Reduced-Dimensional Neural Network Surrogate Construction and Calibration of the E3SM Land Model

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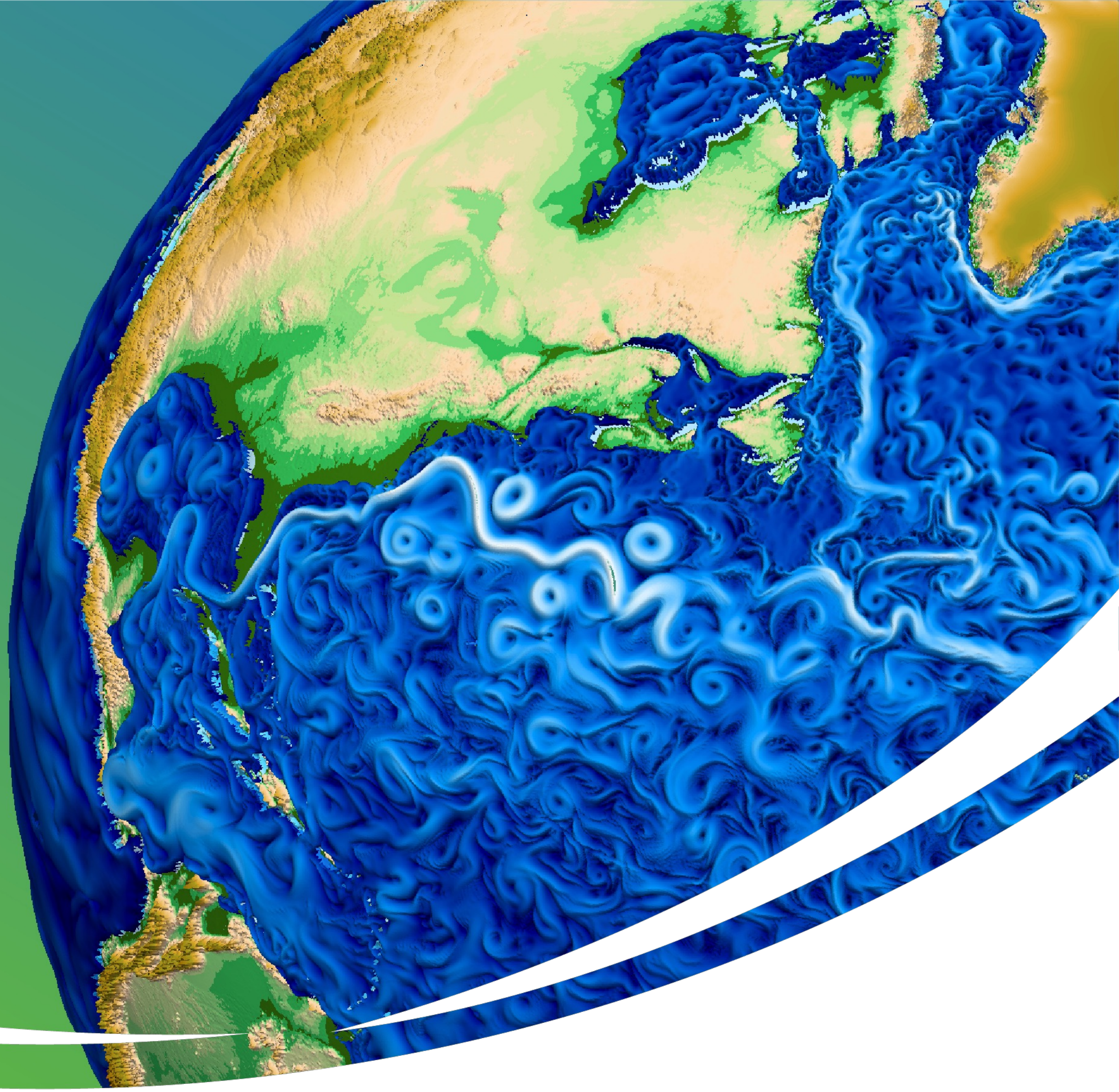

Sandia National Laboratories

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U.S. Department of Energy

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San Francisco
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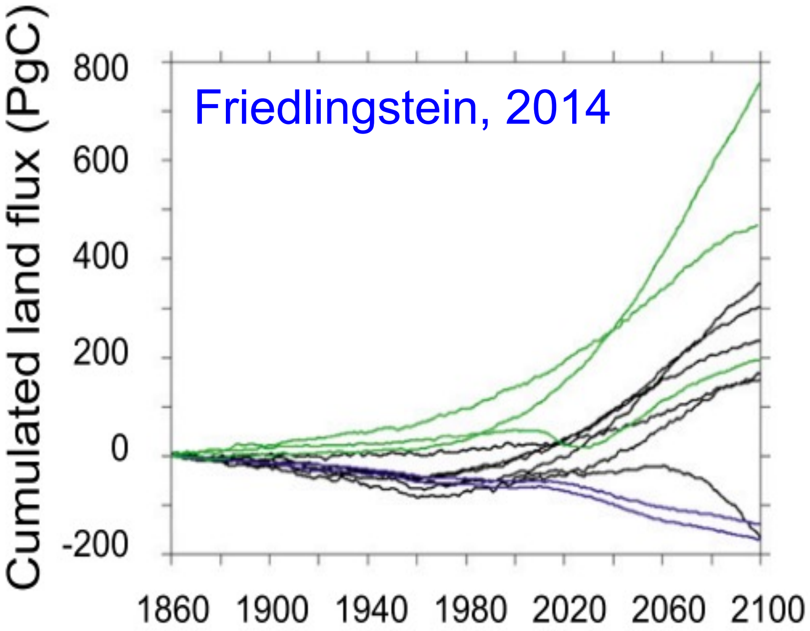
E3SM
Energy Exascale Earth System Model

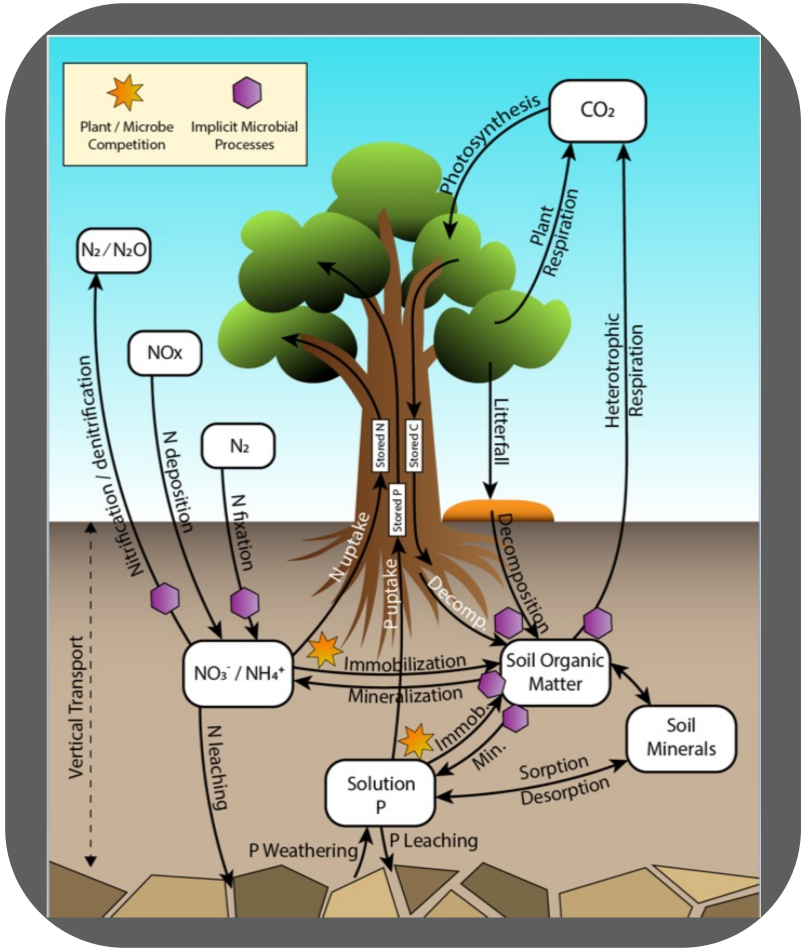
Motivation and Overview

- Need for **model surrogates** for sample-intensive studies, such as …
  - Global sensitivity analysis (forward UQ)
  - Model calibration (inverse UQ)
- Major **challenges**
  - Expensive model evaluation, small ensembles
  - High dimensional (spatio-temporal) outputs



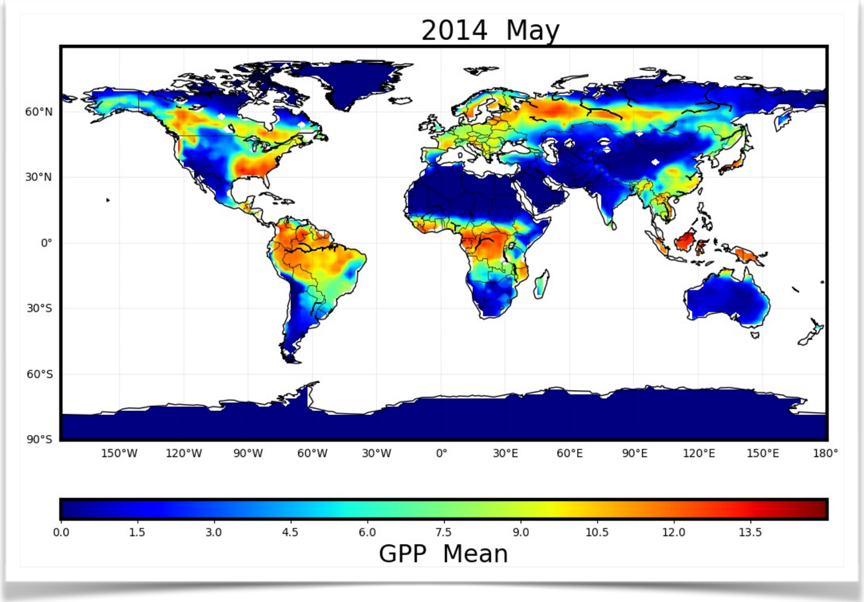
- Reduced-dimensional, inexpensive surrogate construction via Karhunen-Loève expansions and Neural Networks (KLNN)
- Surrogate enables global sensitivity analysis and Bayesian model calibration

