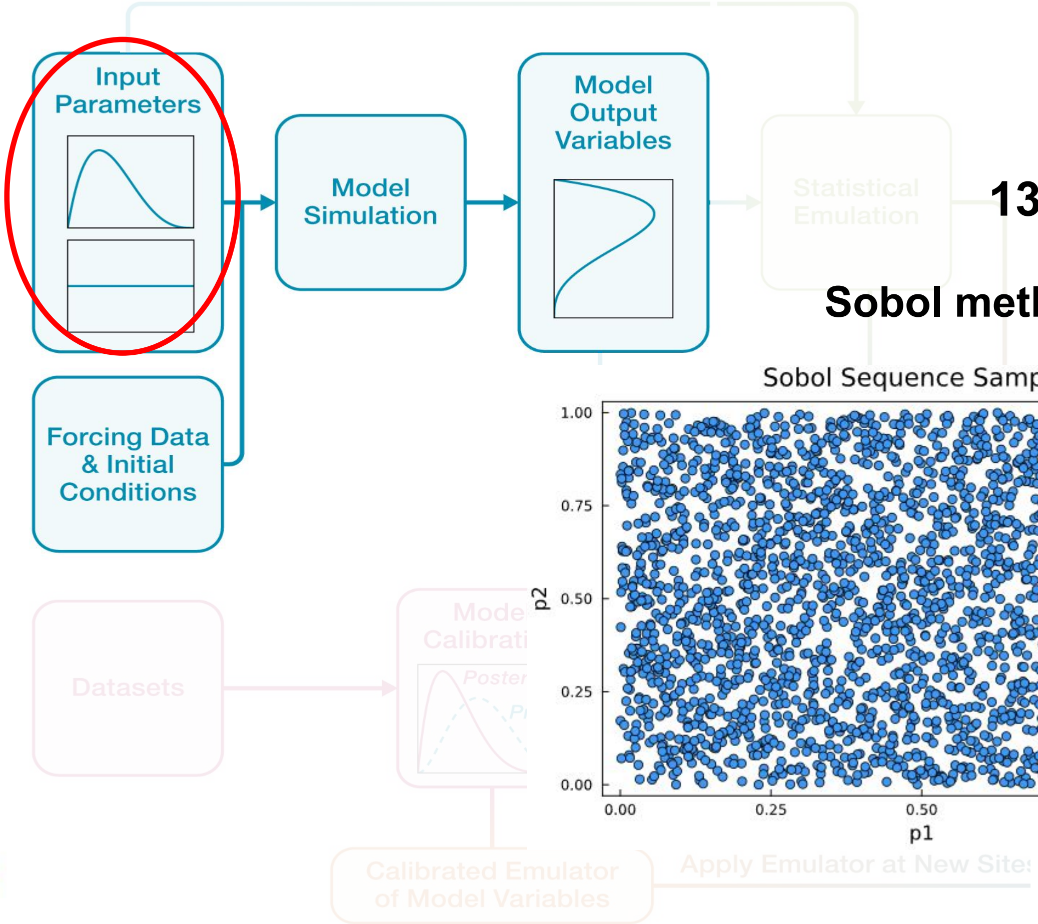



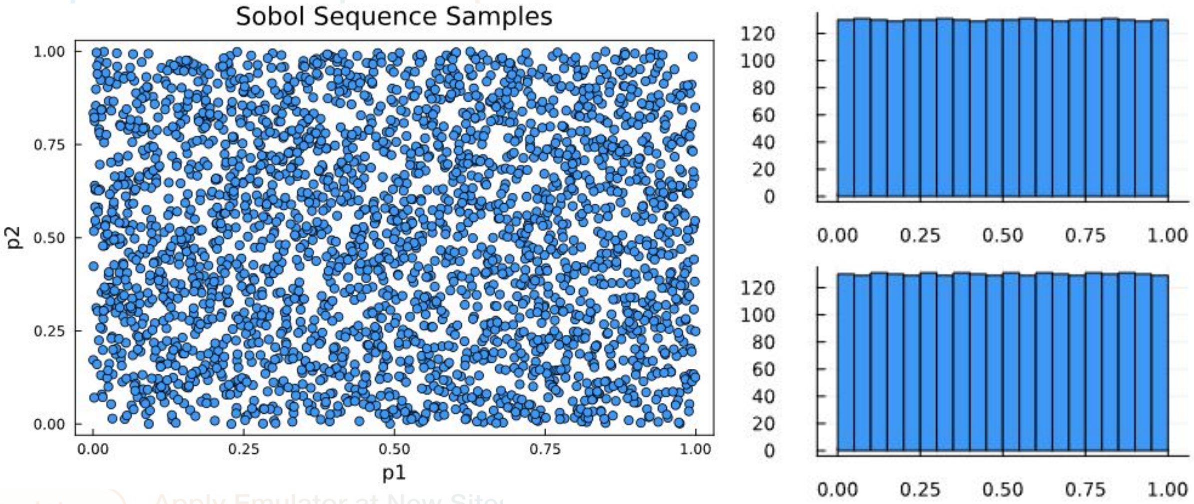
# Perturbed Parameter Ensemble (PPE)

**297 parameters in clm_params.nc-> 26 parameters**




**1300 ensemble members**

**Sobol methods**




Sobol, 1967

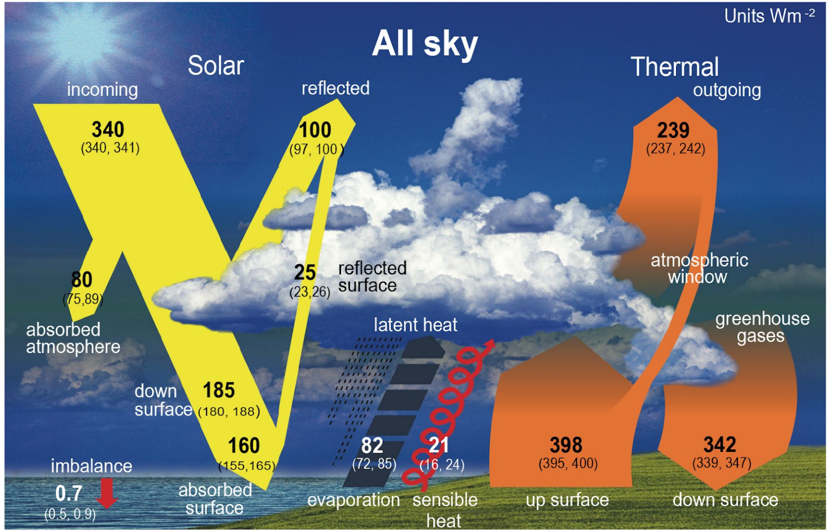
# Quantities of interest

**The Earth's Energy Budget:**

- Sensible heat flux (H)
- Latent heat flux (LE)

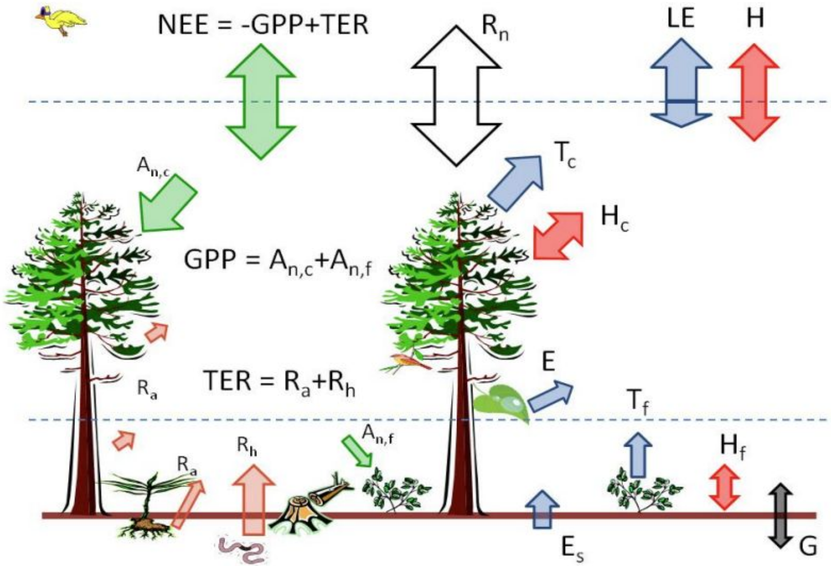
**Carbon and biogeochemical cycle:**

- Gross primary productivity (GPP)
- Net ecosystem exchange (NEE)



