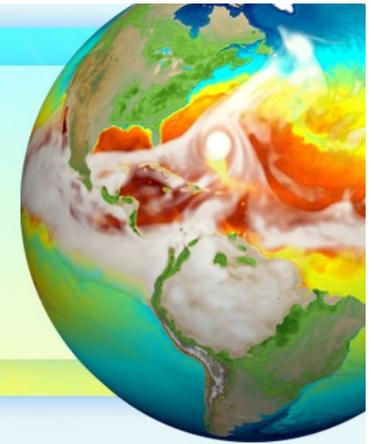


# Quantifying and reducing uncertainty in the E3SM land model using surrogate modeling



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E3SM all hands presentation  
May 27, 2021

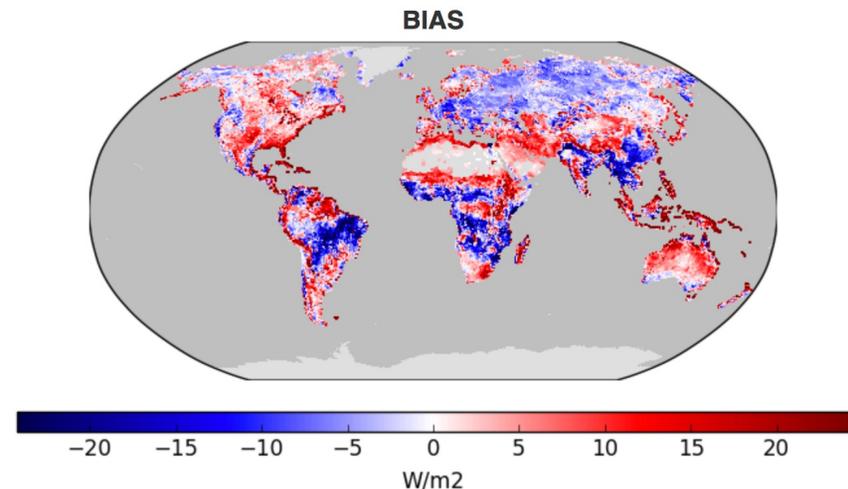
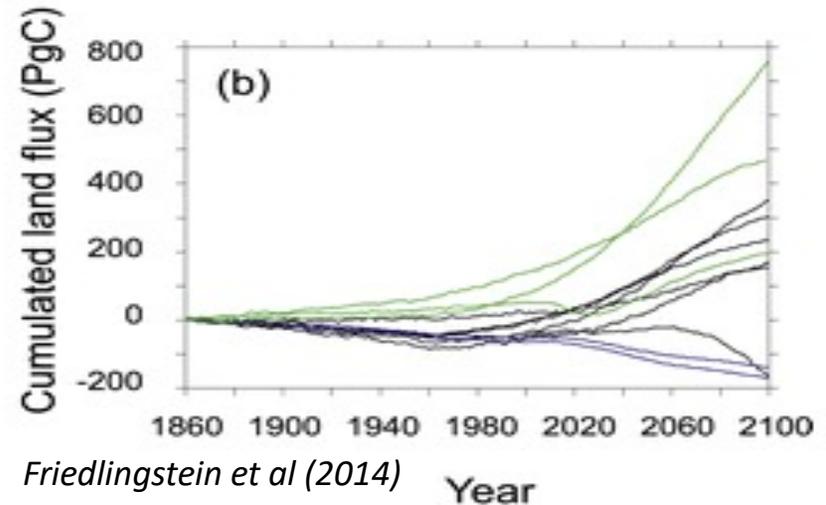


# Overview and motivation: LSMs

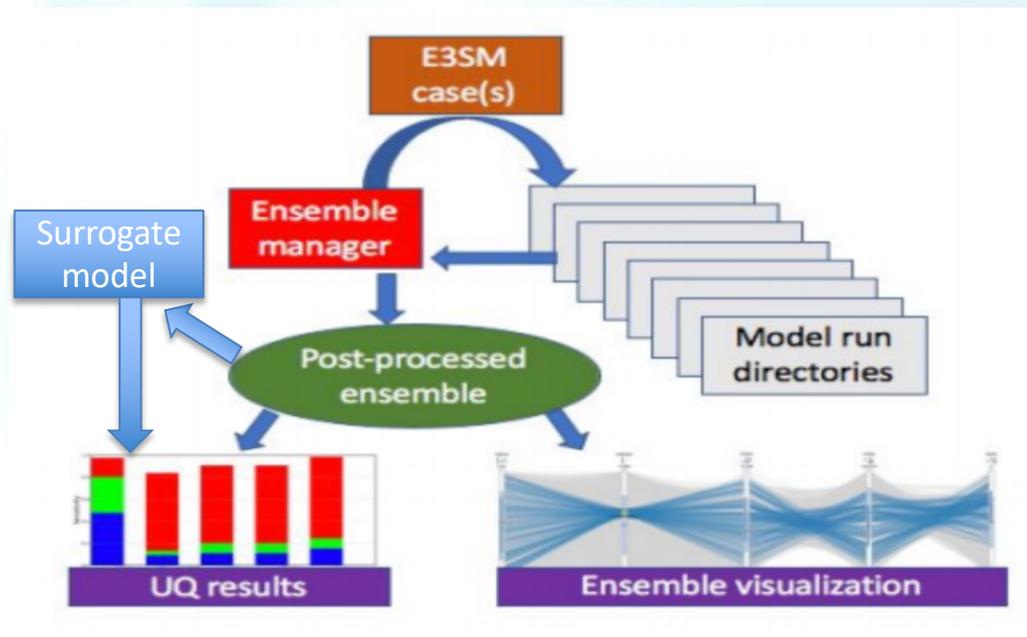
- Uncertainty from Multi-model ensembles
- Large spread in outputs
- Many quantities of interest
- Little formal uncertainty quantification (UQ)
  - Expensive model evaluation
  - High dimensionality

UQ challenges in E3SM :

- What processes drive uncertainty?
- What accounts for the key differences among models?
- Can model calibration using observations (e.g. satellite data) reduce uncertainty?



# The case for large ELM ensembles



- Needed to understand parametric uncertainty
- High dimensionality (uncertain parameters)
- Can be used to construct surrogate models, which enable UQ methods
  - Sensitivity analysis
  - Parameter calibration

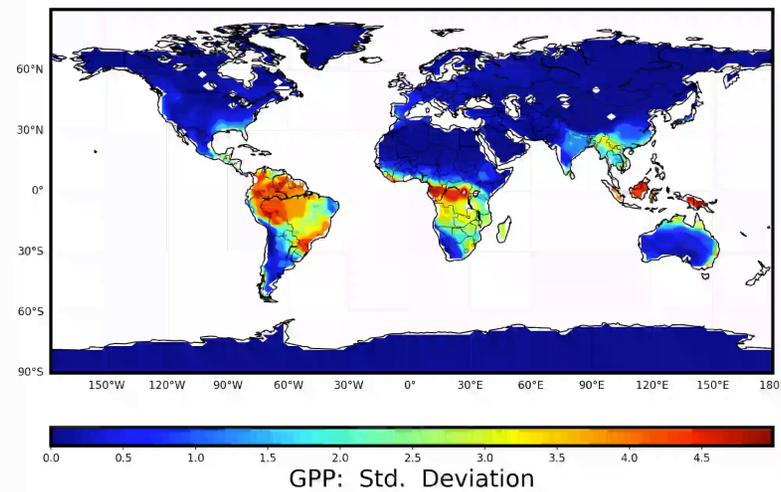
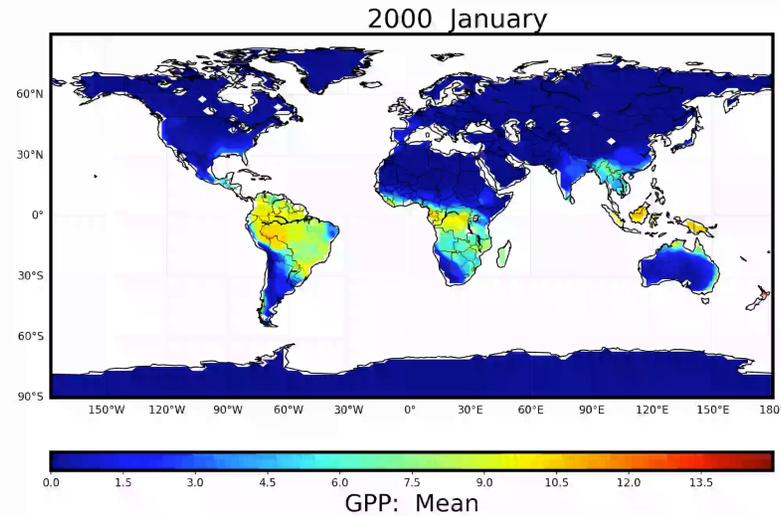
- Single gridcell UQ: Uses mpi-serial version of ELM with mpi4py in the offline land-model testbed (OLMT) to run up to 10k ensemble members
  - Ongoing tasks: ELM-FATES, crop, default ELM
- Global UQ: Generally smaller ensembles (100-200), low resolution