E3SM Land Model (ELM): focus on carbon and energy cycle

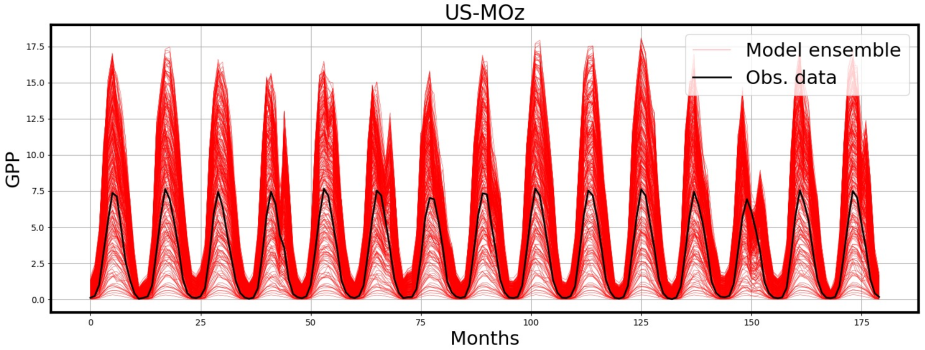


Quantity of Interest: Gross primary productivity (GPP)…

… resolved in space, …

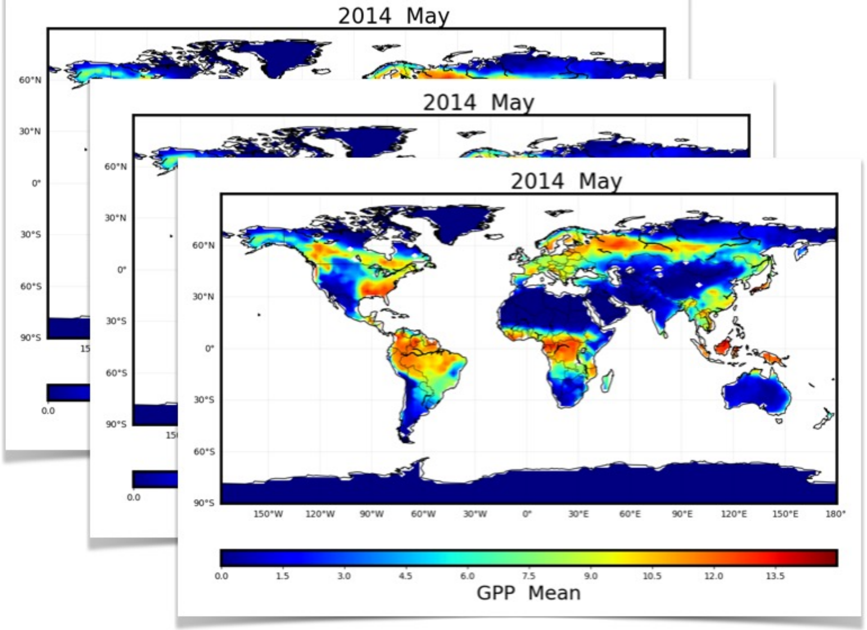


… and in time.



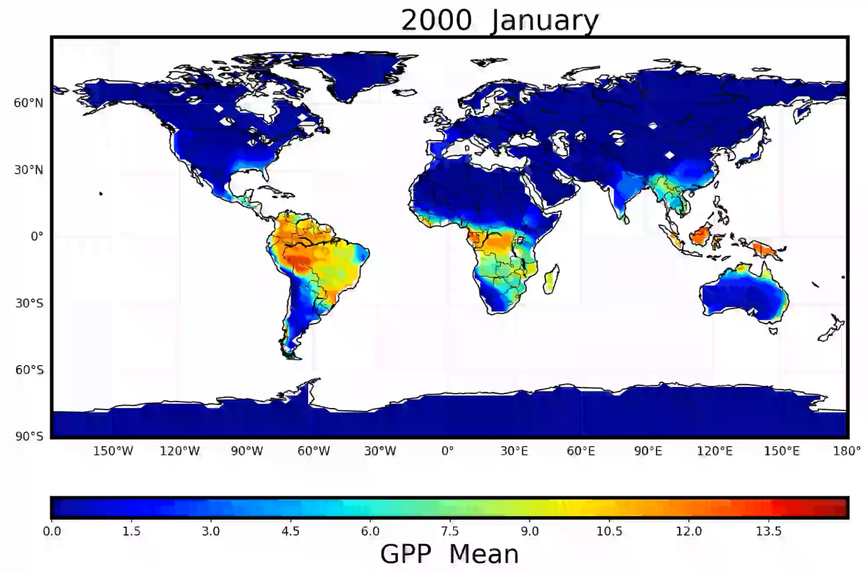
Model Ensemble (275 samples)

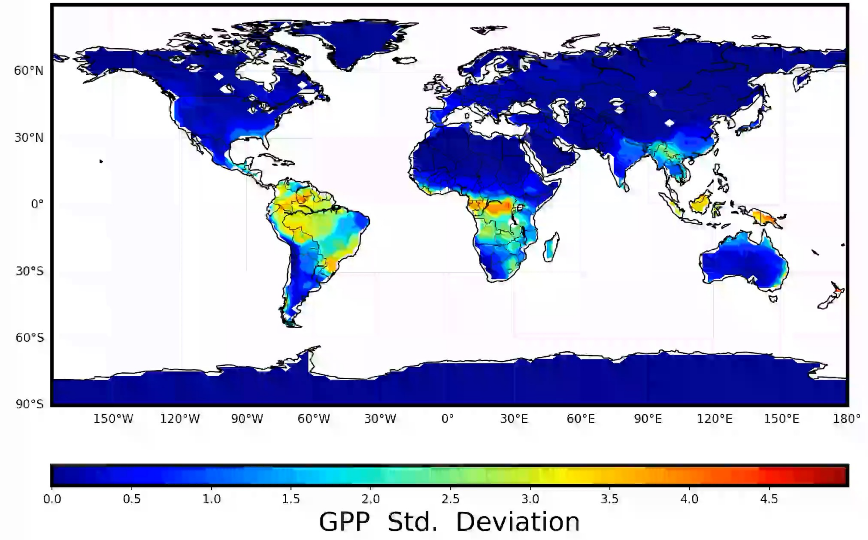
1.9x2.5 resolution, satellite phenology



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





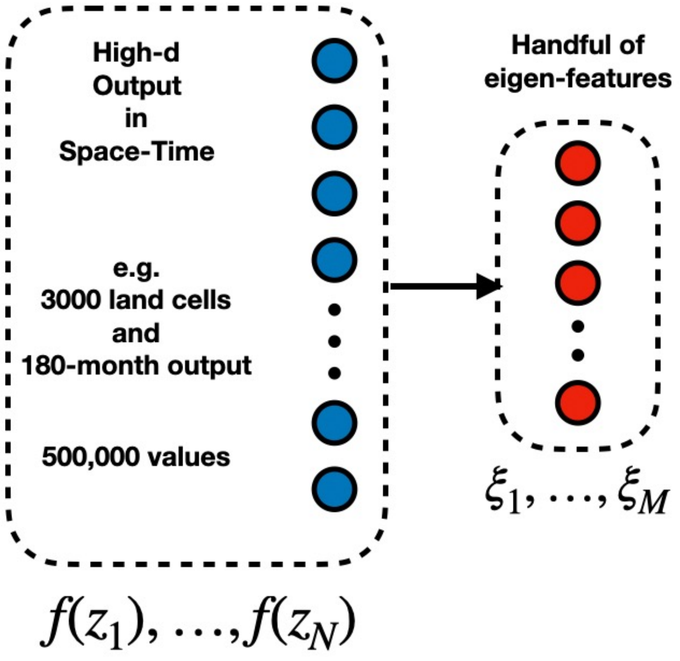
Dimensionality Reduction via Karhunen-Loève Expansion

$$f(\color{red}{\lambda}; \color{blue}{z}) \approx \bar{f}(z) + \sum_{m=1}^{M} \xi_m(\lambda)\sqrt{\mu_m}\,\phi_m(z)$$