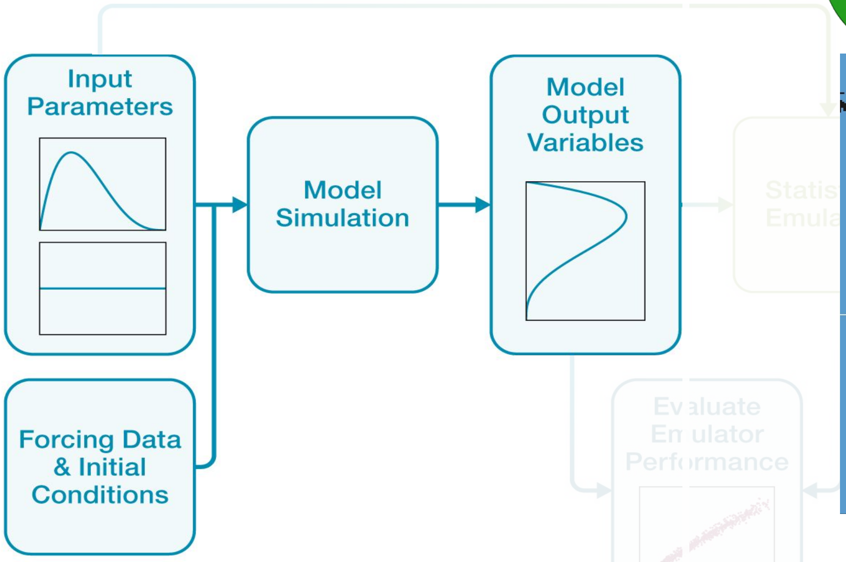



IPCC AR6 Figure 7.2

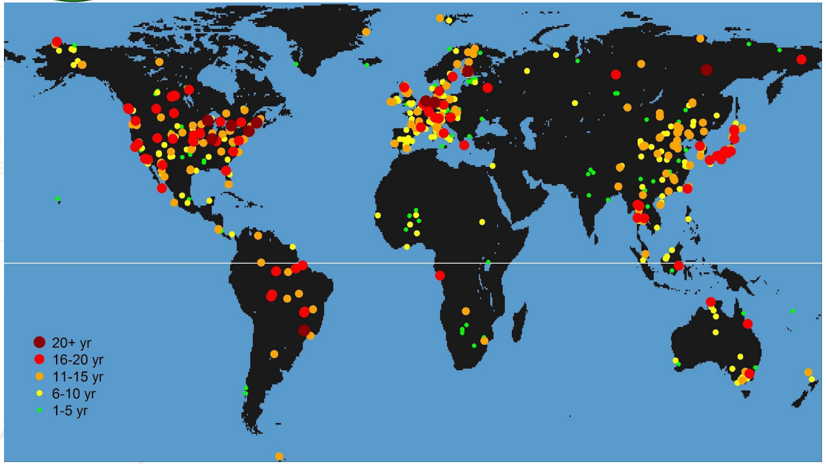


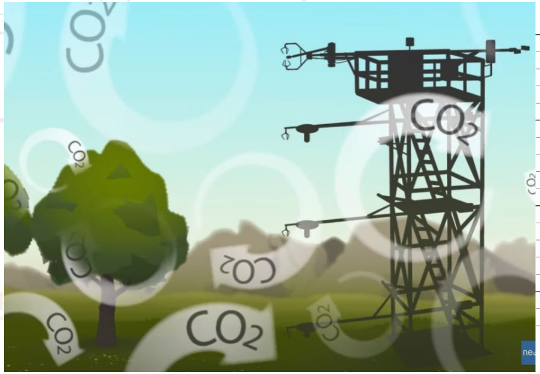

Samuli, 2011

# Observation

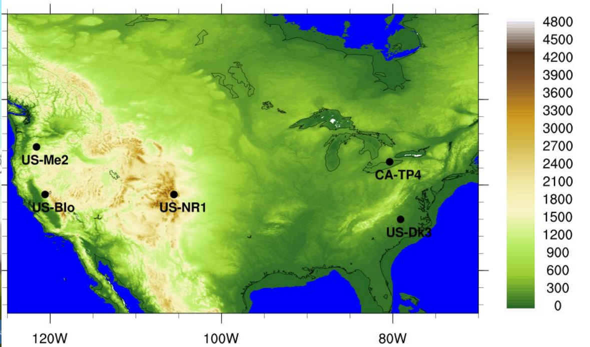



The most recent FLUXNET data product, **FLUXNET2015**

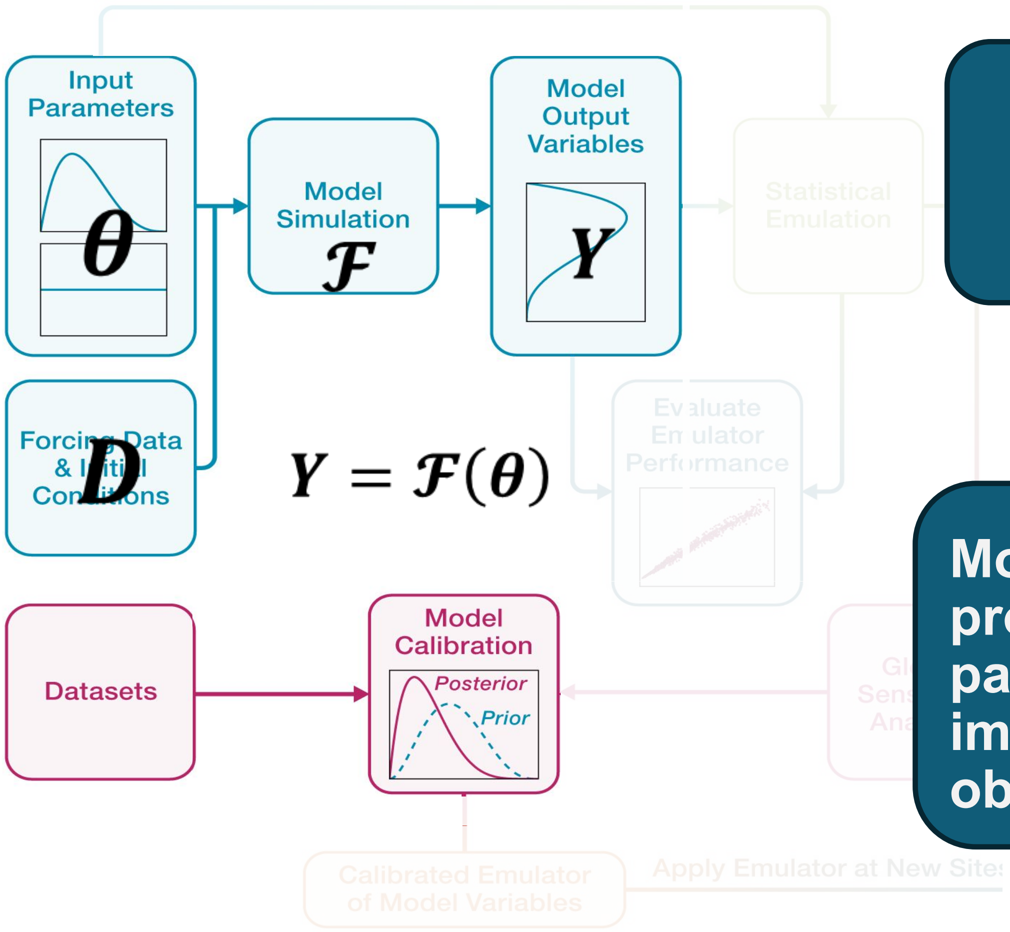



## PFT: Evergreen Needleleaf Trees



# Model calibration-Definition



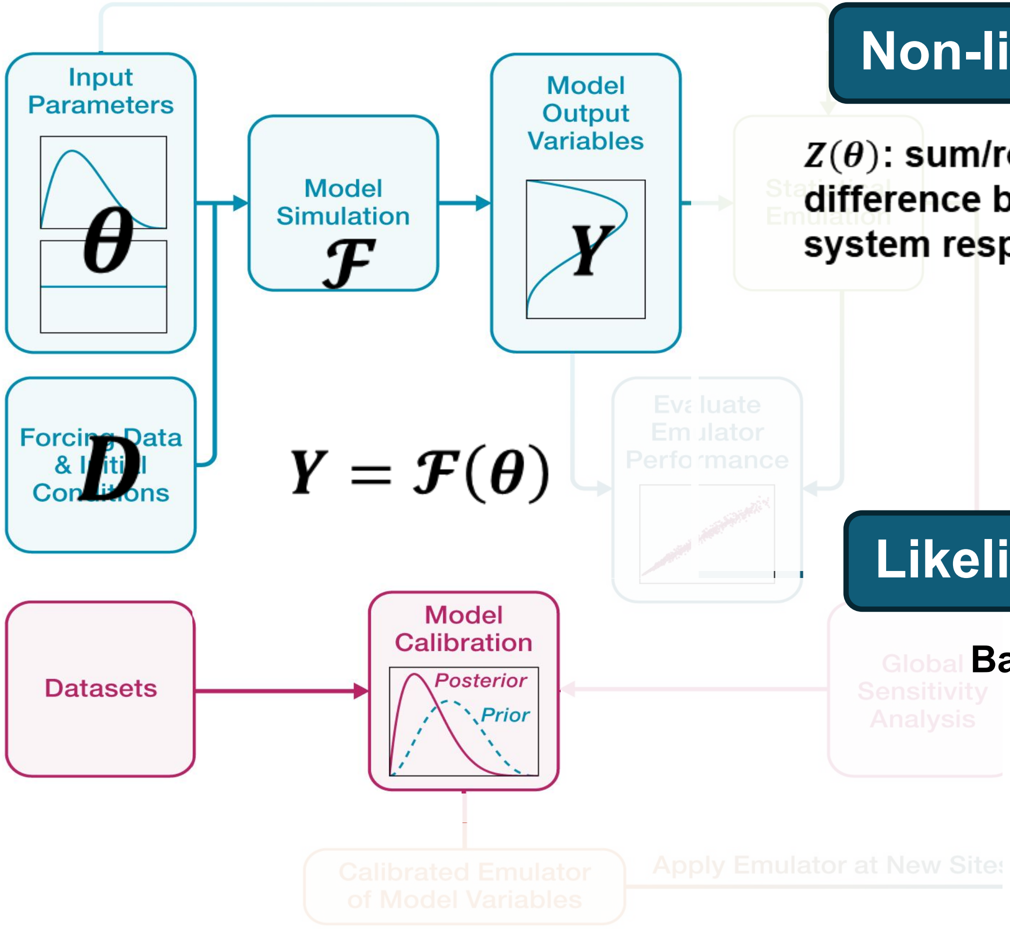

## Question

How can we improve model performance with observation?

## Definition

Model calibration refers to the process of adjusting the parameters of the model to improve its agreement with observed data.