# A global ELM ensemble

- Focused on GPP (gross primary productivity)
  - Primary input for land C-cycle,
  - strong coupling with transpiration
- 10 parameters analyzed using 275 ensemble members (1.9x2.5 resolution), satellite phenology

Parameter	Description	Min	Max	Default range
flnr	Fraction of leaf in in RuBisCO	0	0.25	[0.042,0.176]
mbbopt	Stomatal slope (Ball-Berry)	2	13	[4,9]
bbbopt	Stomatal intercept (Ball-Berry)	1000	40000	[10000,40000]
roota_par	Rooting depth distribution	1	10	[3,10]
vcmahx	Activation energy for Vcmax	50000	90000	72000
vcmahx	Engropy for Vcmax	640	700	670
jmaxha	Activation energy for jmax	50000	90000	72000
dayl_scaling	Day length factor	0	2.5	2
dleaf	Characteristic leaf dimension	0.01	0.1	[0.01,0.1]
xl	Leaf/stem orientation index	-0.6	0.8	[-0.5,0.65]

# GPP (gC m<sup>-2</sup> day<sup>-1</sup>) ensemble

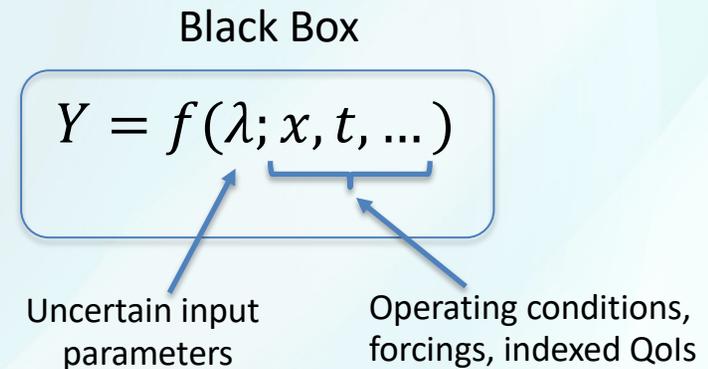


# Goal: create a surrogate model

Surrogate model is a “good-enough” approximation of the full model over a range of parameter variability.

... otherwise called

- Metamodels
- Response surfaces
- Emulators
- Low-fidelity model

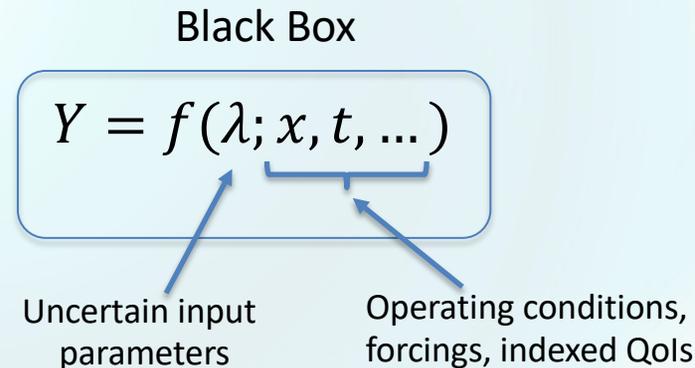


Surrogate models are needed for computationally intensive tasks:

- Parameter estimation
- Optimization
- Experimental/computational design
- Forward uncertainty propagation

$$f(\lambda; x, t, \dots) \approx f_{surr}(\lambda; x, t, \dots)$$

# Curse of dimensionality hits twice!



**Challenge:** **High-d input:** large number of uncertain parameters

**High-d output:** large number of Qols over high-res grid

**Fix:** Sensitivity analysis to select the most important parameters

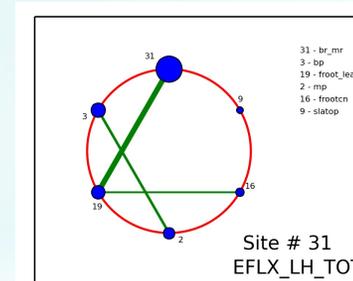
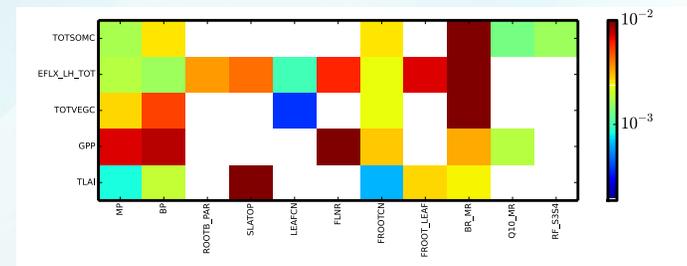
Principal component analysis to reduce dimensionality

# Global Sensitivity Analysis (GSA) enables parameter selection

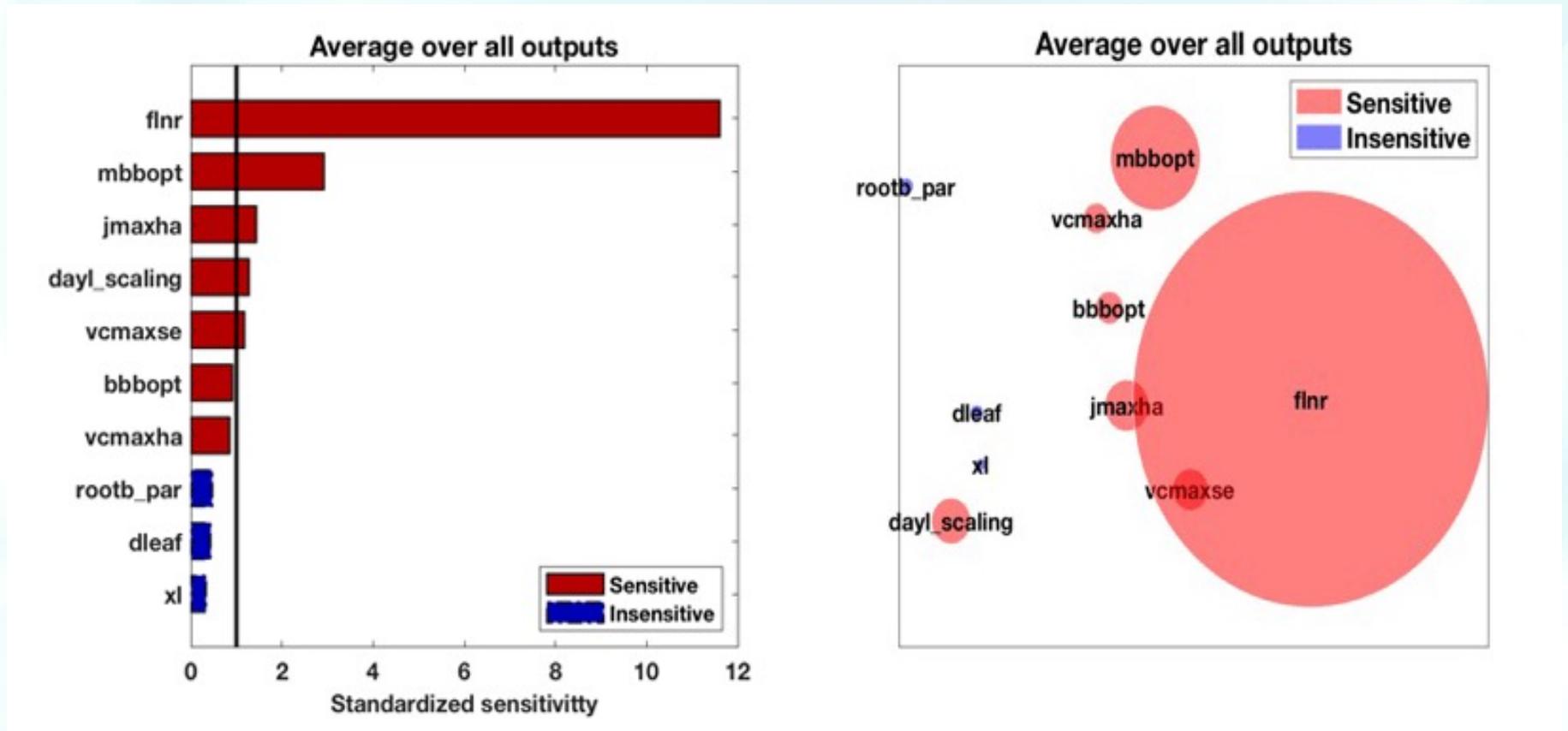
... otherwise called Sobol indices, variance-based decomposition  
Attribute fractions of output variance to input parameters