Uncertain parameters

"Certain" conditions

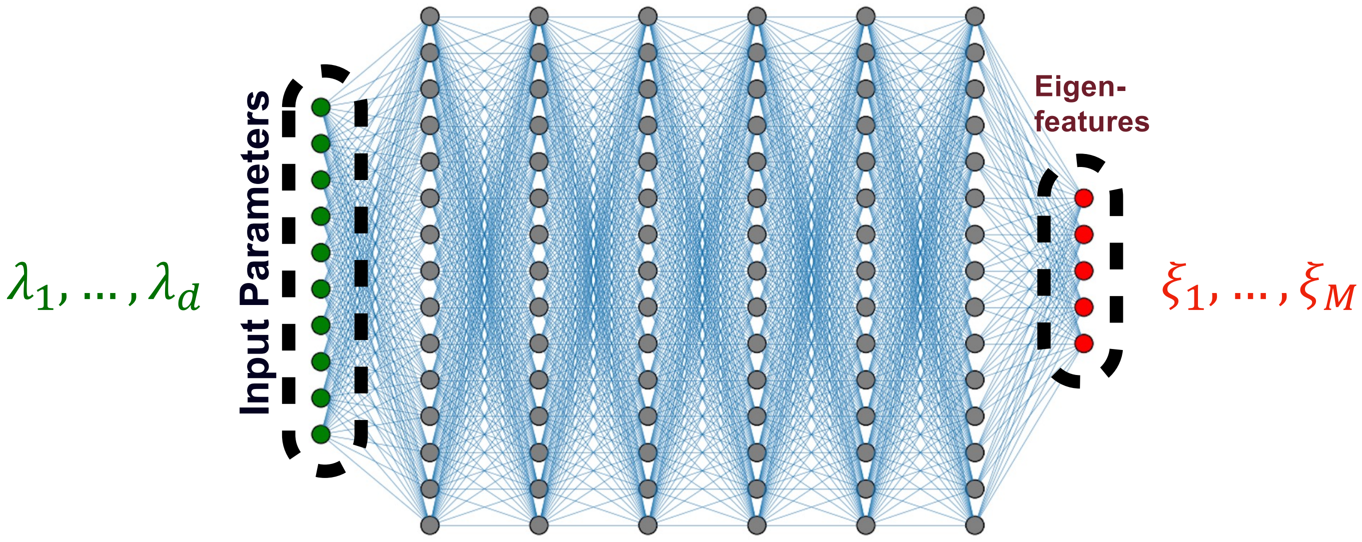
- Spatio-temporal model output $f(\lambda; z)$, where $z = (x, y, t)$
- Output field has large dimensionally $N = N_x \times N_y \times N_t$
- Eigenpairs $(\mu_m, \phi_m(z))$ are found via eigen-solve
- Analysis reduces to $M \ll N$ eigenfeatures $\xi_1, \ldots, \xi_m$
- Under the hood: this is essentially an SVD



KL+NN = reduced dimensional spatio-temporal surrogate

The goal is to construct a surrogate with respect to uncertain parameters λ, such that $f(\lambda; z_i) \approx f_s(\lambda; z_i)$ for all conditions z_i.

Instead of building surrogate for each individual z_i for $i = 1, \dots, N$,
we construct neural network (NN) surrogate for $\xi_1, \dots, \xi_M$ where $M \ll N$.



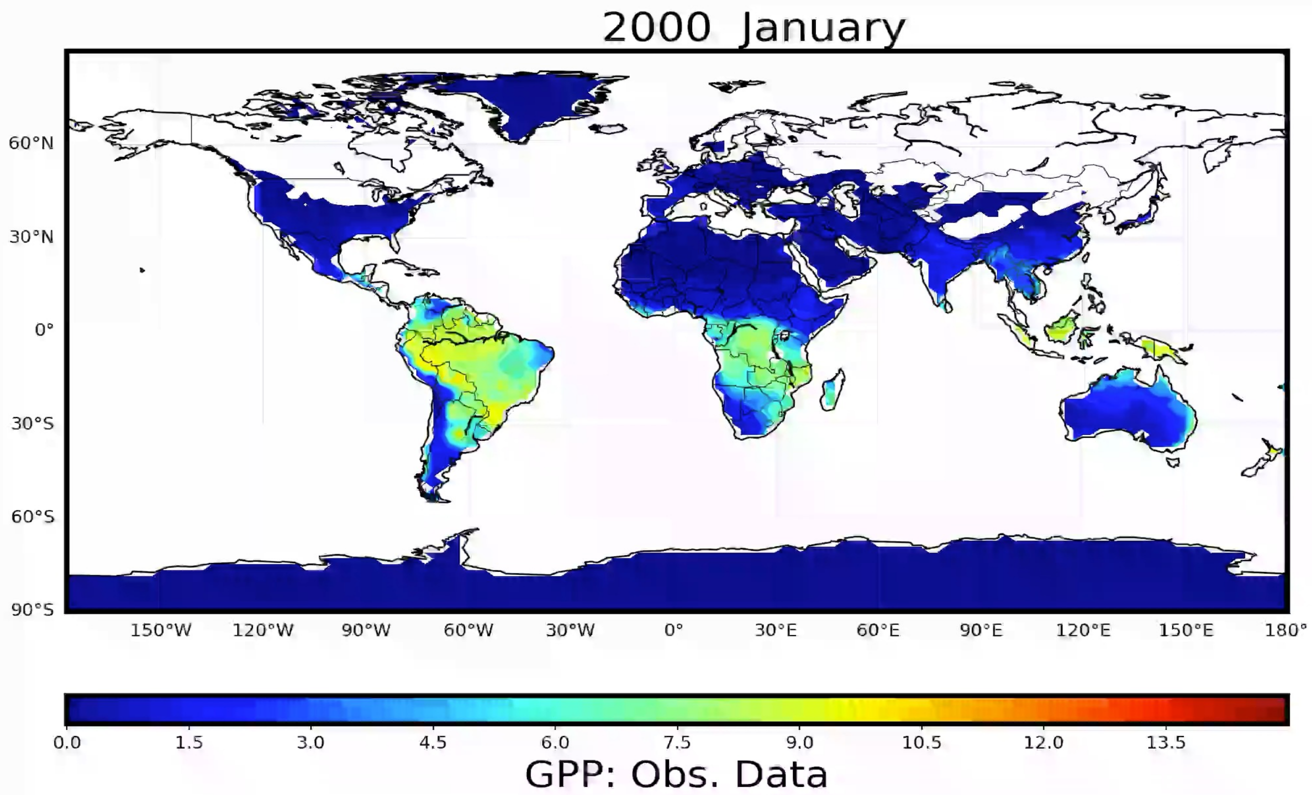
$$f(\lambda; z) \approx \overline{f}(z) + \sum_{m=1}^{M} \xi_m(\lambda) \sqrt{\mu_m} \phi_m(z)$$

$\xi_m^{NN}(\lambda)$

Reference Data

FLUXCOM: A gridded GPP benchmark upscaled from FLUXNET network using meteorology, remote sensing

https://www.fluxcom.org/



Bayes' formula $p(\lambda \mid g) \propto p(g \mid \lambda)\, p(\lambda)$

$f(\lambda; z)$

ELM:
1.9x2.5 resolution,
satellite phenology

KLNN Surrogate:

$$\bar{f}(z) + \sum_{m=1}^{M} \xi_m^{NN}(\lambda)\sqrt{\mu_m}\phi_m(z)$$

$f_s(\lambda; z)$

Prior $p(\lambda)$

Bayesian Likelihood

Posterior $p(\lambda \mid g)$

Posterior sampling is done via Markov chain Monte Carlo

FLUXCOM: A gridded GPP benchmark upscaled from FLUXNET network using meteorology, remote sensing

$g(z)$

Bayesian Likelihood is constructed in the reduced space

Bayes' formula $$p(\lambda|g) \propto p(g|\lambda)p(\lambda)$$

KLNN surrogate:

$$f(\lambda; z) \approx \bar{f}(z) + \sum_{m=1}^{M} \xi_m^{NN}(\lambda)\sqrt{\mu_m}\phi_m(z)$$

Project observed data to the KL eigenspace:

$$g(z) \approx \bar{f}(z) + \sum_{m=1}^{M} \eta_m\sqrt{\mu_m}\phi_m(z)$$

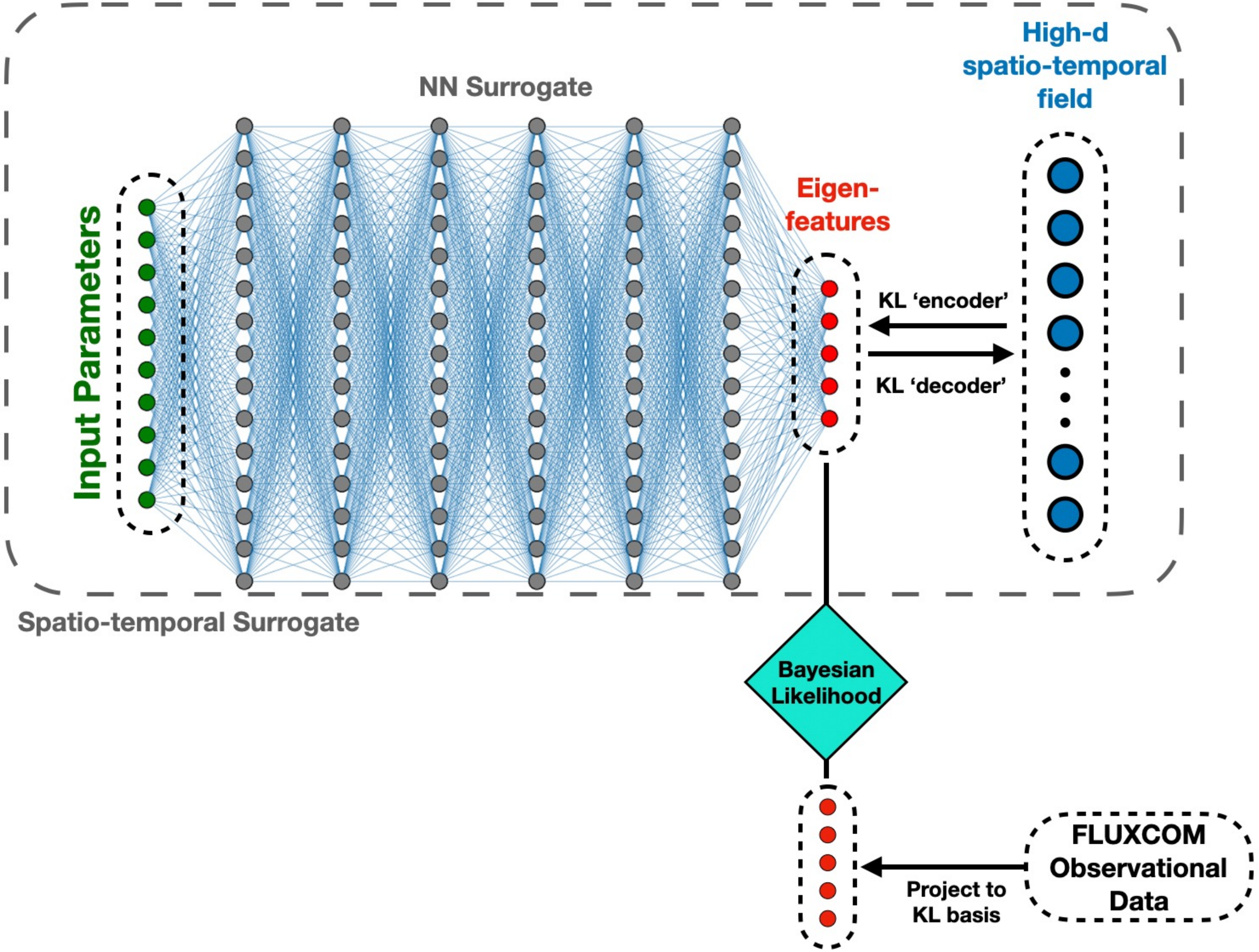
Pointwise likelihood (naïve) :

$$L_g(\lambda) \equiv p(g|\lambda) \propto \exp\left(-\sum_{i=1}^{N}\frac{(g(z_i) - f(\lambda; z_i))^2}{2\sigma_i^2}\right)$$