# Model calibration-Classes




## Classes

### Non-likelihood-based calibration

**$Z(\theta)$: sum/root mean of squared residuals (i.e., the difference between the observed and simulated system response)**

$$SSE = \sum_{i=1}^{n}(y_i - m_i)^2$$

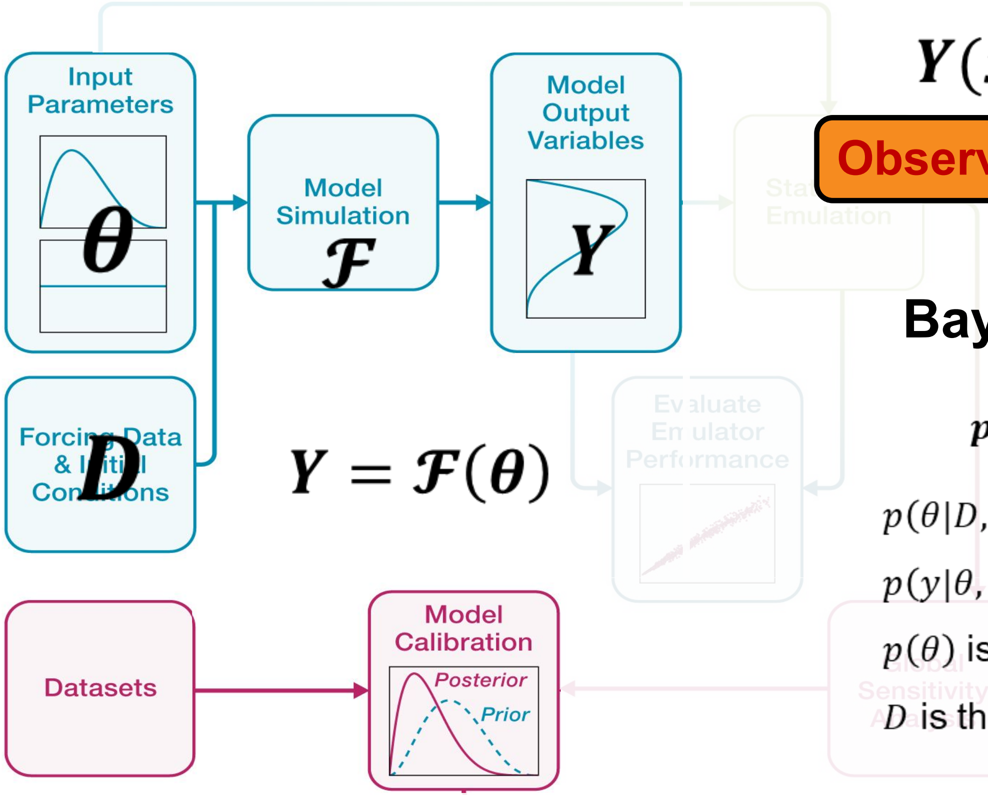
$$RMSE = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(y_i - m_i)^2}$$

### Likelihood-based calibration

**Bayes' theorem:**

$$P(A|B) = \frac{P(B|A)\cdot P(A)}{P(B)}$$

# Model calibration




$$Y = \mathcal{F}(\theta)$$

## Likelihood-based calibration

$$Y(x,t) = m(x,t;\theta) + \epsilon(x,t)$$

**Observation** **model** **residual**

**Bayes' theorem:**

$$p(\theta|D,y) = \frac{p(y|\theta,D)p(\theta)}{p(y,D)} \propto p(y|\theta,D)p(\theta)$$

$p(\theta|D,y)$ is the **posterior probability** of $\theta$ given Y

$p(y|\theta,D)$ is the **likelihood** of $\theta$ given Y

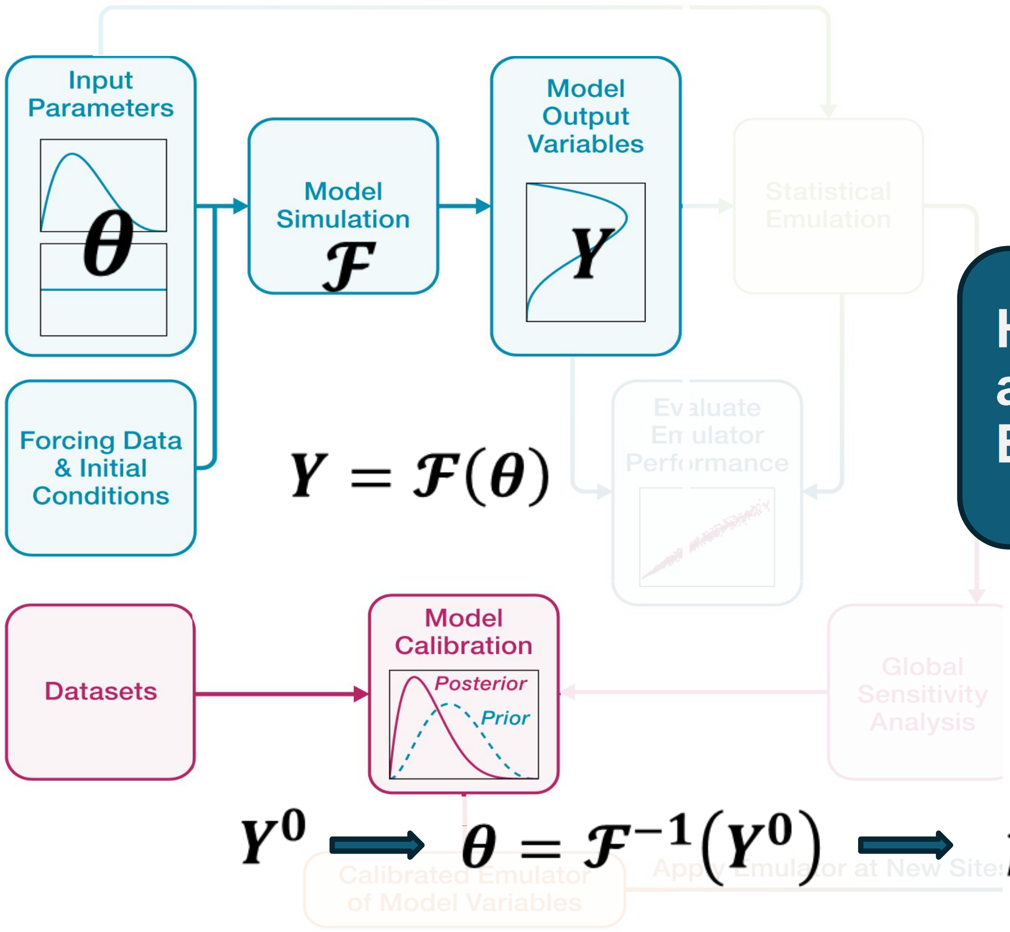
$p(\theta)$ is the **priori probability** of $\theta$

$D$ is the driver condition

$$Y^0 \longrightarrow \theta = \mathcal{F}^{-1}(Y^0) \longrightarrow p(\theta|Y^0) \propto p(Y^0|\theta)p(\theta)$$

# Model calibration

## Likelihood-based calibration




$$Y = \mathcal{F}(\theta)$$

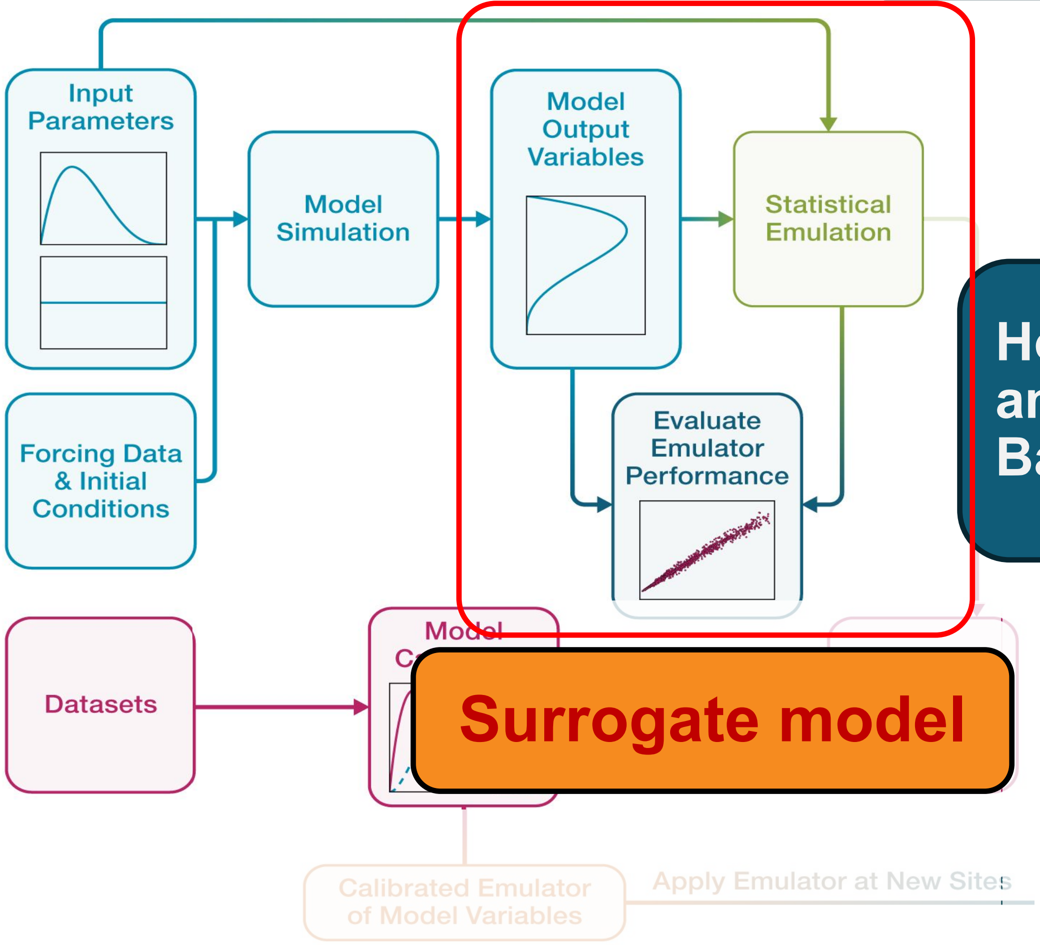
## Technical Problem

**How to accomplish the huge amount of sampling in the Bayesian inference?**

$$Y^0 \longrightarrow \theta = \mathcal{F}^{-1}(Y^0) \longrightarrow p(\theta|Y^0) \propto p(Y^0|\theta)p(\theta)$$