- i.e., how much output variance would reduce if a given parameter is fixed to its nominal value
- also generalizes to joint sensitivities: joint parameter impact to a given QoI



# Sensitivities of global average GPP



# Spatio-temporal surrogate model via Karhunen-Loève and Polynomial Chaos

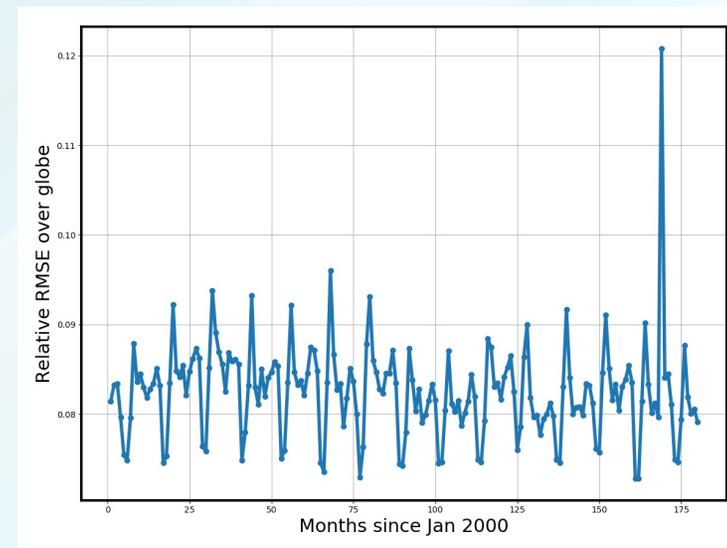
$$f(\lambda; x, t) \stackrel{\text{KL}}{\approx} \sum_{k=0}^K f_k(\lambda) \varphi_k(x, t) \stackrel{\text{PC}}{\approx} \underbrace{\sum_{k=0}^K \sum_{j=0}^J f_{kj} \phi_j(\lambda) \varphi_k(x, t)}_{f_{\text{surr}}(\lambda; x, t)}$$

**Karhunen-Loève (KL) expansion** is essentially a continuous version of principal component analysis

**Polynomial chaos (PC) expansion** is essentially a polynomial regression with respect to uncertain parameters

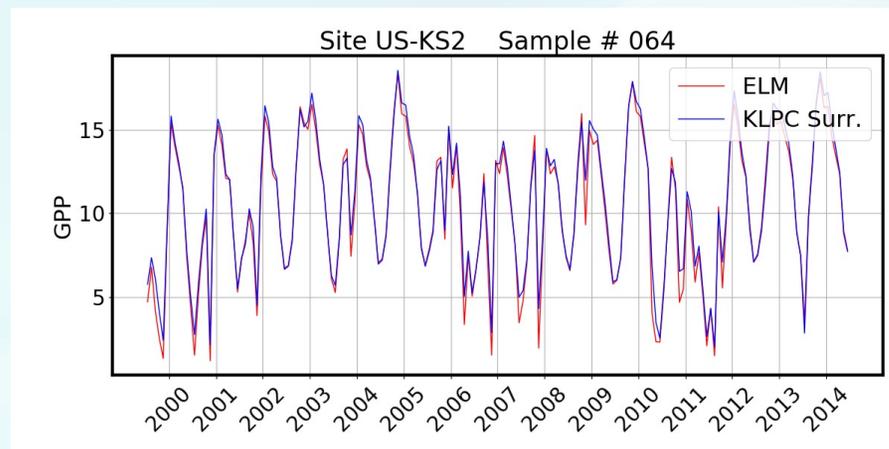
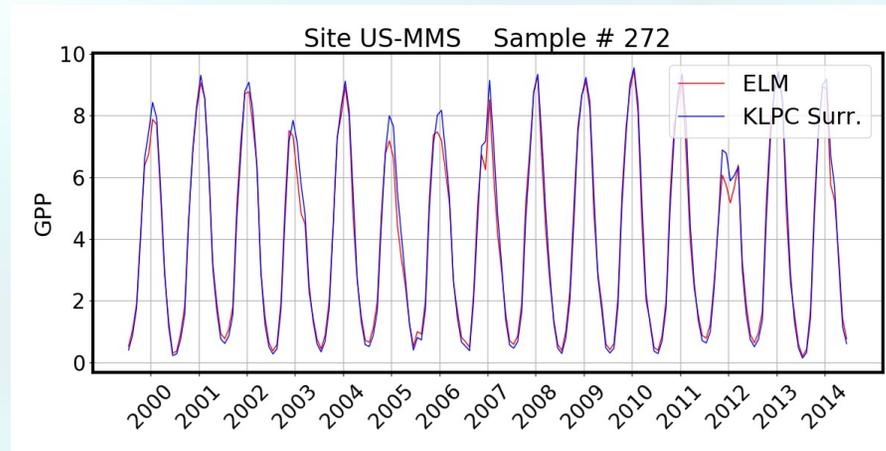
# Spatio-temporal KL-PC surrogate is globally within 10% accuracy

- 3183 land cells over 180 months is > 500,000 outputs
- Instead of 500K surrogates, we build about 2K surrogates, one for each eigen-component
- End result: a single surrogate, resolved in space and time, with about 10% relative error compared to true ELM
- Surrogate ELM is extremely cheap to evaluate and is being used online to calibrate the parameters
- Room to improve: neural networks!!



# ELM vs Surrogate:

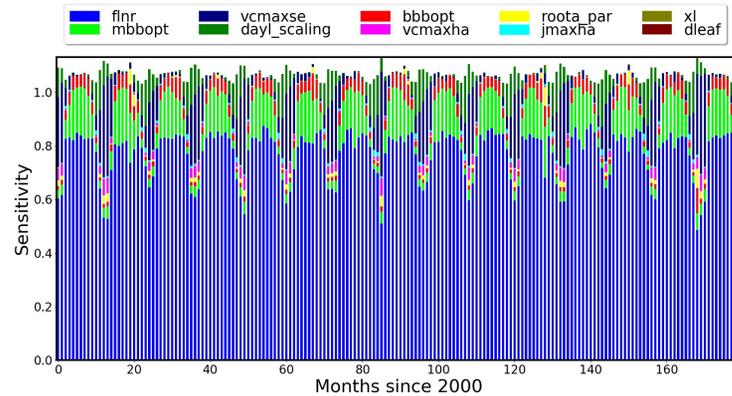
accuracy can be improved with higher order KL or PC