Reduced likelihood :

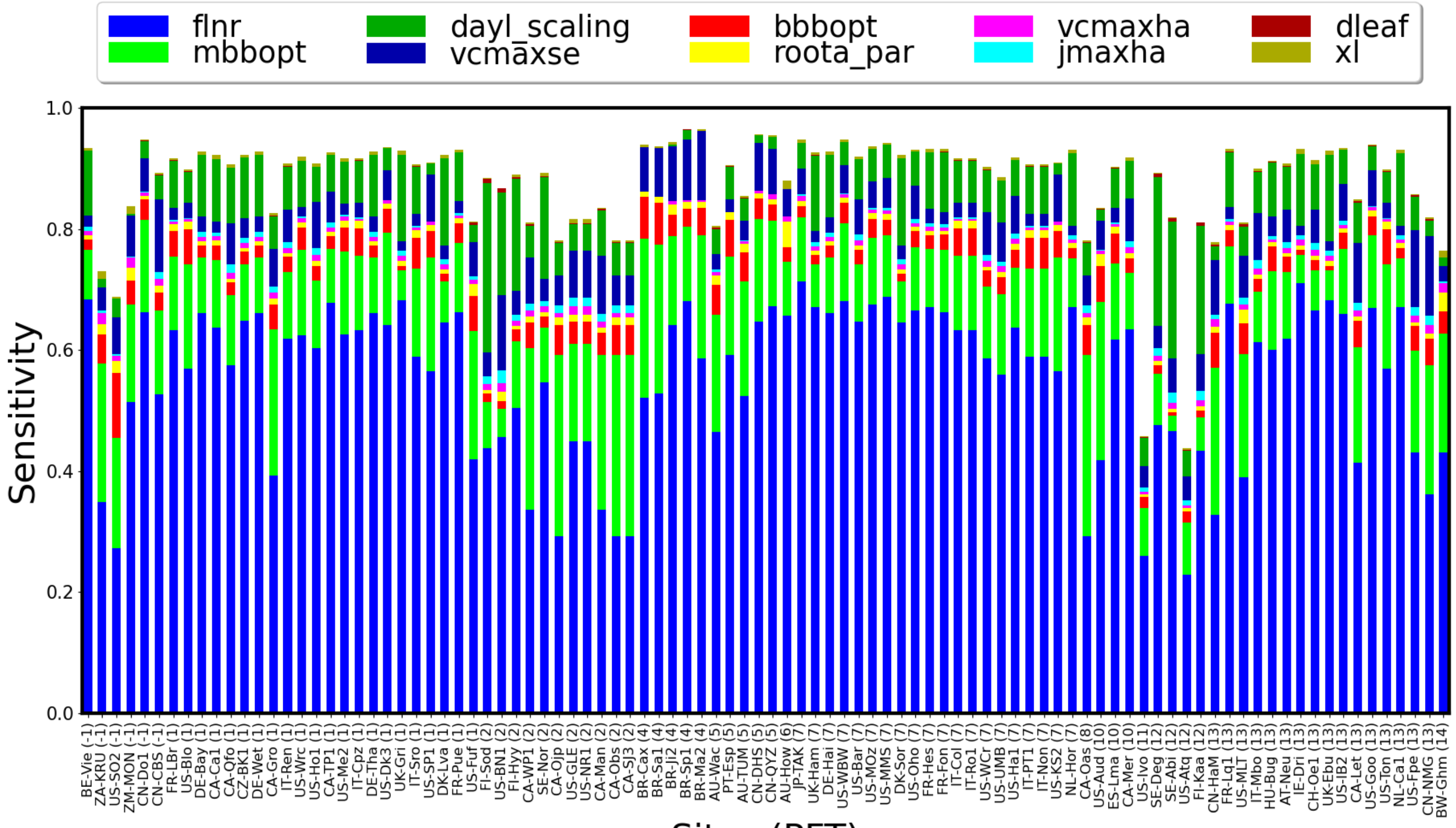
$$L_g(\lambda) \equiv p(g|\lambda) \propto \exp\left(-\sum_{m=1}^{M}\frac{(\eta_m - \xi_m^{NN}(\lambda))^2}{2\sigma^2}\right)$$

Eigenfeatures ξ_m's are uncorrelated, zero-mean, unit variance,
hence iid gaussian likelihood is a much better assumption in the reduced space.

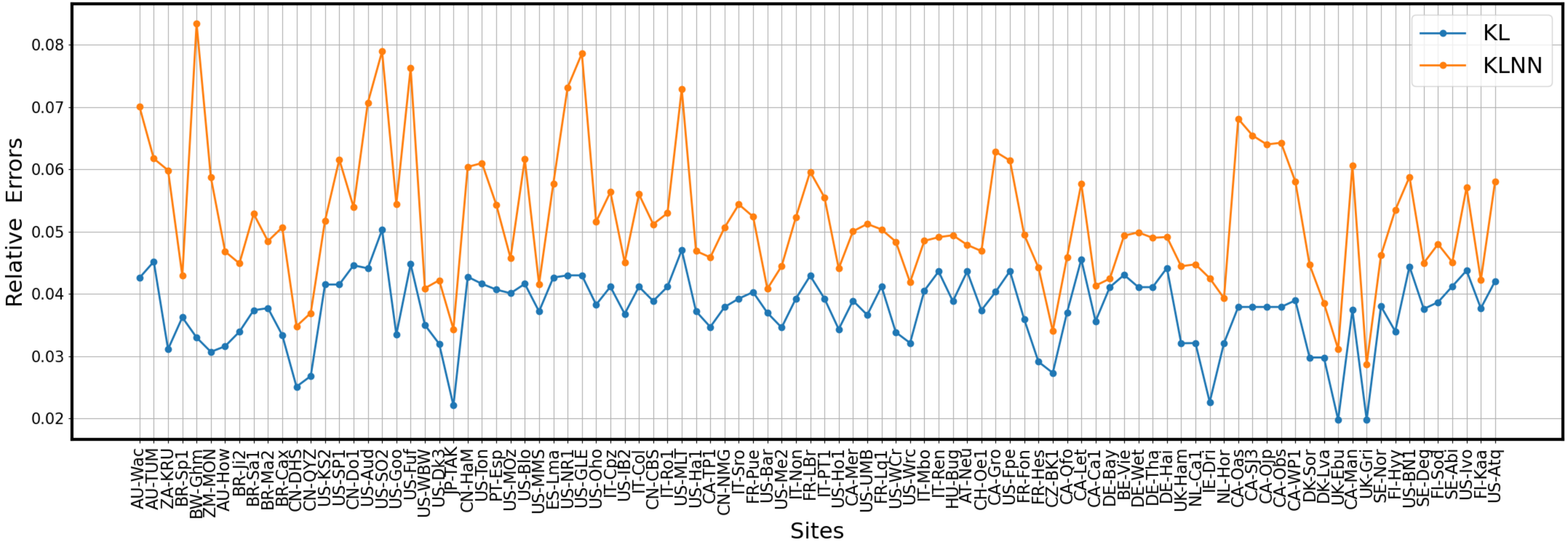


Surrogate-enabled calibration workflow incorporates both forward and inverse UQ tasks

Sensitivity at 96 FLUXNET sites: RuBisCO leaf fraction as the most impactful parameter



Instead of 96x180=**17280** surrogates, we build a single NN surrogate in the reduced, **8**-dimensional latent space