# Statistical Emulation

## Likelihood-based calibration

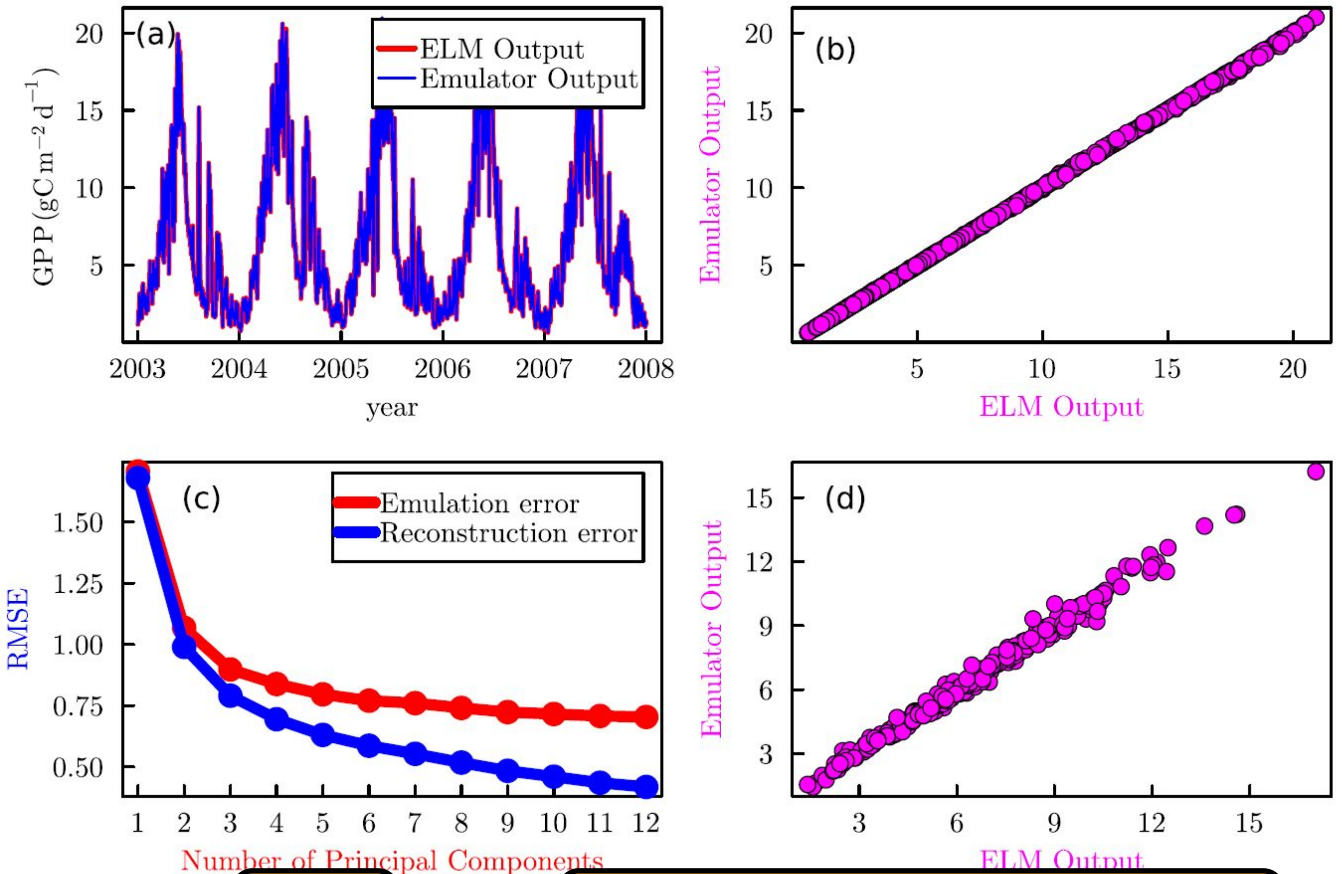



## Technical Problem

How to accomplish the huge amount of sampling in the Bayesian inference?

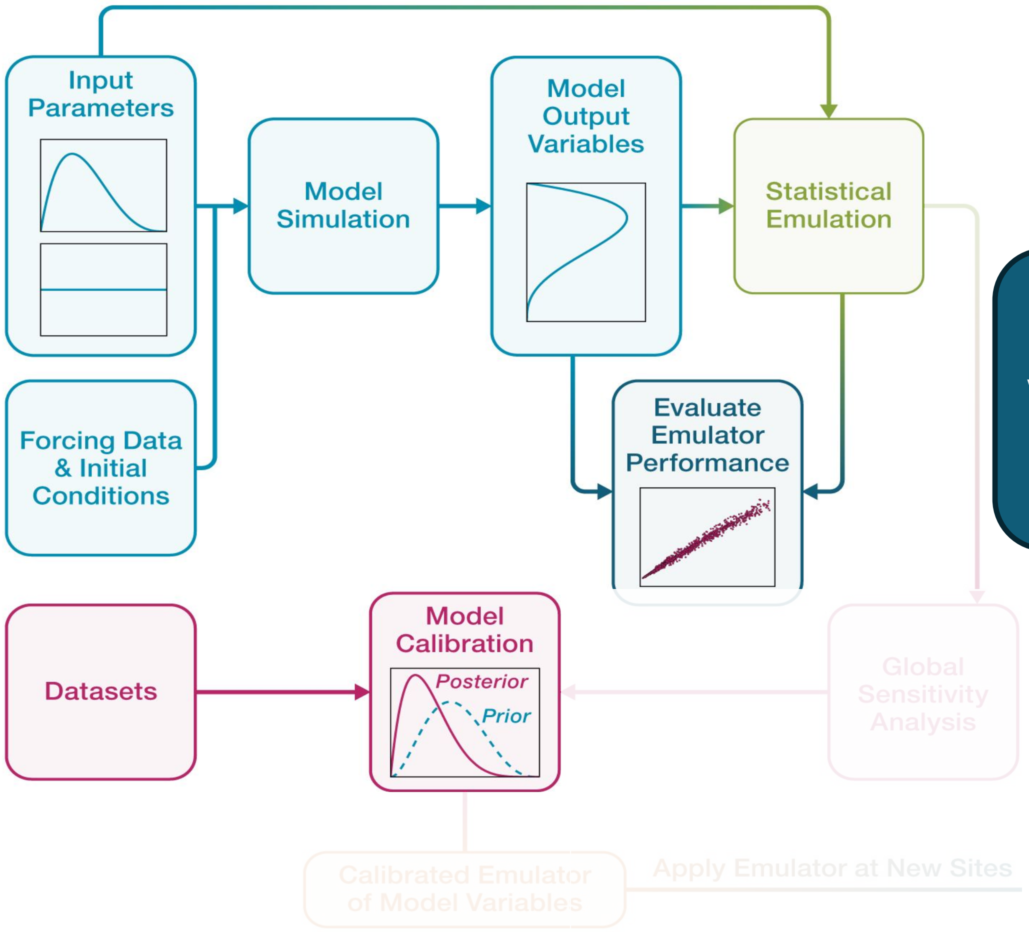
$$\mathcal{E}(\boldsymbol{\theta}) \sim \mathcal{F}(\boldsymbol{\theta})$$

# How good is the emulator? QoI: GPP US-Me2




**~10s** VS. **~15hours (72 cores)**

# Global sensitivity analysis




## Scientific Question

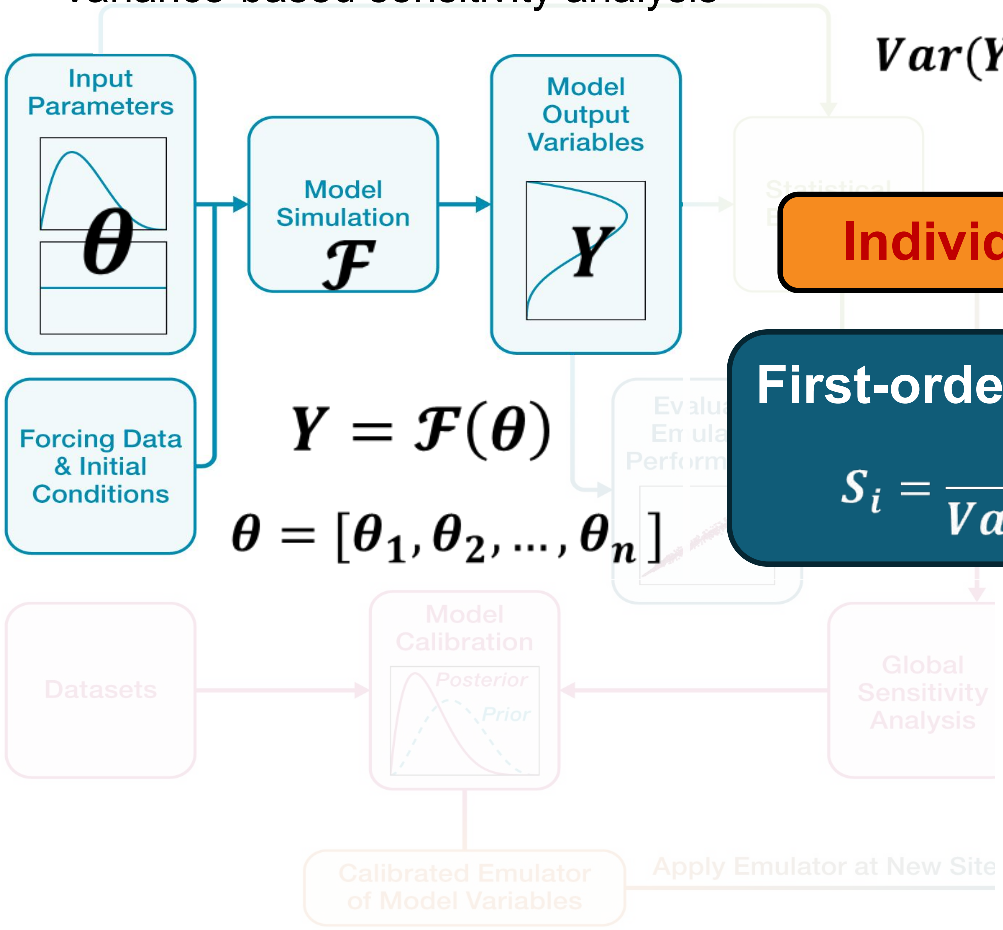
**For the quantity of interest, which parameters are the most sensitive (important)?**

# Sobol Global Sensitivity Analysis (GSA)

Variance-based sensitivity analysis

$$Var(Y) = \sum_{i=1}^{d} V_i + \sum_{i<j}^{d} V_{ij} + \cdots + V_{1,2,\ldots,n}$$