# Gridcell-level sensitivities

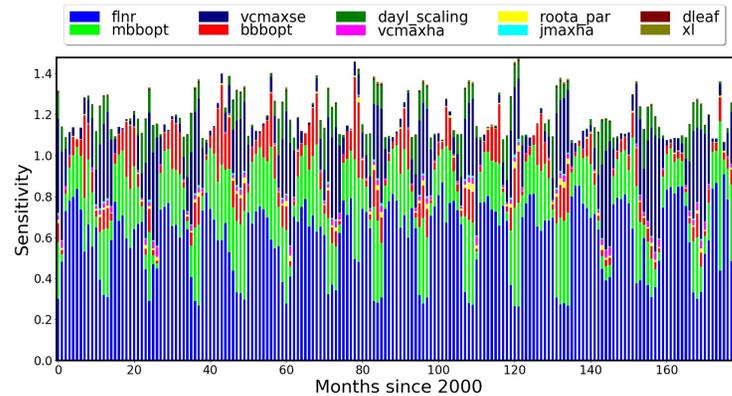
## Site US-Ha1

Deciduous forest  
Massachusetts, USA

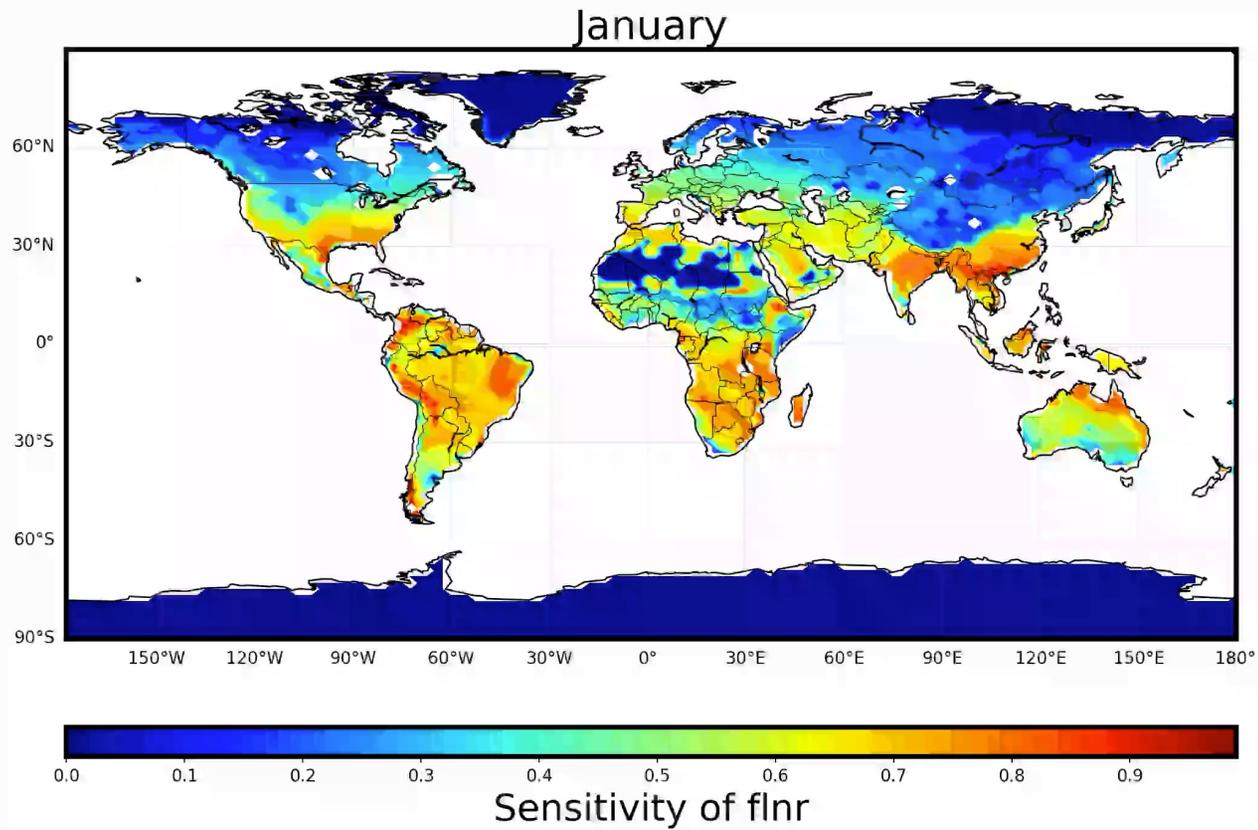


## Site US-Fpe

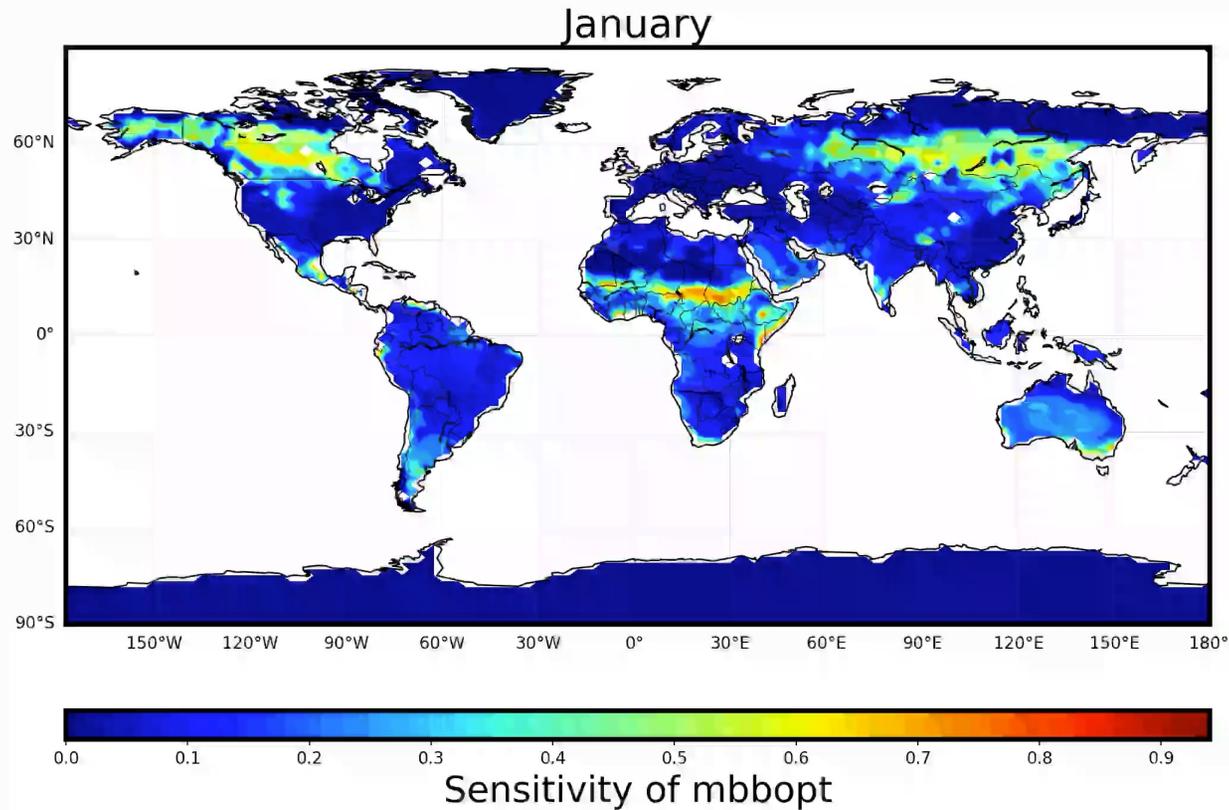
Grassland  
Montana, USA



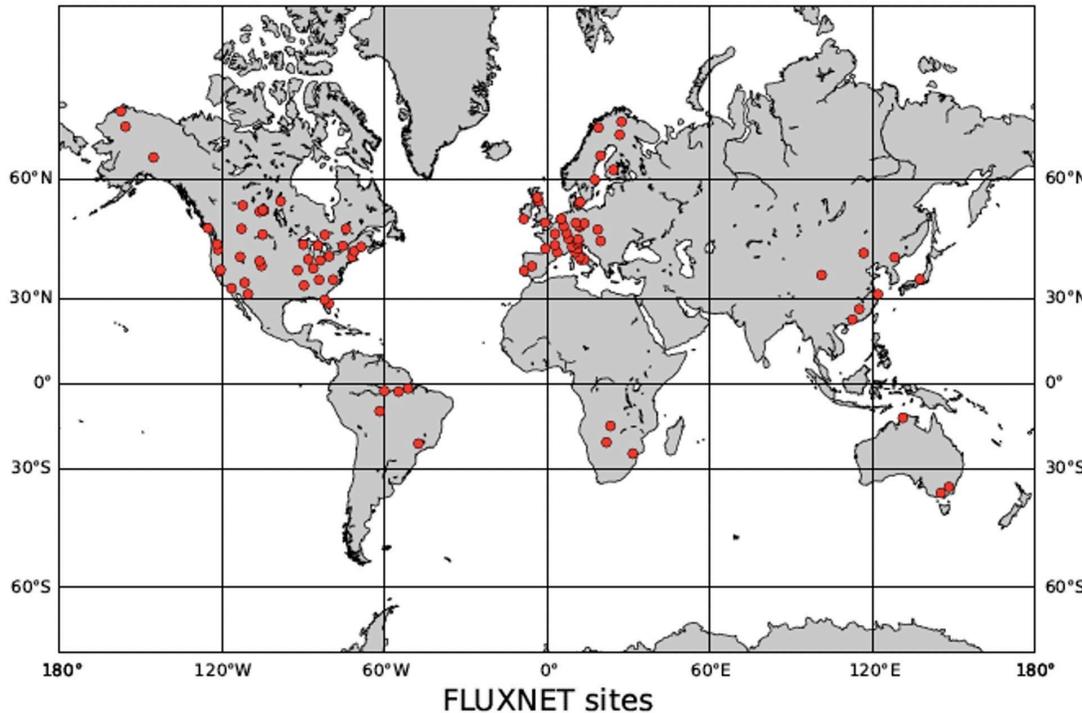
# Sensitivity to flnr (fraction of leaf N in RuBisCO)