E3SM
Energy Exascale
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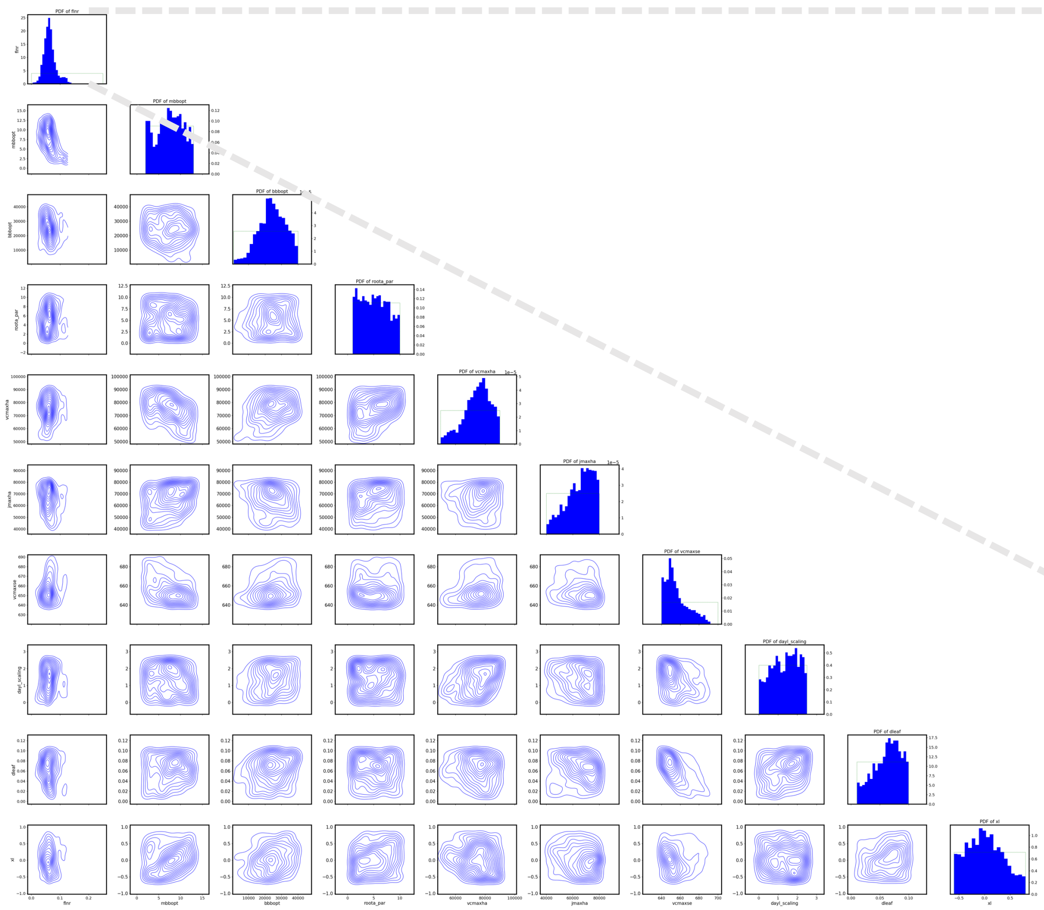
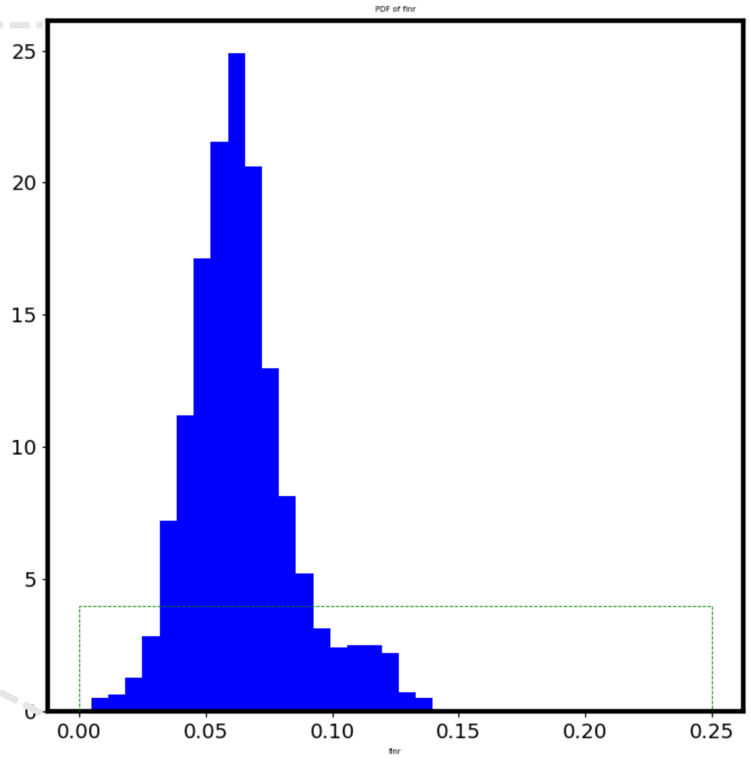
Bayesian MCMC calibration enabled by KLNN surrogate





RuBisCO leaf fraction (**flnr**) is the most constrained parameter

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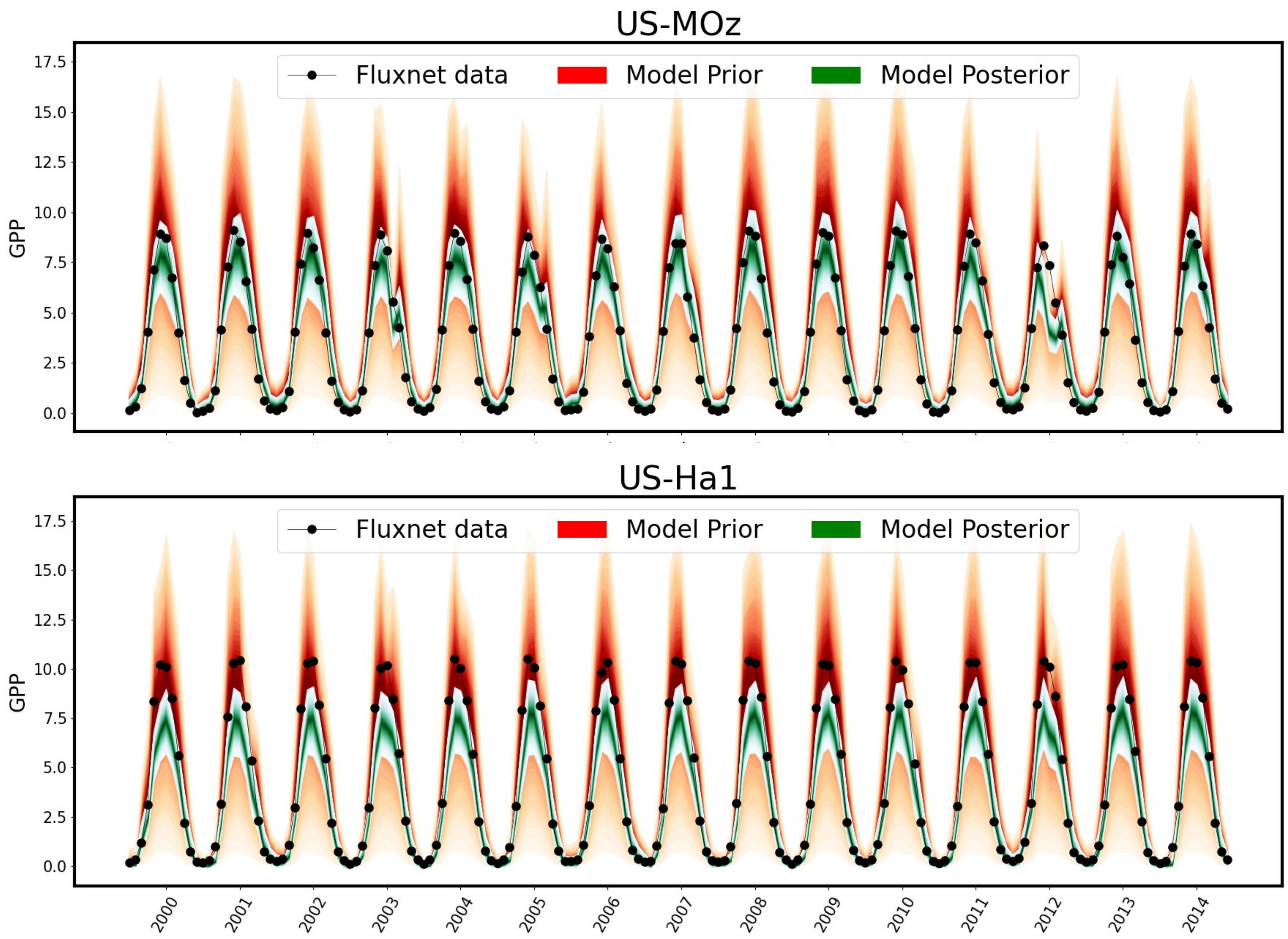
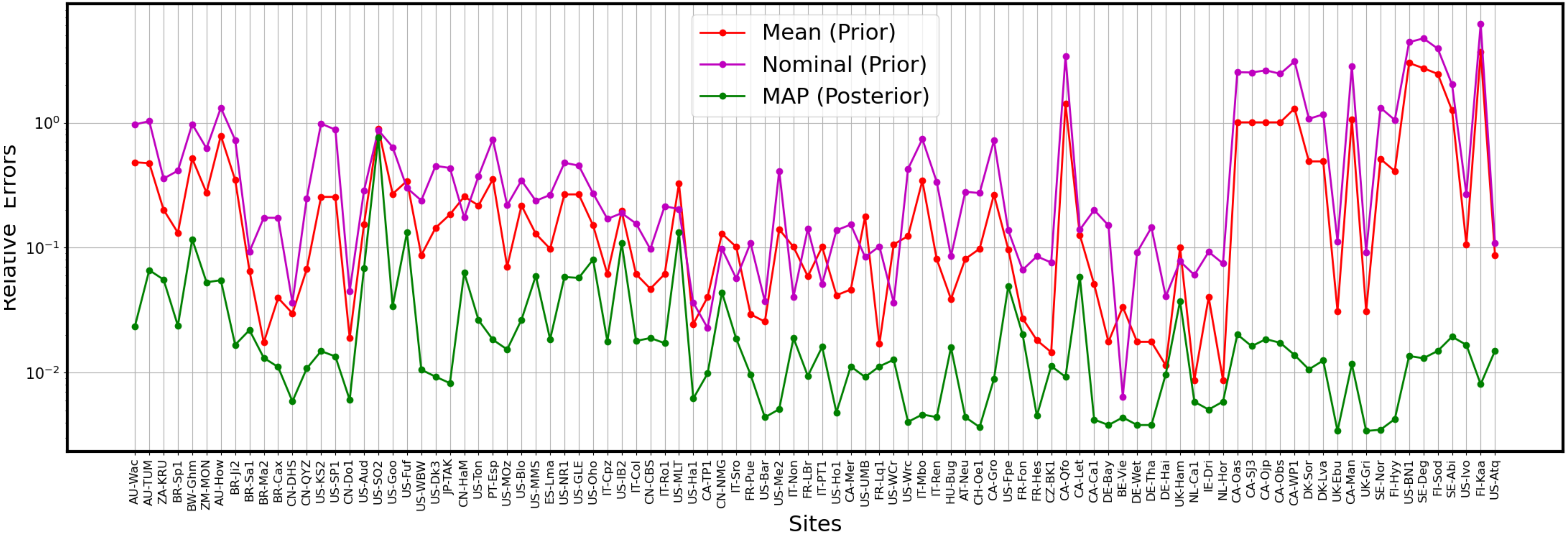
Time evolution of GPP at select FLUXNET sites