**Individual effect** + **Interactions**




$$Y = \mathcal{F}(\theta)$$

$$\theta = [\theta_1, \theta_2, \ldots, \theta_n]$$

**First-order index**

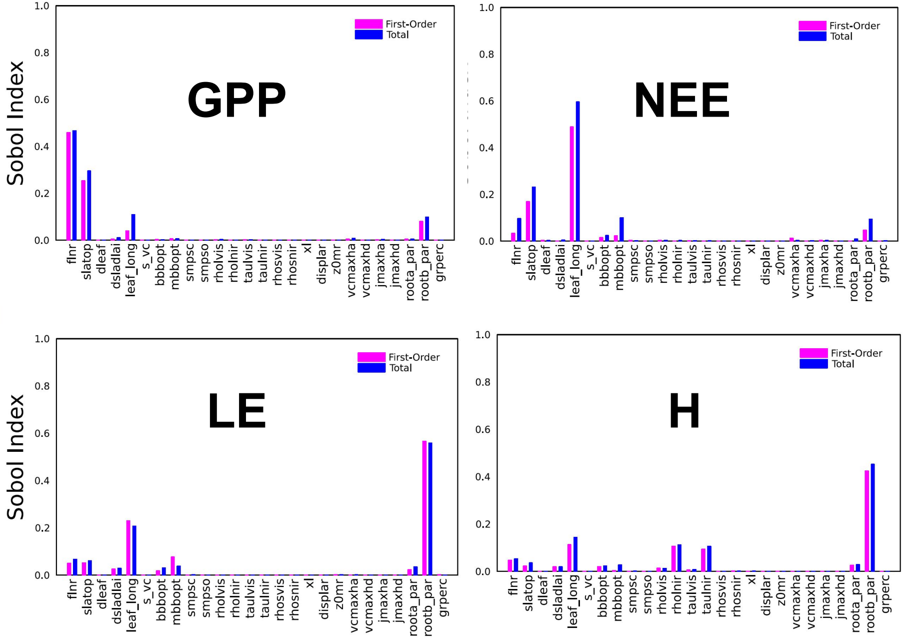
$$S_i = \frac{V_i}{Var(Y)}$$

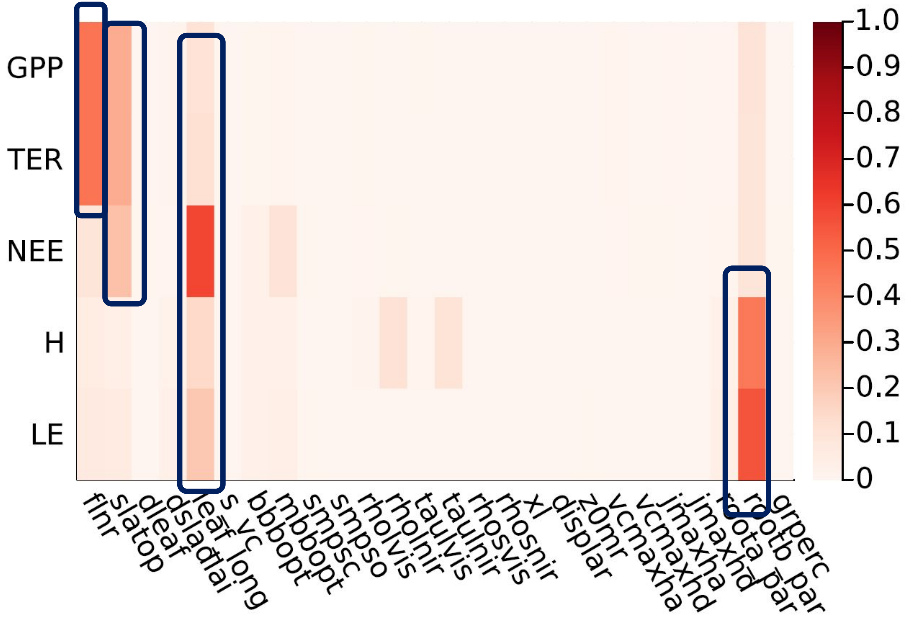
**Total-effect index**

$$S_{Ti} = \frac{E_{X_{\sim i}}(Var_{X_i}(Y|X_{\sim i}))}{Var(Y)}$$

# Sobol GSA result

## Same site (US-Me2), different variables



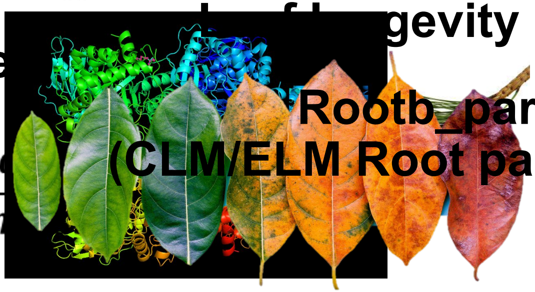




**Slatop (Specific leaf are**

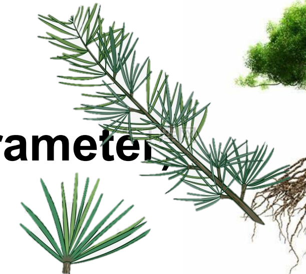
**Flnr (the fraction of leaf nitrogen in Rubisco)**

$$Slatop = \frac{leaf\ a}{dry\ m}$$

**gevity**



**Rootb_par (CLM/ELM Root parameter**



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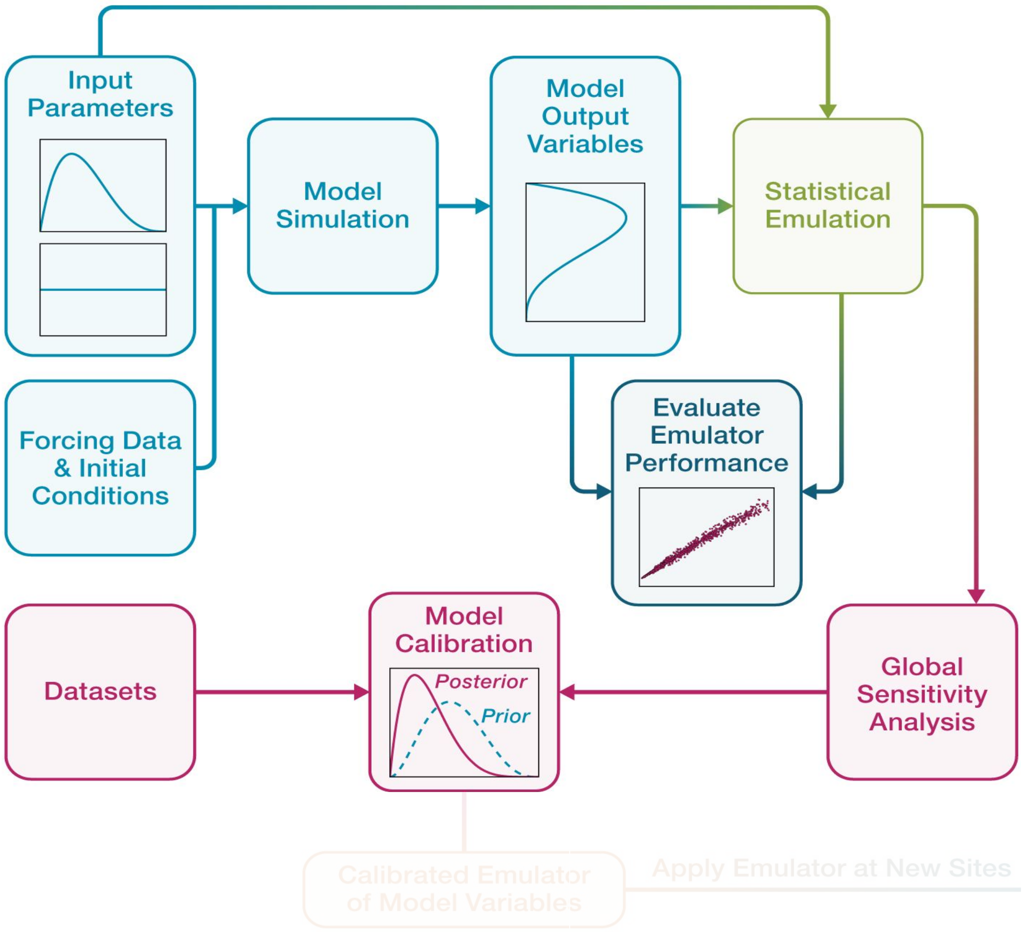
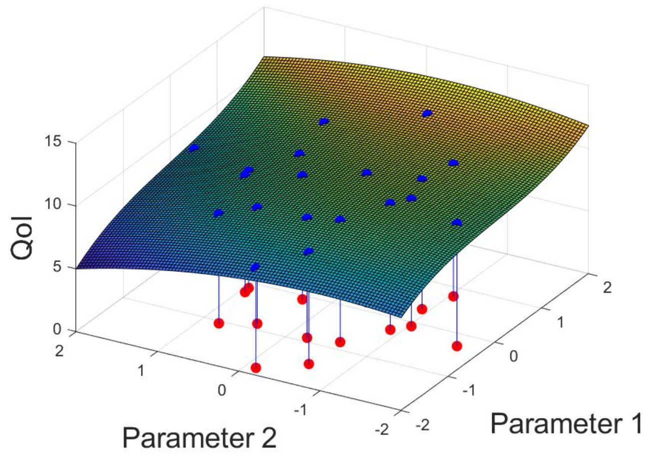
# Model calibration - Probabilistic model