# Sensitivity to $m_{BBopt}$ (stomatal slope)



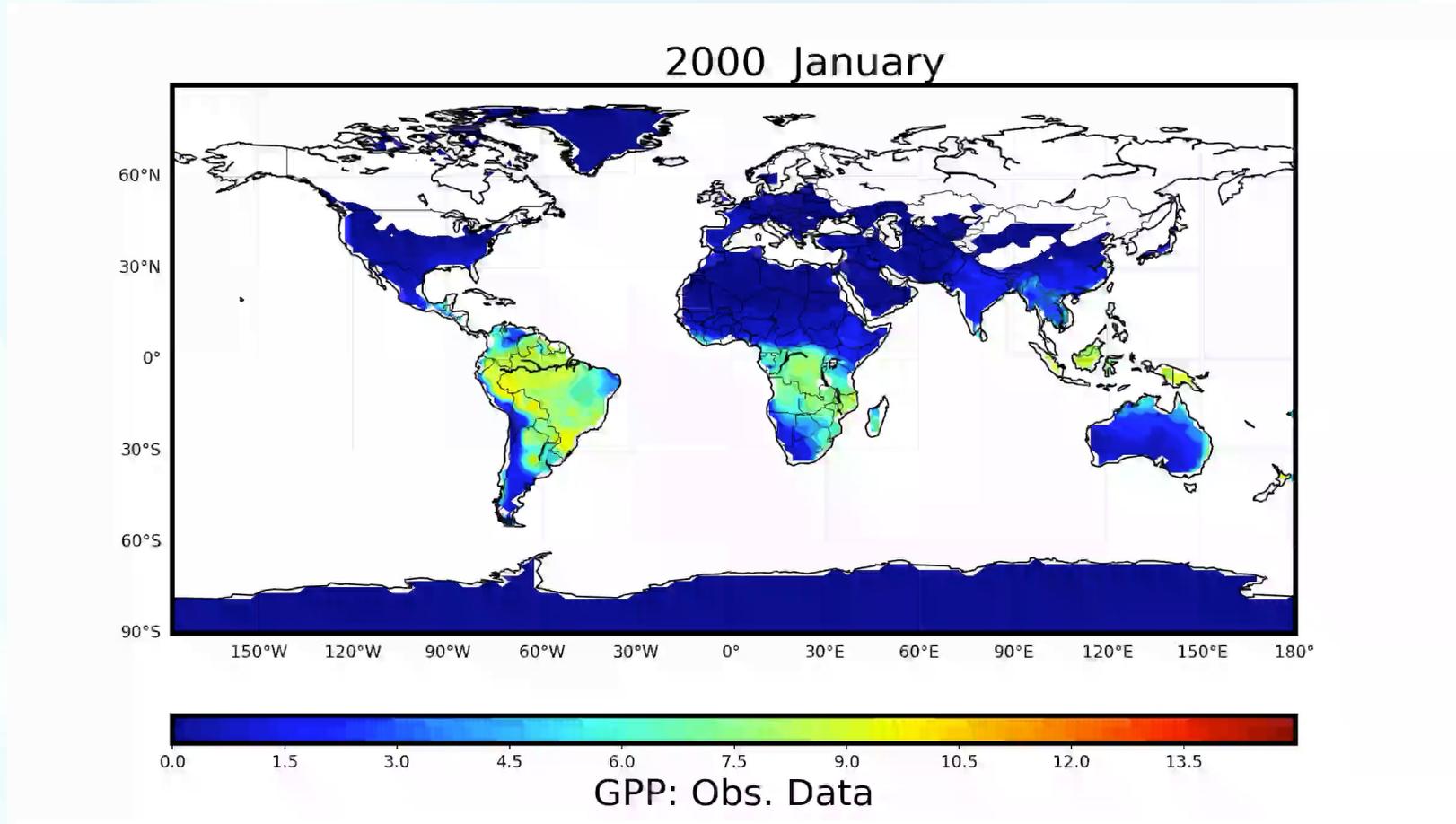
# Constraining ELM with FLUXNET



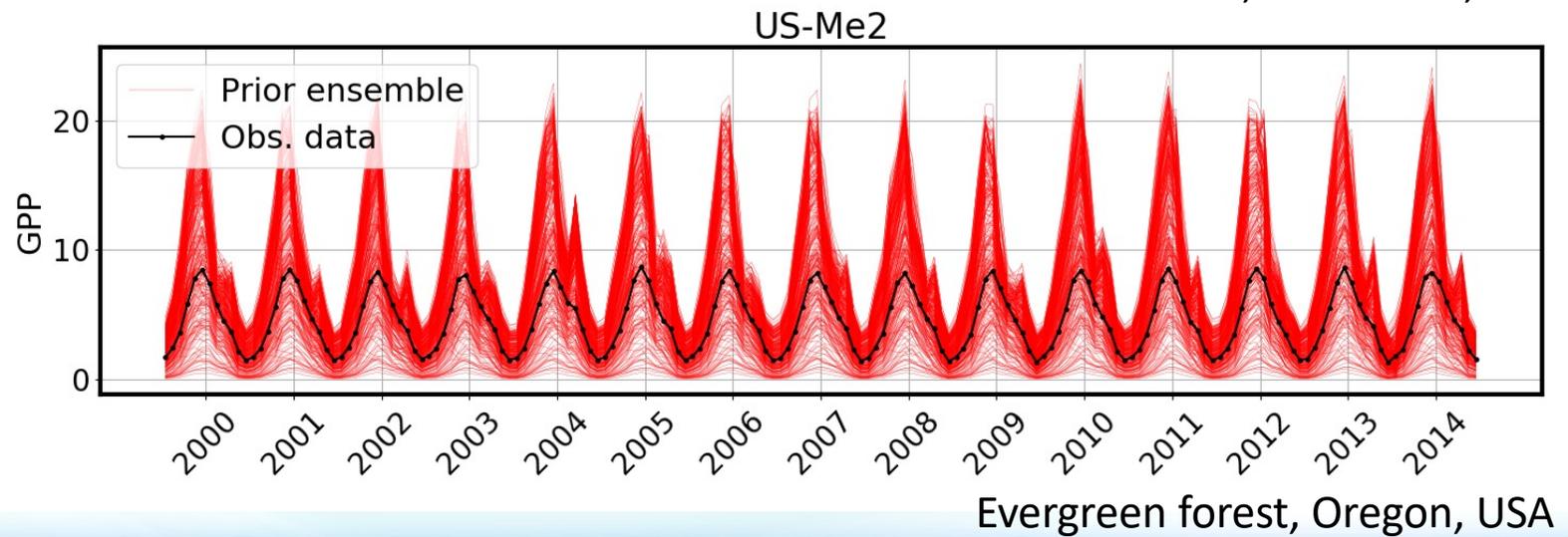
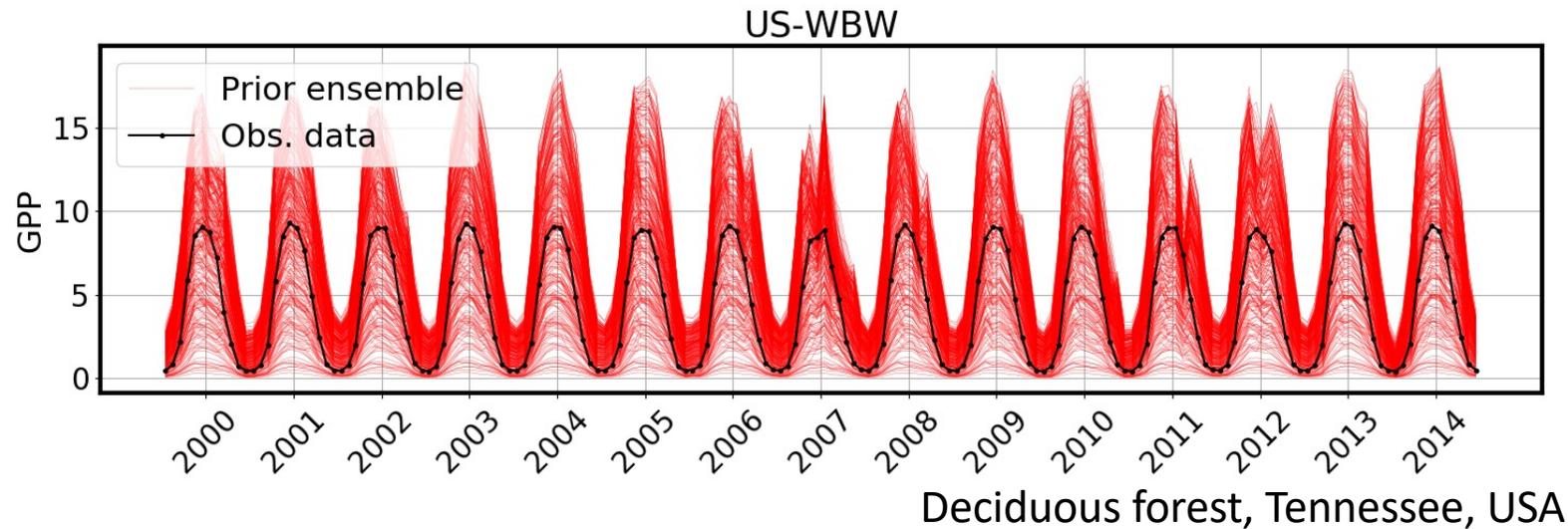
- FLUXNET towers measure CO<sub>2</sub>, water, energy fluxes
- FLUXCOM: A gridded GPP benchmark upscaled from FLUXNET network using meteorology, remote sensing
- In this study: 96 high-quality sites selected for calibration