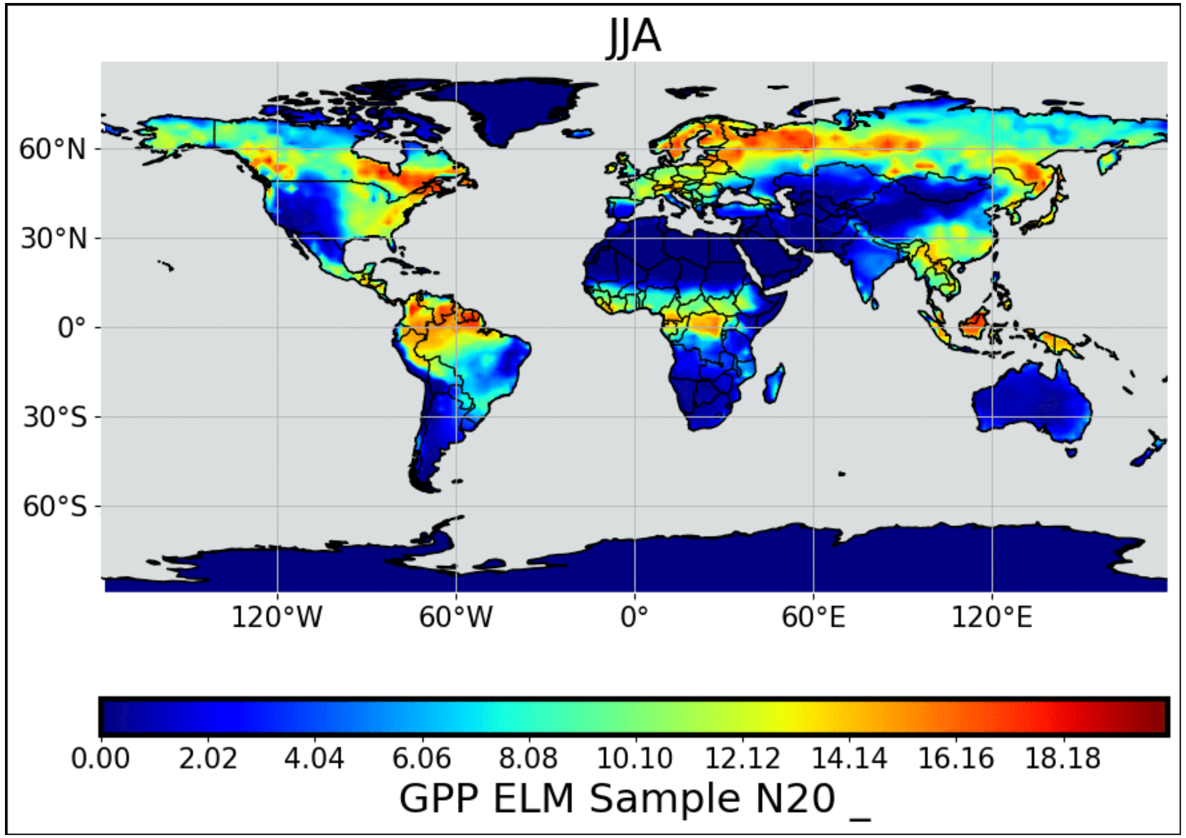


Calibration brings model prediction closer to reference data

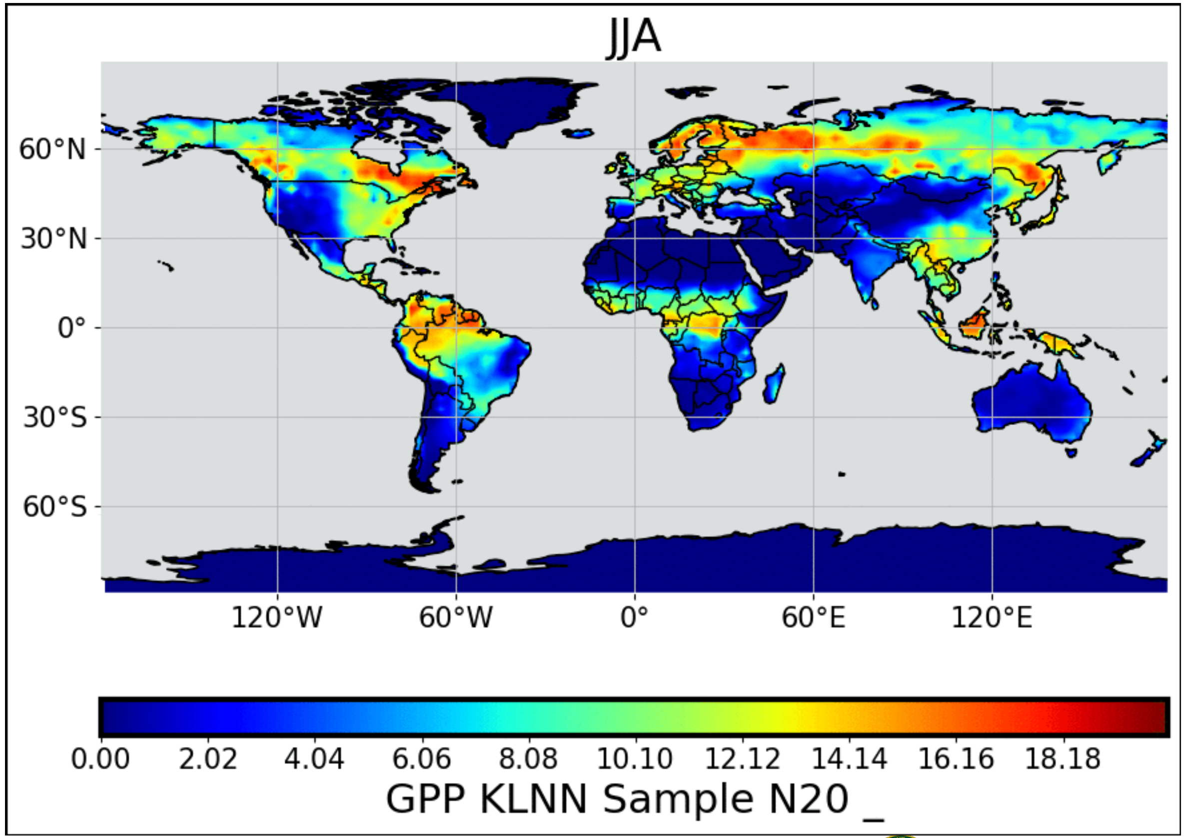


Dimensionality reduction from 4000 cells x 4 seasons = **16000** to **11**-dimensional latent space