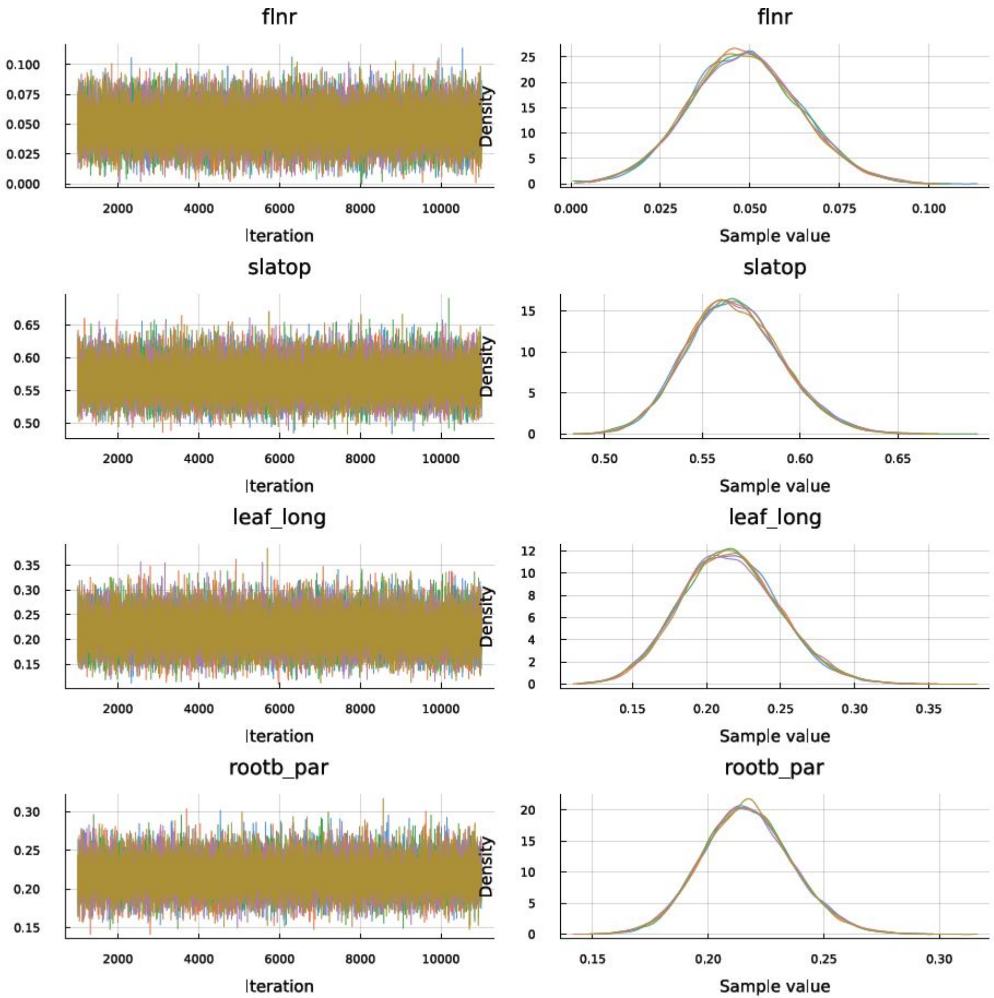

**4 leading model parameters**

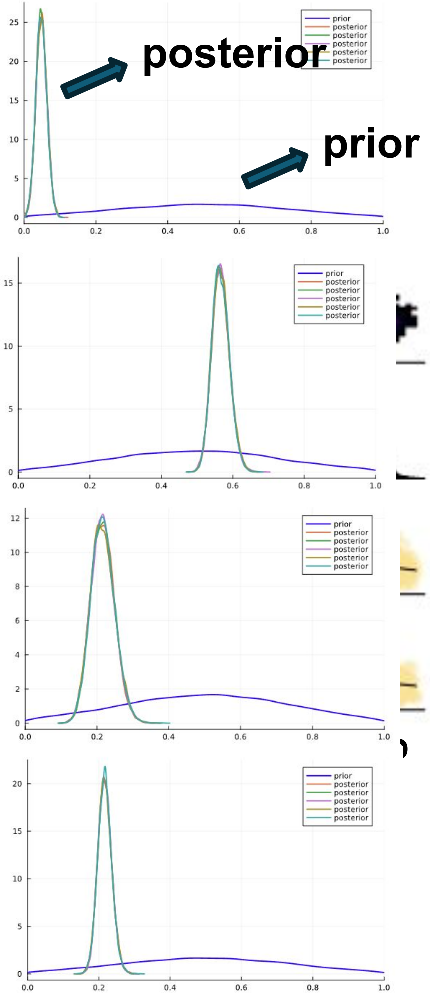
**200 ensemble members**

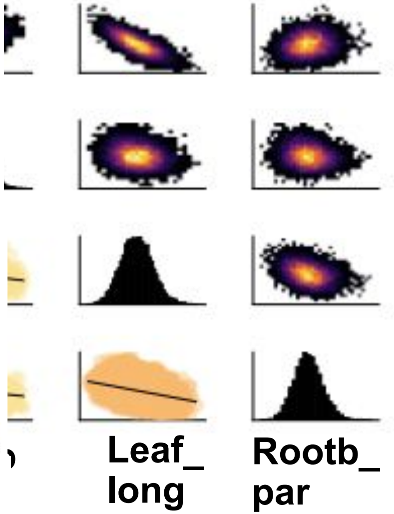


# Model calibration to US-Me2 with fluxnet data

*FASSt* - Simulation

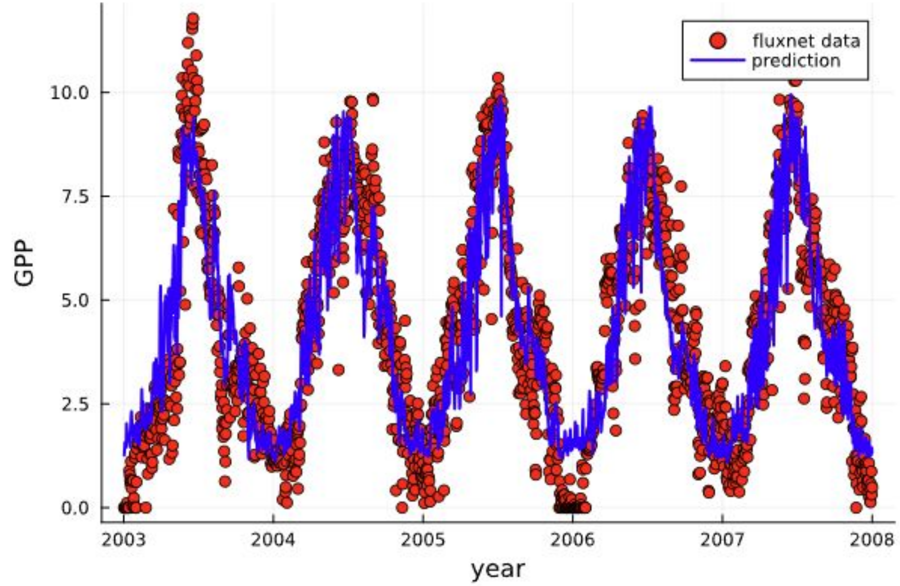


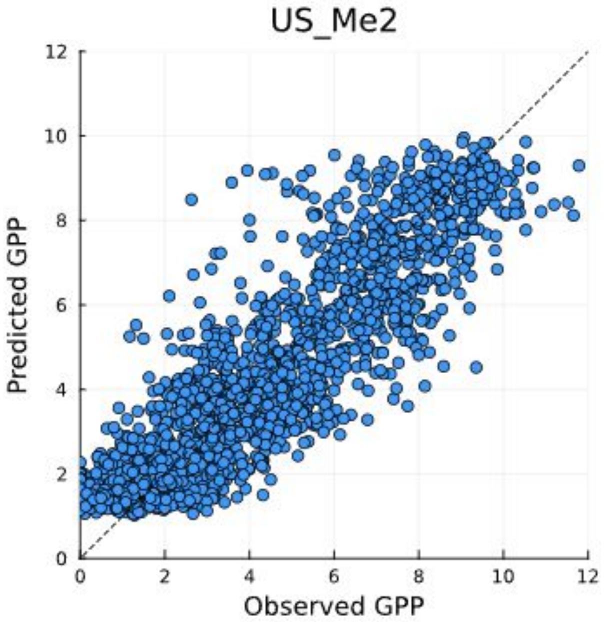



# Calibrated prediction at the same site

**US-Me2**

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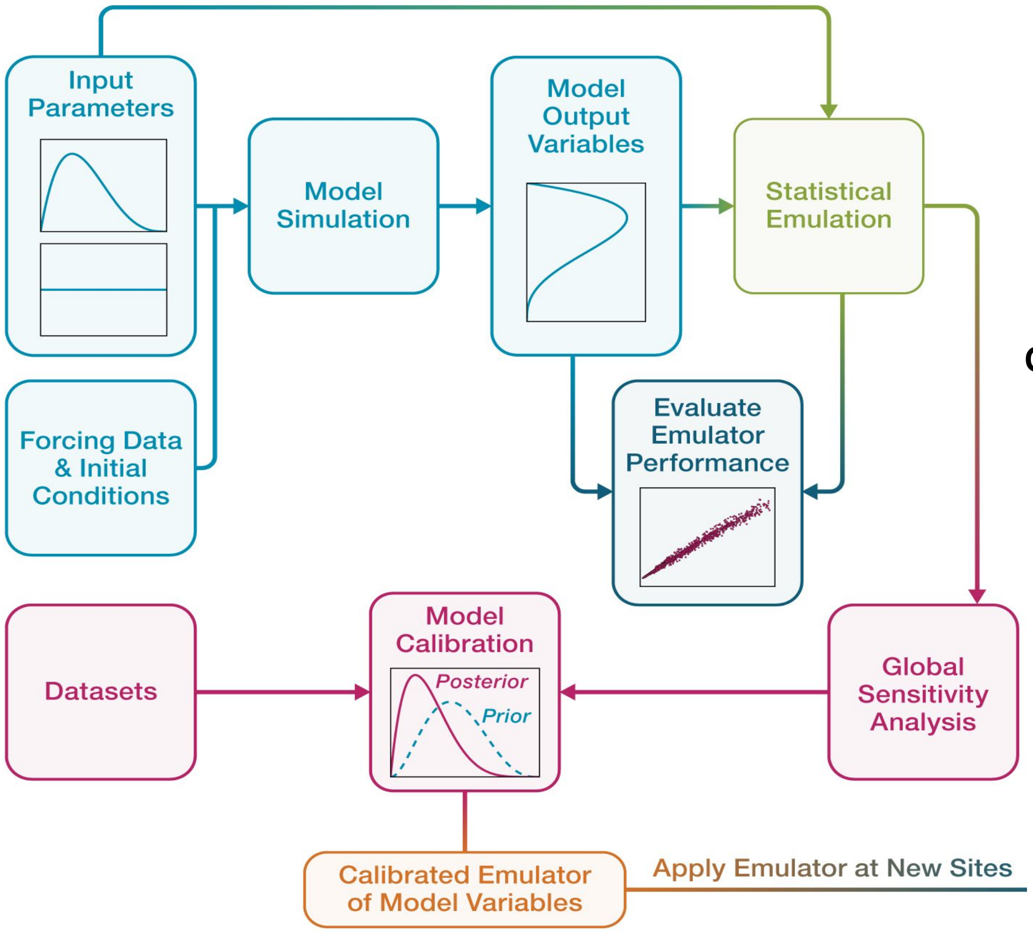
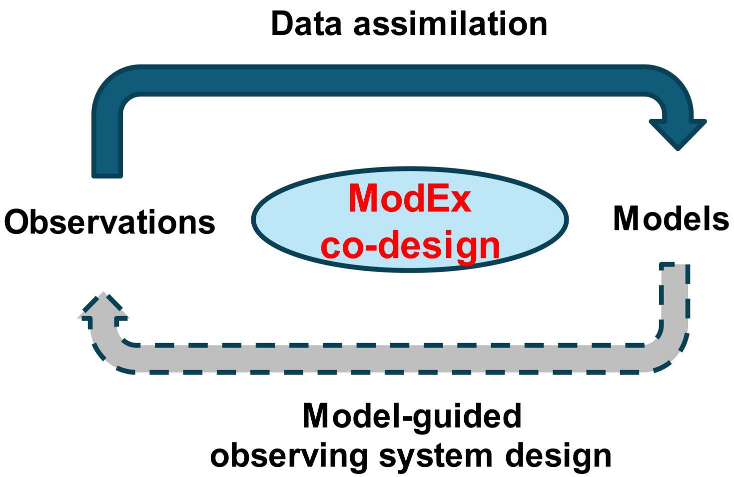
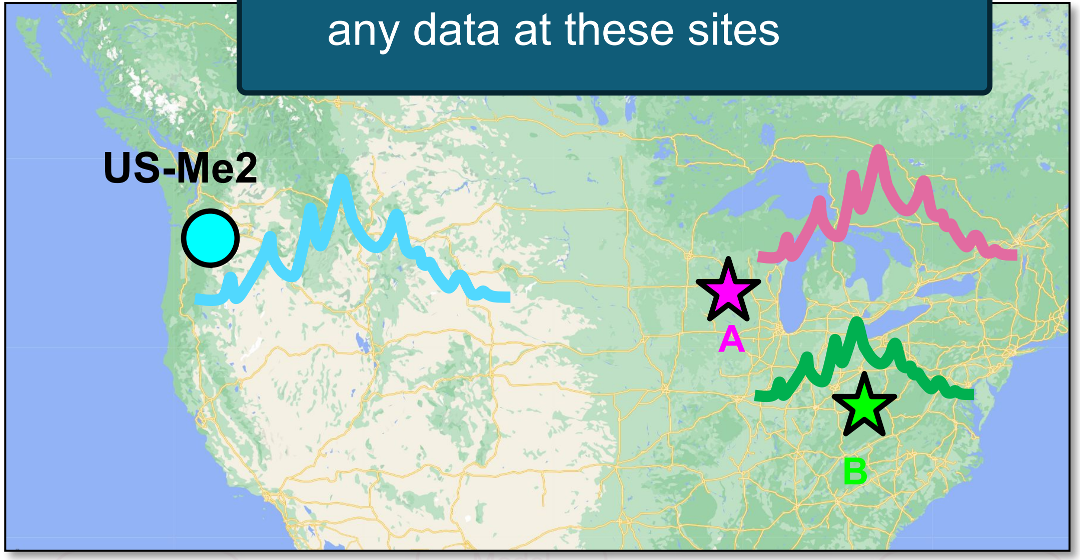
# Optimal Experimental Design (OED)

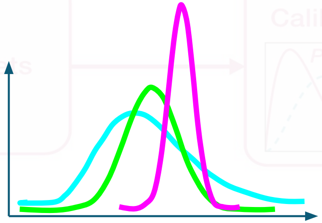


# Optimal Experimental Design (OED)

**Problem:** we haven't measured any data at these sites



**Model uncertainty**
(parameter or prediction)

Select the location whose data, *if measured*, reduces model uncertainty the most