- This analysis focuses on calibration at multiple gridcells, but methodology can be used to calibrate gridded observations/benchmarks (e.g. FLUXCOM)

# FLUXCOM data, visualized

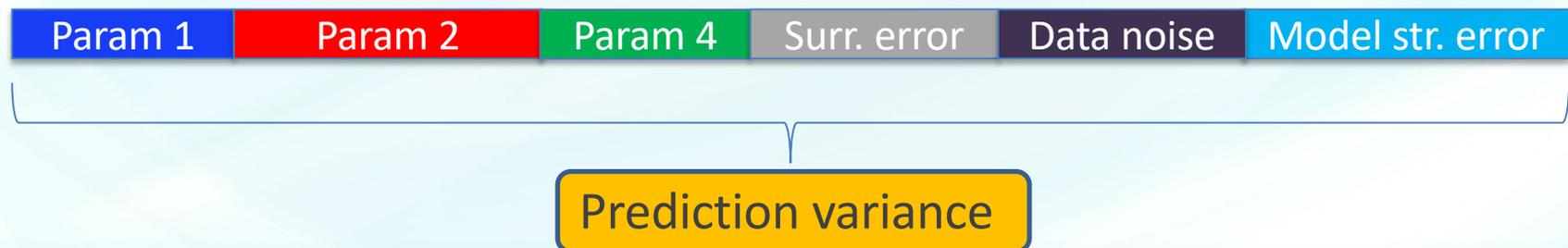


# Model ensemble with GPP data



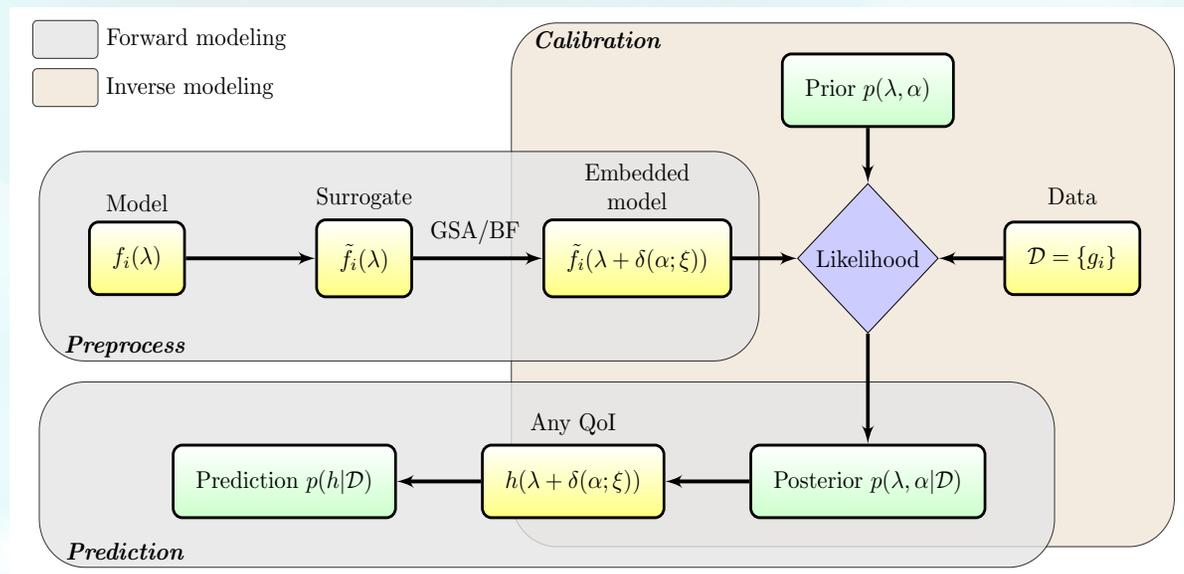
# Bayesian approach is main tool for parameter calibration

- Bayesian inference allows incorporation of various sources of uncertainty
- Markov chain Monte Carlo (MCMC) for building posterior PDFs
  - Ugly high-dimensional parameter PDFs, but advanced MCMC methods are available
- Requires many online evaluations of the model
  - **This is why we needed the surrogate!**
- Predictive uncertainty decomposition augmented with surrogate error and observational noise, and *model structural error*



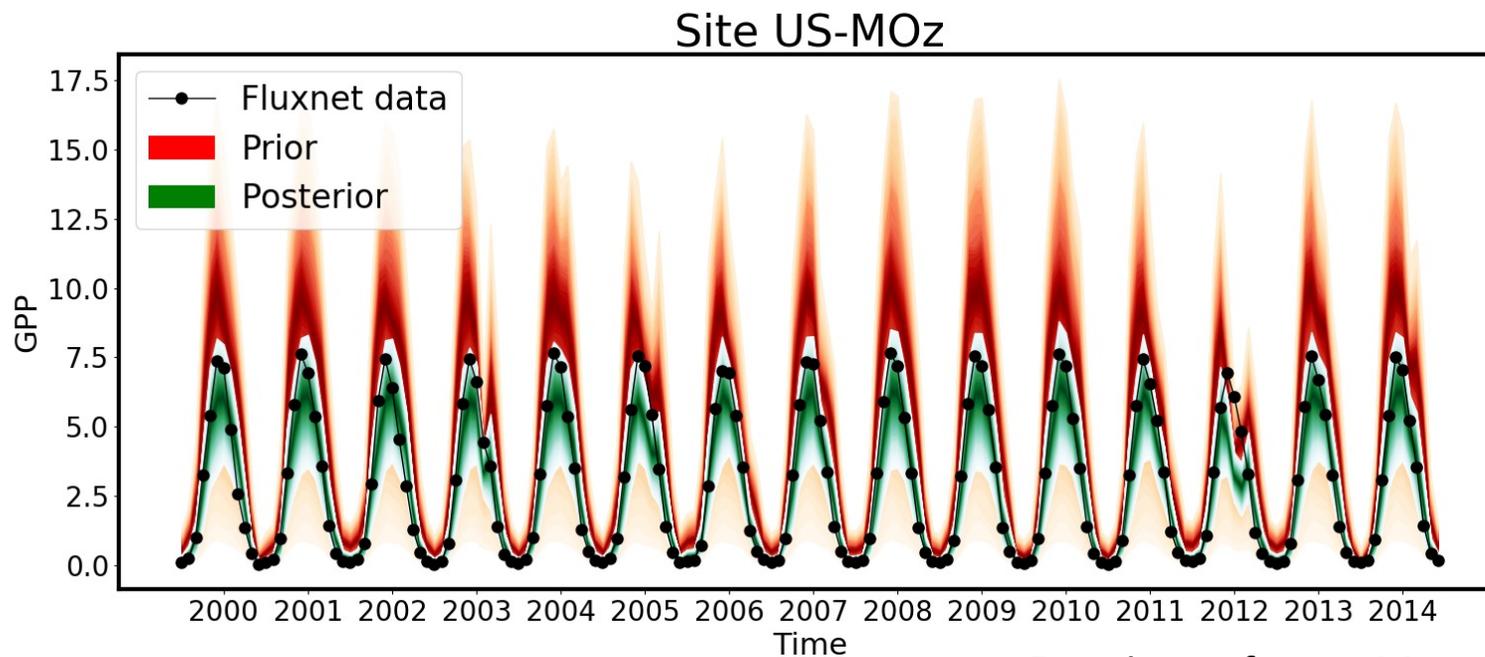
# Calibration with *Embedded Model Structural Error*