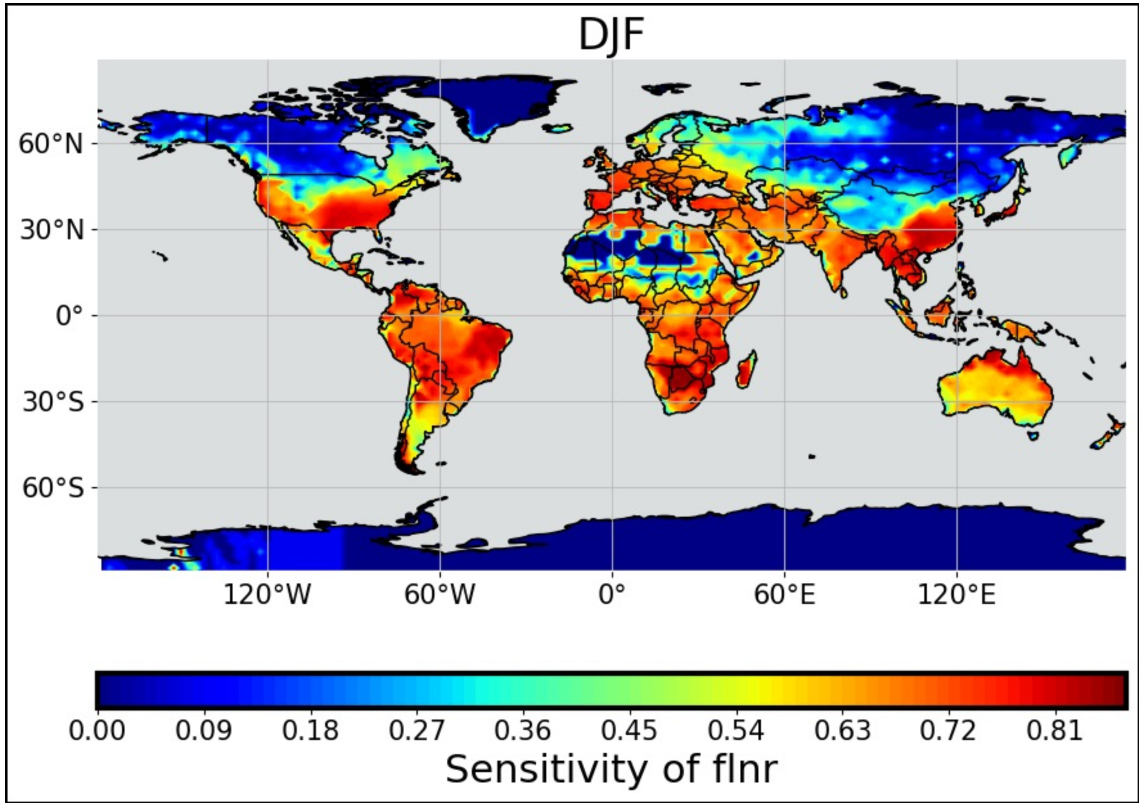
ELM Model Samples

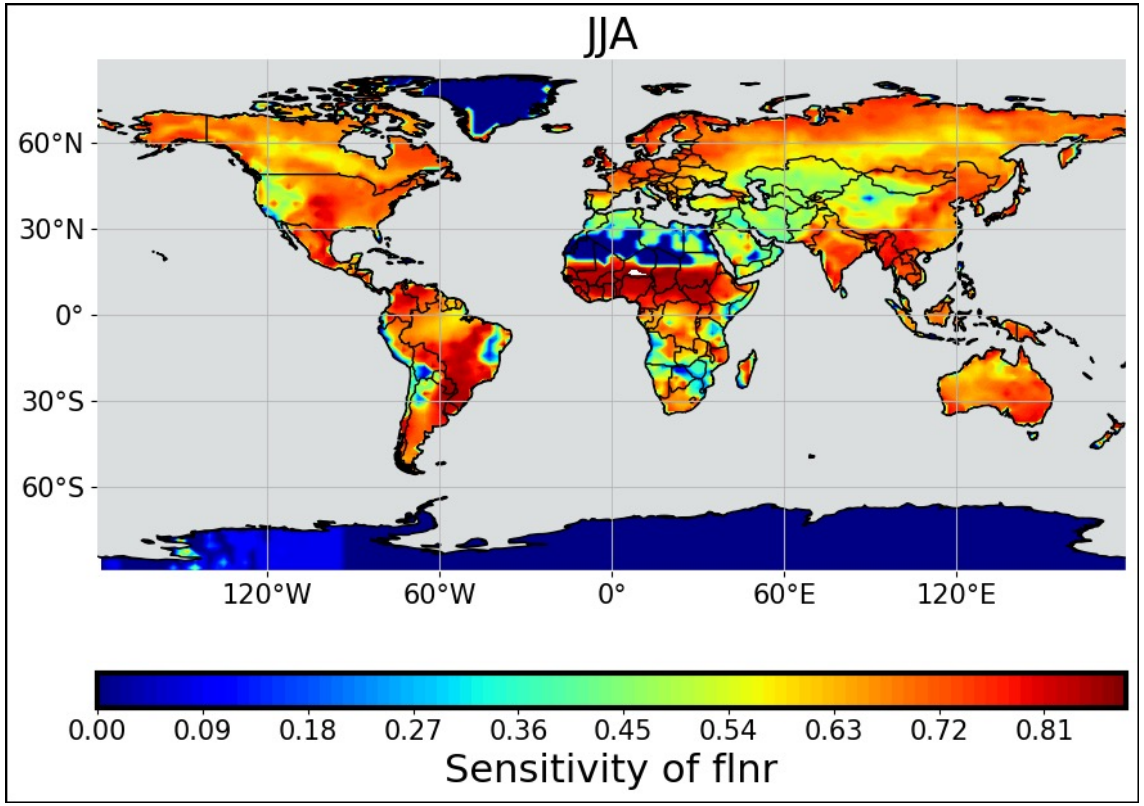


KLNN Surrogate Samples



flnr sensitivity across the globe

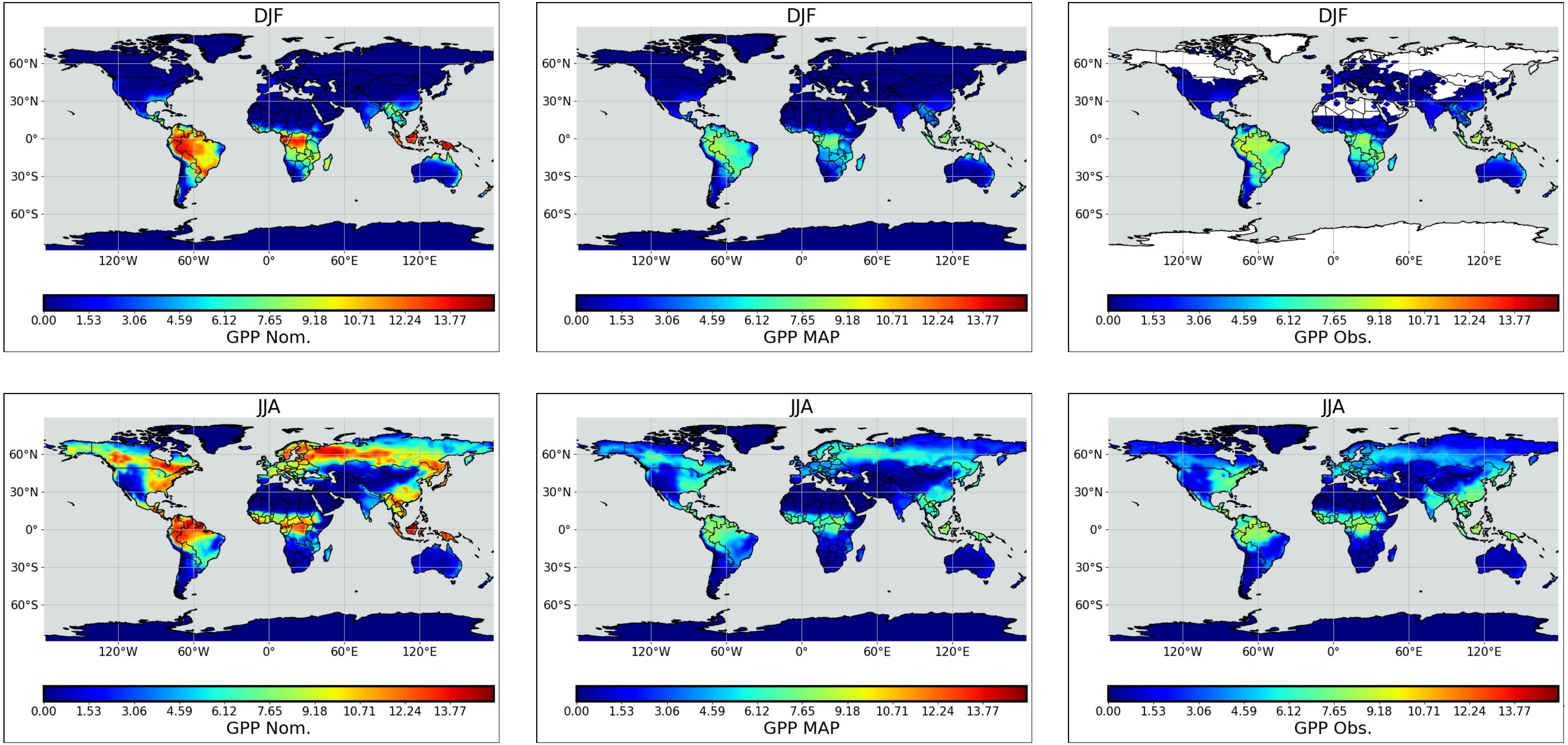




	Nominal parameter (prior)	Max a posteriori (MAP)	Reference data

Winter

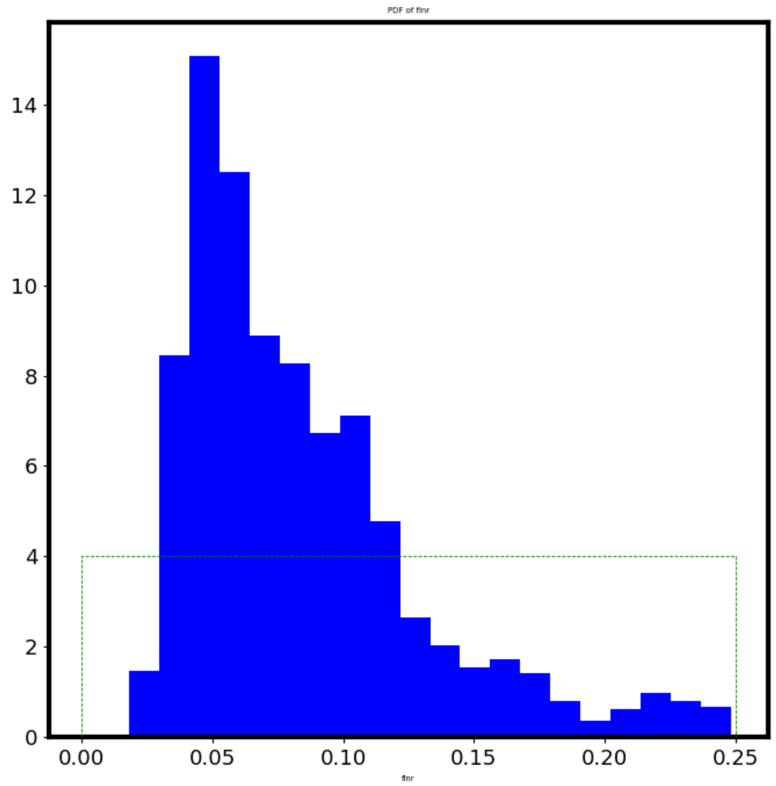
Summer



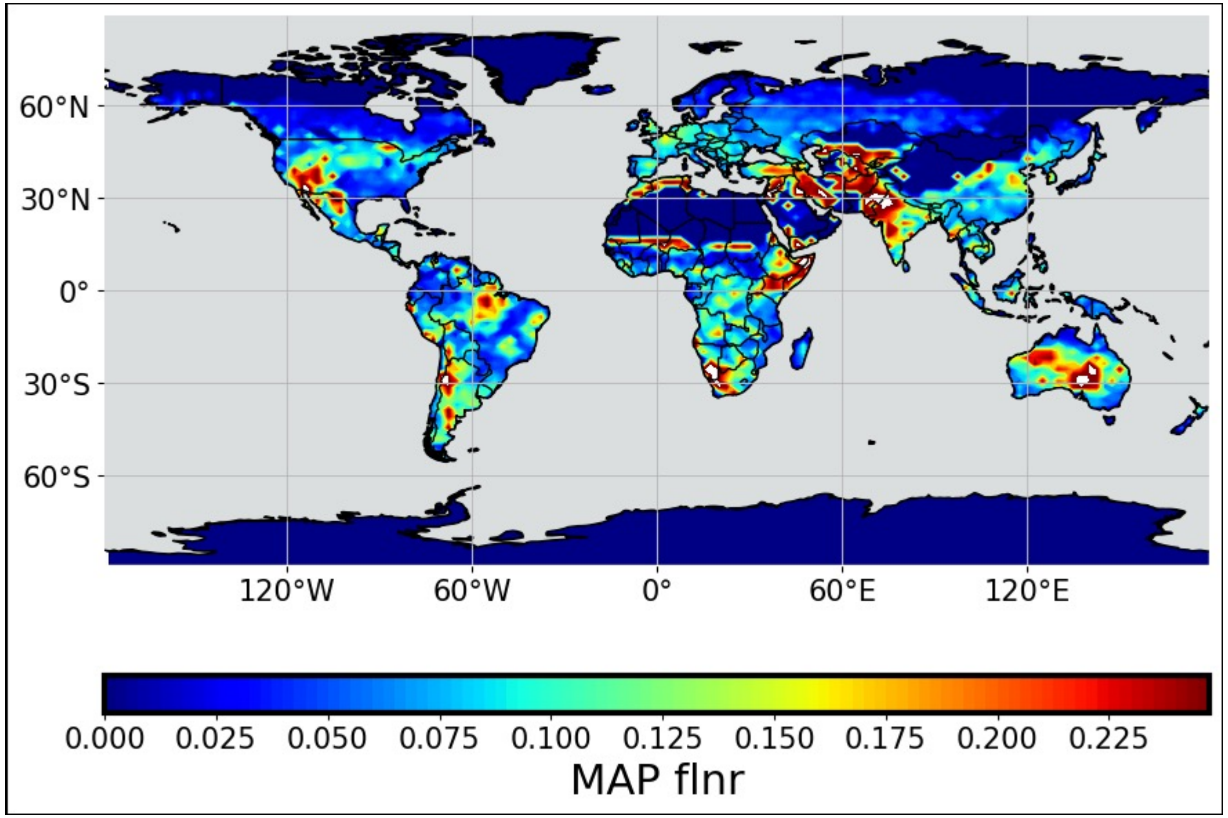
Two calibration regimes

Ongoing work: PFT-dependent reparameterization to improve model's ability to match reference data.

Fixed global flnr parameter



Local flnr parameter



Summary

- Karhunen-Loève (KL) decomposition reduces the spatio-temporal output dimensionality, taking advantage of correlations over space and time.

- Neural network (NN) surrogate in the reduced eigenspace leads to a spatio-temporal **KLNN** surrogate that is a small fraction of ELM cost.

- KLNN surrogate enables sampling based global sensitivity analysis and Bayesian calibration performed in the eigenspace.

- Several orders of magnitude reduction of output dimensionality, and of the simulation cost with ~5% accuracy impact.
- *Ongoing work: PFT-dependent reparameterization to improve model's ability to match reference data.*