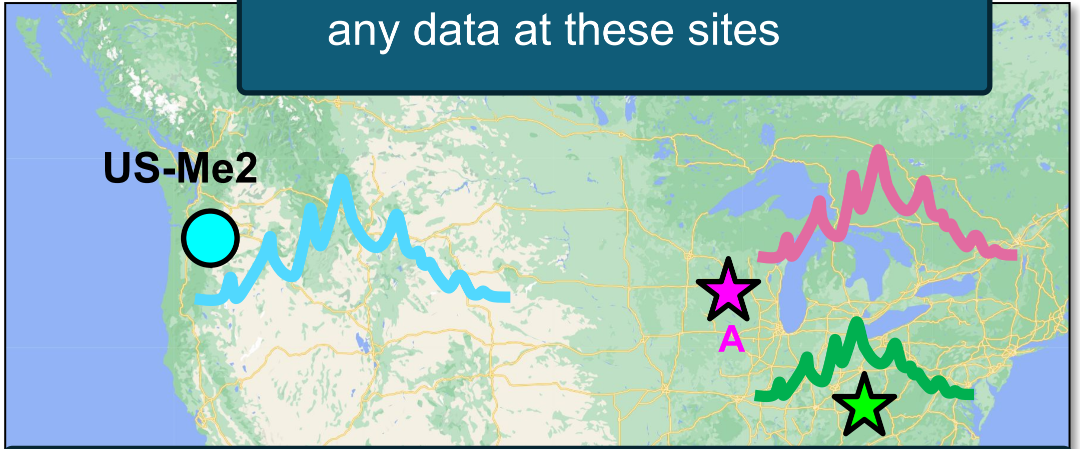
**Solution**

**OSSE Step**
Simulated observations with calibrated emulator

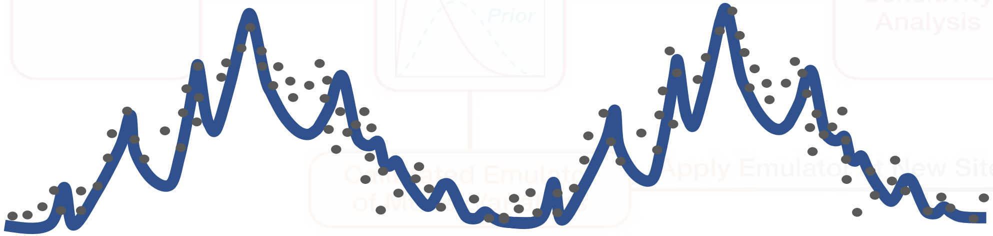
Of the two proposed new site locations (A and B), which one should we choose?

# Observing system simulation experiment (OSSE)

**Problem:** we haven't measured any data at these sites



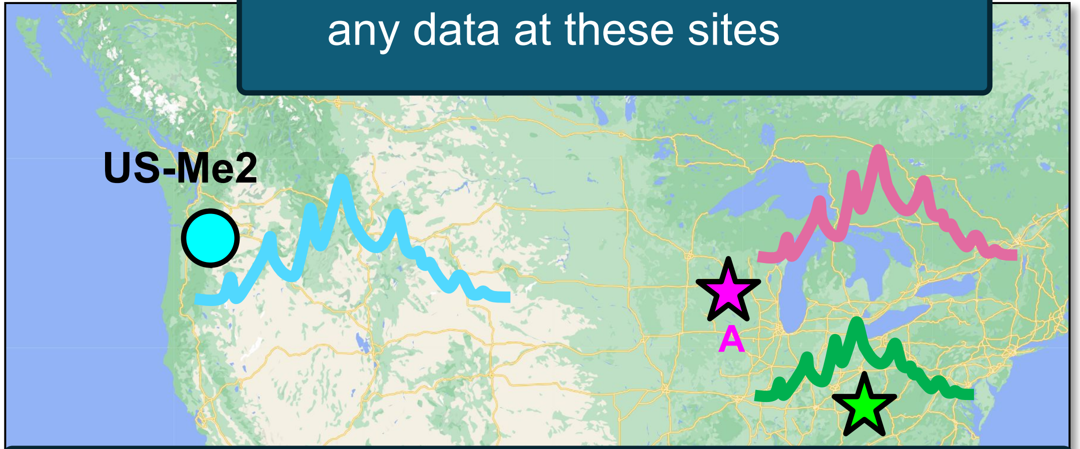

**Step1:** run the model & train the emulator
**Step2**: simulate observations (add unmodeled variability, model bias, instrument error)



## Solution

# Observing system simulation experiment (OSSE)

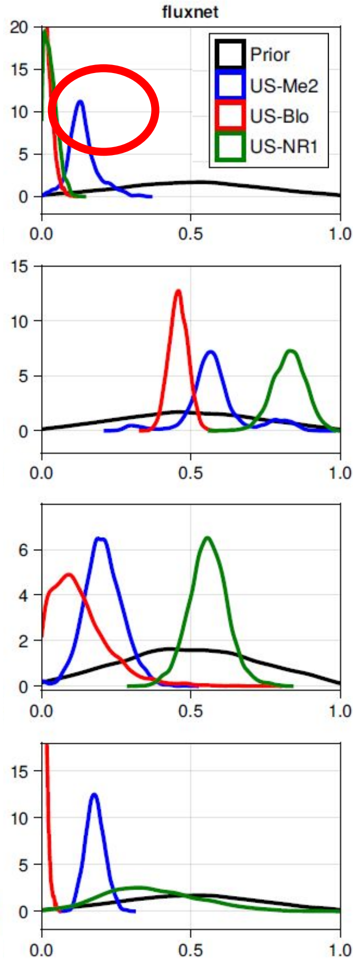
**Problem:** we haven't measured any data at these sites




**Step1:** run the model & train the emulator
**Step2**: simulate observations (add unmodeled variability, model bias, instrument error)