- Model structural error embedding approach [*Sargsyan et. al., 2015, 2018*]
  - Embedded, but not intrusive, i.e. black-box
  - Meaningful extrapolation to full set of QoI predictions
  - Disambiguation between model error and data noise
  - Removes parameter biases and overfitting



# Prior vs posterior predictions...

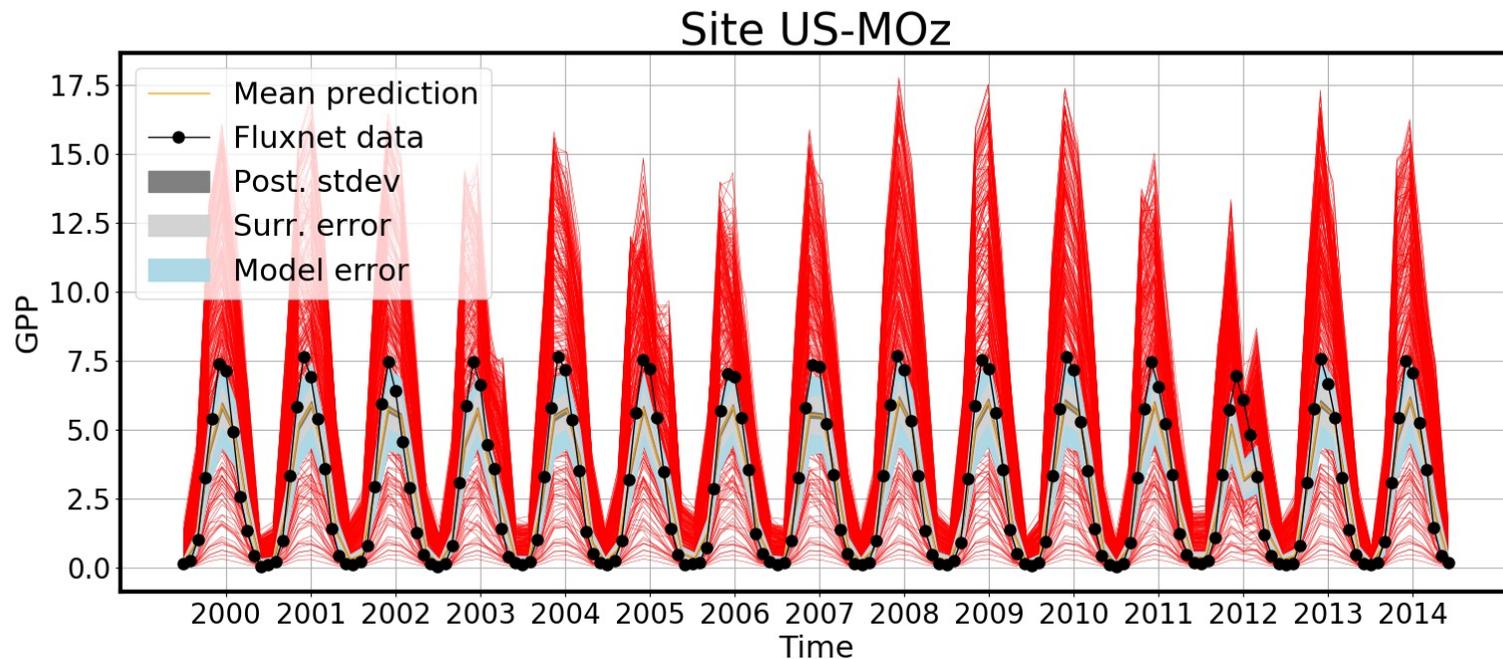
Uncertainty reduction: zoom in the parameter space regions relevant to obs. data



Deciduous forest, Missouri, USA

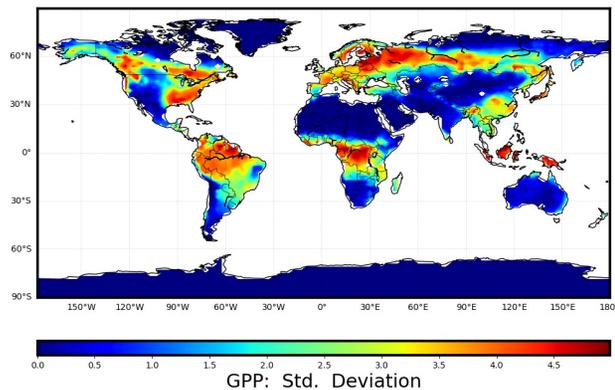
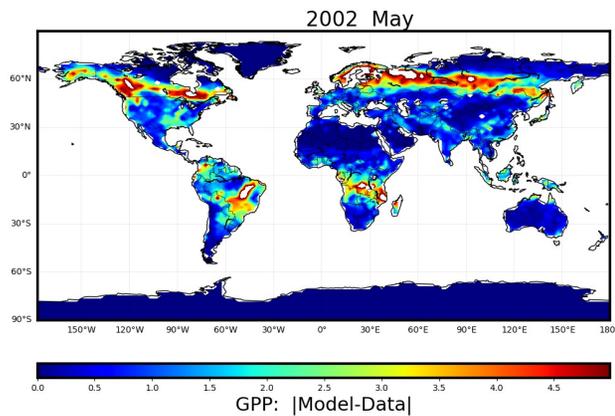
# ... with uncertainty decomposition

Model structural error is usually the largest contributor of predictive variance

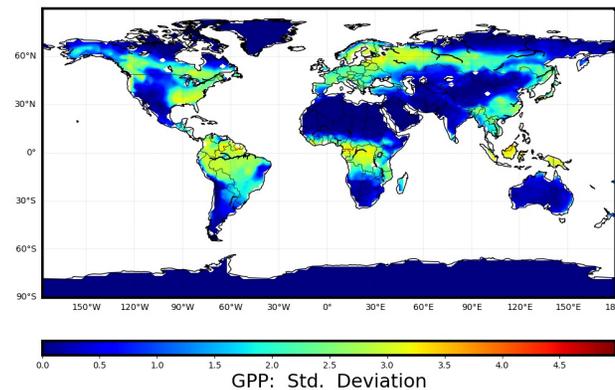
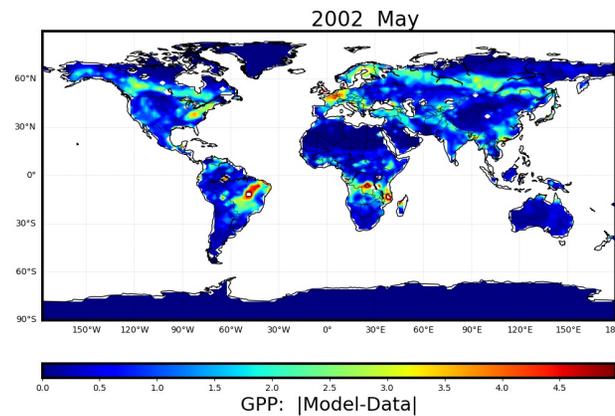