## Solution

# Posterior distribution for three sites




Posterior parameter distribution

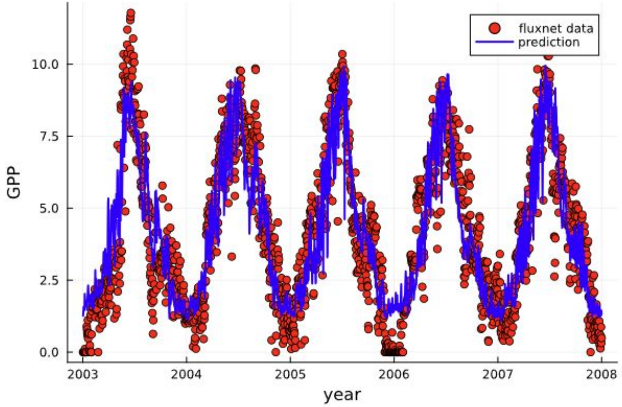
+

GP emulator

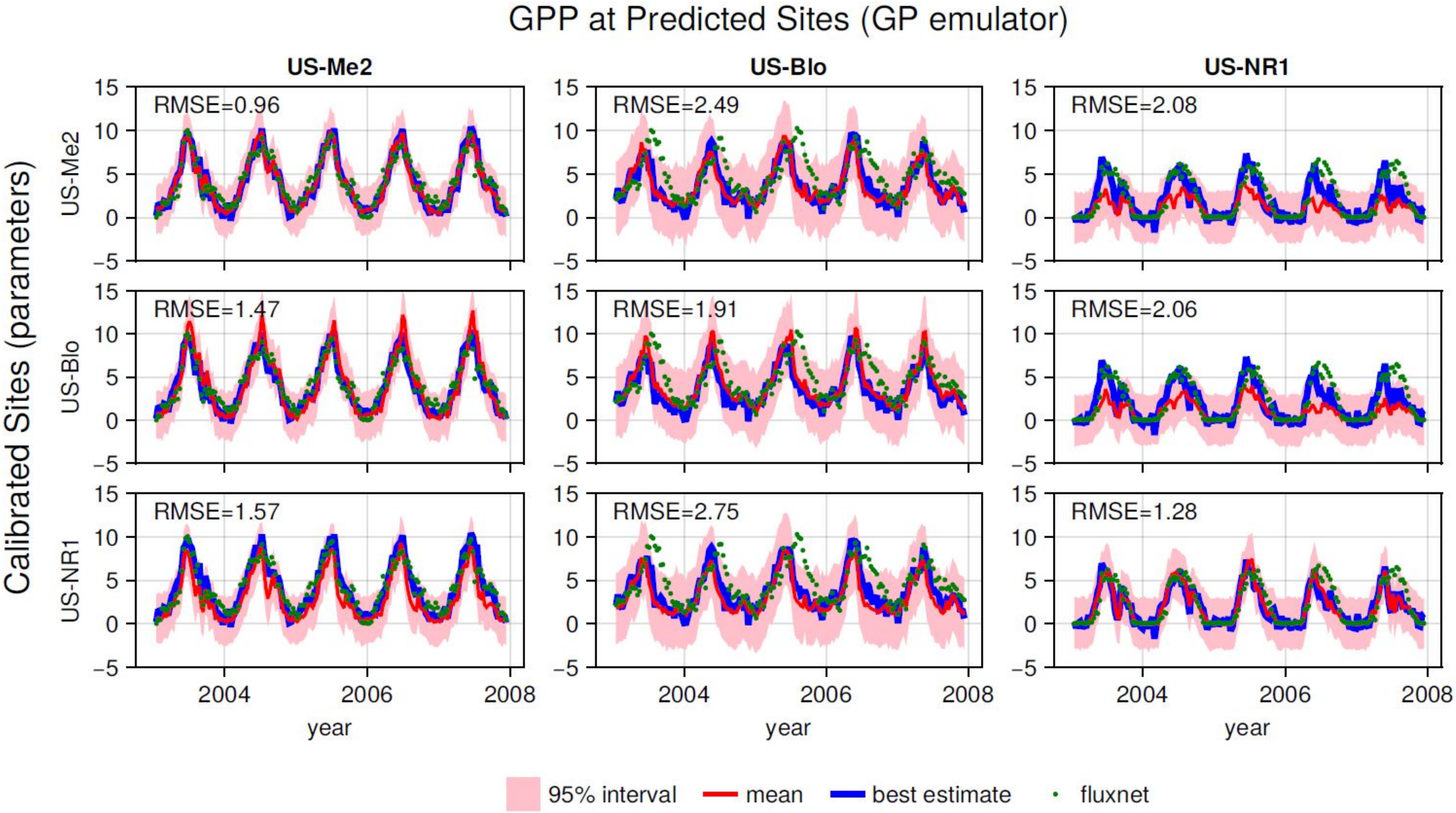
Calibration sites

Prediction sites

Prediction (Simulated Observation)

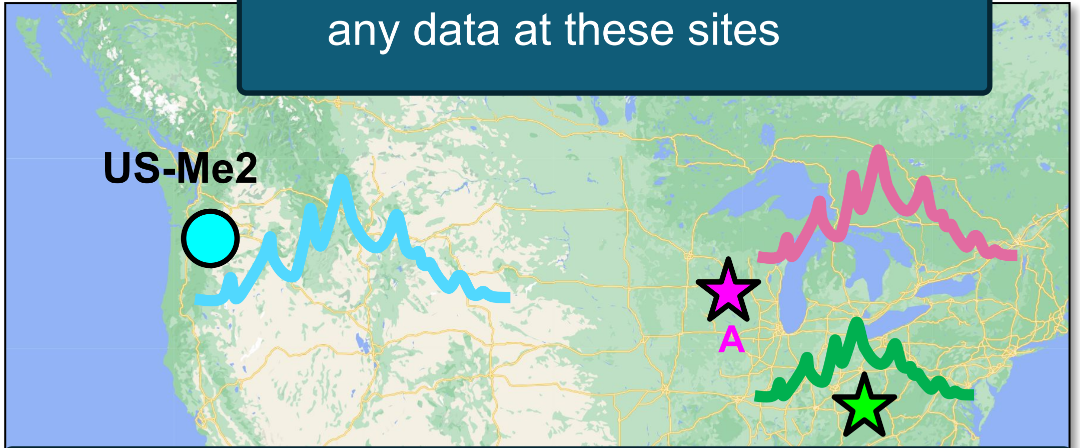


# Site heterogeneity-prediction at different sites

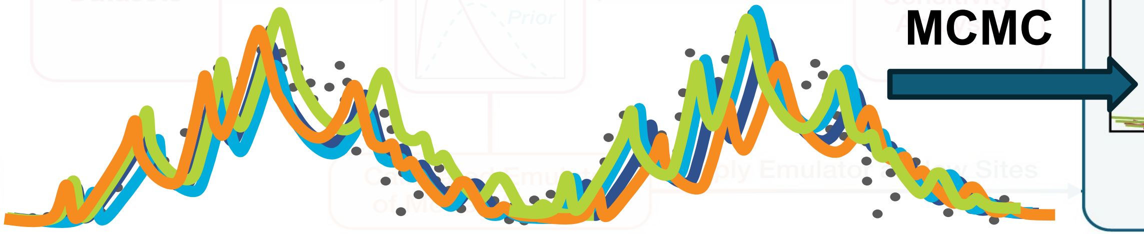


# OSSE-Simulated uncertainty reduction

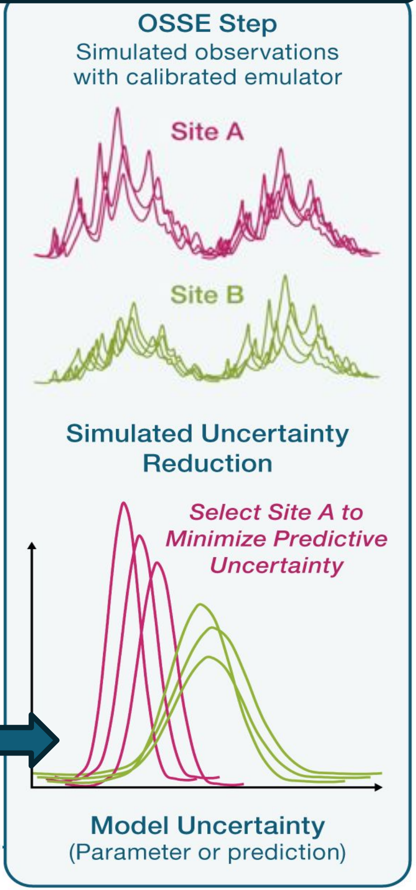
**Problem:** we haven't measured any data at these sites




**Step1:** run the model & train the emulator
**Step2**: simulate observations (add unmodeled variability, model bias, instrument error)

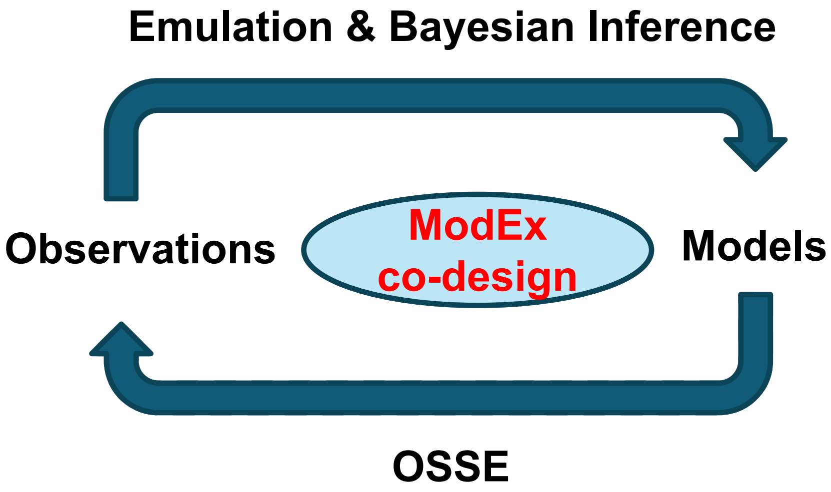



## Solution



# Summary

## Technical perspective




Provide a novel, adaptable computational framework for model-observing system co-design (Where to measure?)

## Scientific perspective

GSA: identified the leading sensitive parameters, e.g. flnr, slatop, leaf_longevity, etc. (What to measure?)

MCMC: Site heterogeneity might overwhelm parameter uncertainty (promoting new questions for next-step studies)

# Backup slides