# Calibration reduces predictive mean error and predictive standard deviation

Prior

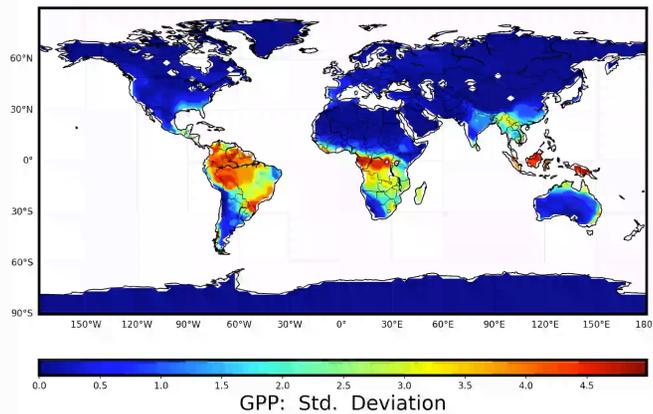
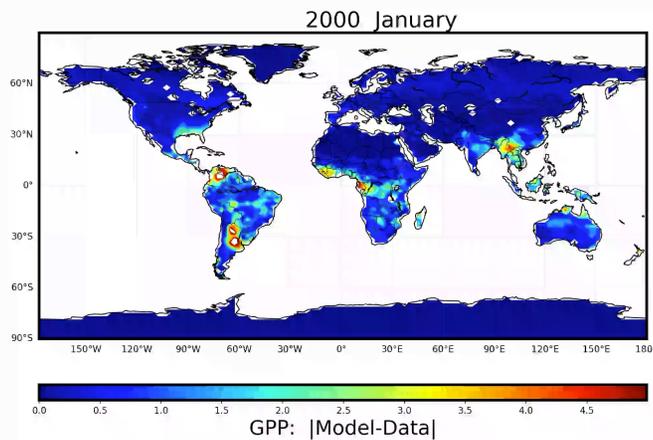


Posterior

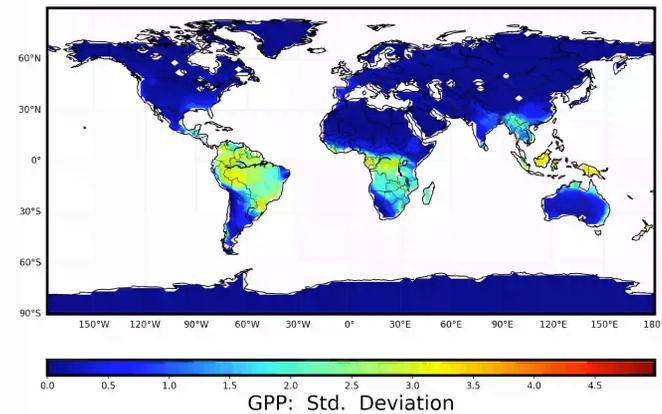
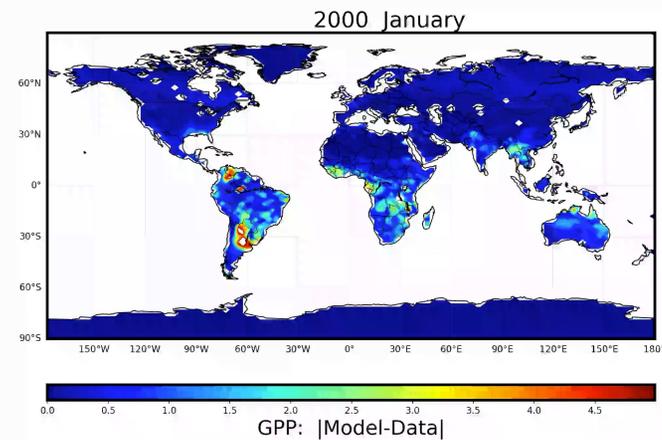


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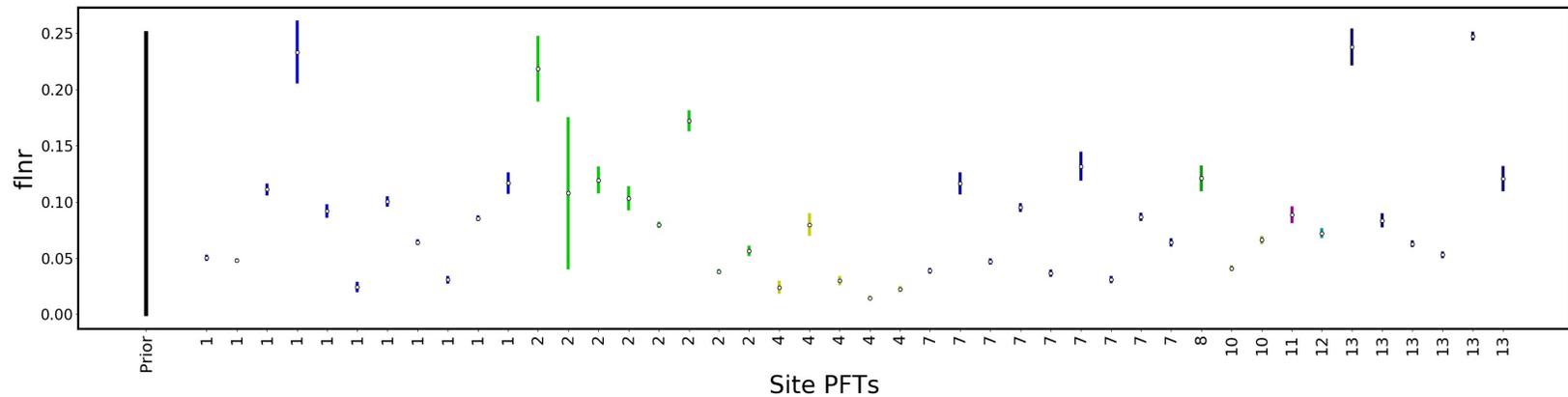


Posterior

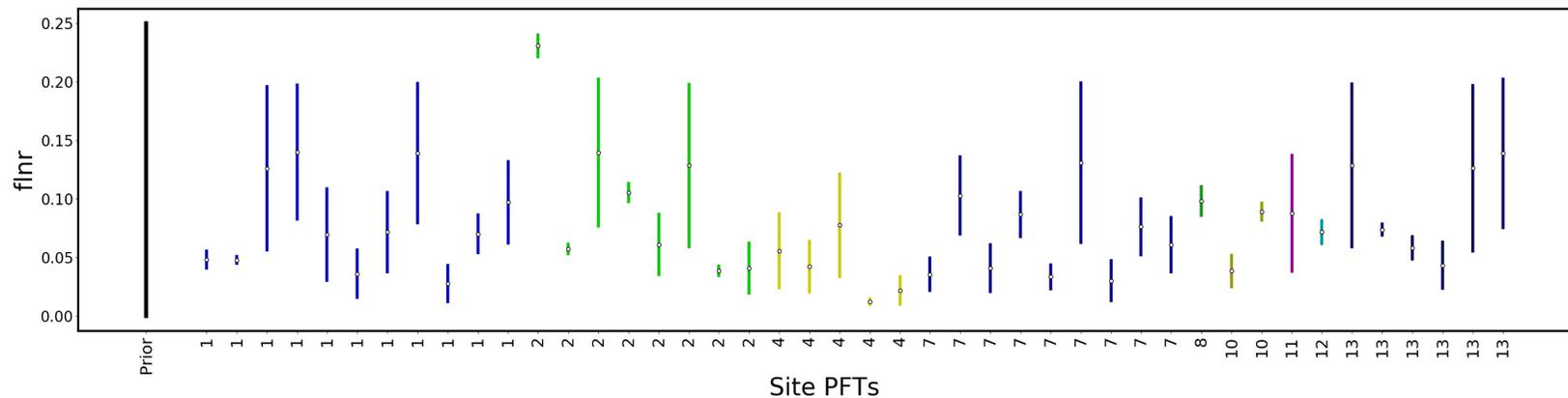


# Calibrated parameter values across FLUXNET sites

**Without model error:** Overfitting, i.e. high variability in flnr across sites within and across PFTs



**With model error:** fair representation of unknown flnr (still narrower than prior!)



# Summary

- **Constructed spatio-temporal surrogate to approximate ELM**
  - Karhunen-Loève + Polynomial Chaos expansions
  - Surrogate is orders of magnitude less expensive than ELM
- **Global sensitivity analysis or variance decomposition is a free bi-product**
- **Bayesian calibration using online evaluation of the surrogate**
  - Embedded model structural error provides the missing uncertainty component
  - Reduction of predictive uncertainty in light of FLUXCOM data
  - Full decomposition of predictive uncertainty

Param 1

Param 2

Param 4

Surr. error

Data noise

Model str. error

## Next:

- **Build a global land-model calibration framework**
  - Construct ensembles with land biogeochemistry active (higher expense)
  - Determine sensitive parameters for land variables that couple to Earth system
  - Engage with ILAMB to prioritize datasets to be used to integrate with ELM
  - Find best parameters to use in future offline and coupled experiments