Additional Material

Bayesian Likelihood in the reduced space

KLNN surrogate:

$$f(\lambda; z) \approx \bar{f}(z) + \sum_{m=1}^{M} \xi_m^{NN}(\lambda)\sqrt{\mu_m}\phi_m(z)$$

Project observed data to the KL eigenspace:

$$g(z) \approx \bar{f}(z) + \sum_{m=1}^{M} \eta_m\sqrt{\mu_m}\phi_m(z)$$

Pointwise likelihood (old) :

$$L_g(\lambda) \equiv p(g|\lambda) \propto \exp\left(-\sum_{i=1}^{N}\frac{(g(z_i) - f(\lambda; z_i))^2}{2\sigma_i^2}\right)$$

Data model (old) :

i.i.d. Normal

$$g(z_i) = f(\lambda; z_i) + \sigma_i\epsilon_i$$

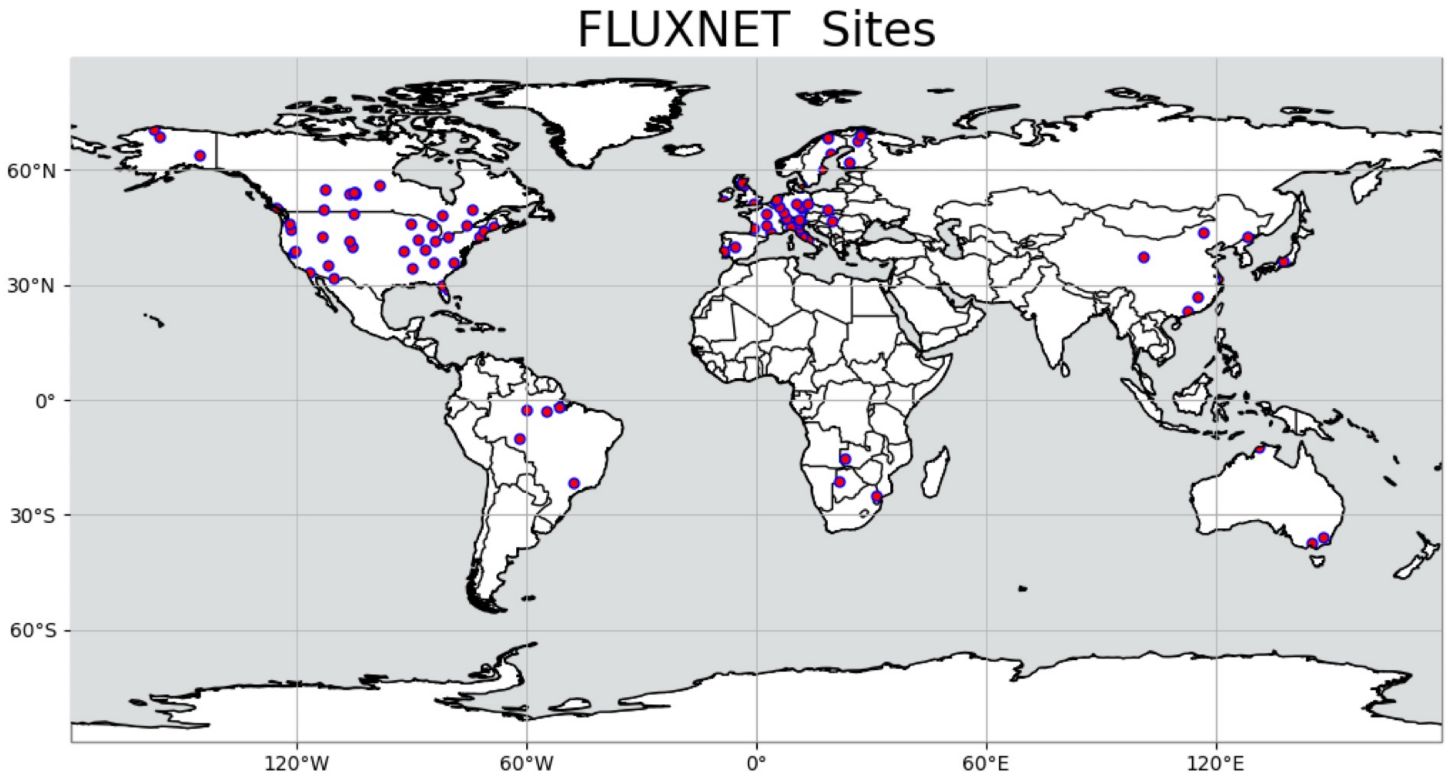
$$L_g(\lambda) \equiv p(g|\lambda) \propto \exp\left(-\sum_{m=1}^{M}\frac{(\eta_m - \xi_m^{NN}(\lambda))^2}{2\sigma^2}\right)$$

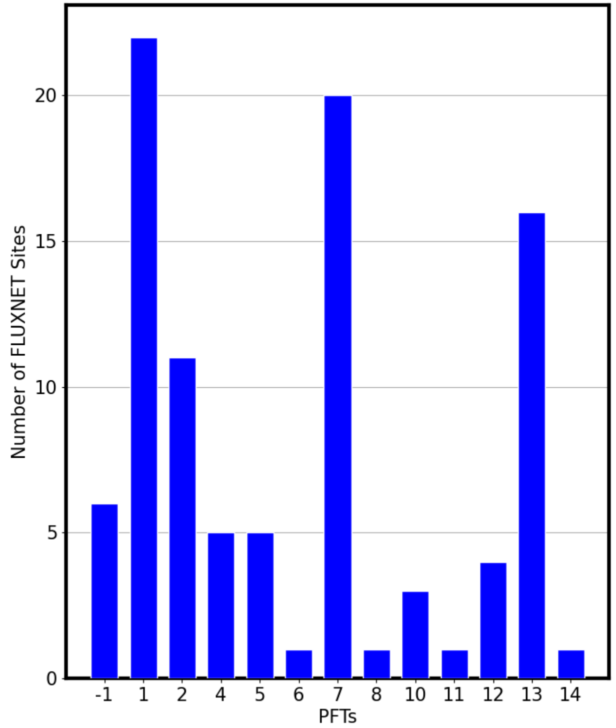
Data model (new) :

$$\eta_m = \xi_m^{NN}(\lambda) + \sigma\tilde{\epsilon}_m$$

MVN (physics-based)

$$g(z_i) = f(\lambda; z_i) + \sum_{m=1}^{M}\tilde{\epsilon}_m\sqrt{\mu_m}\phi_m(z_i)$$


FLUXNET Sites
60°N
30°N
0°
30°S
60°S
120°W
60°W
0°
60°E
120°E


Number of FLUXNET Sites
PFTs
0
5
10
15
20
-1
1
2
4
5
6
7
8
10
11
12
13
14

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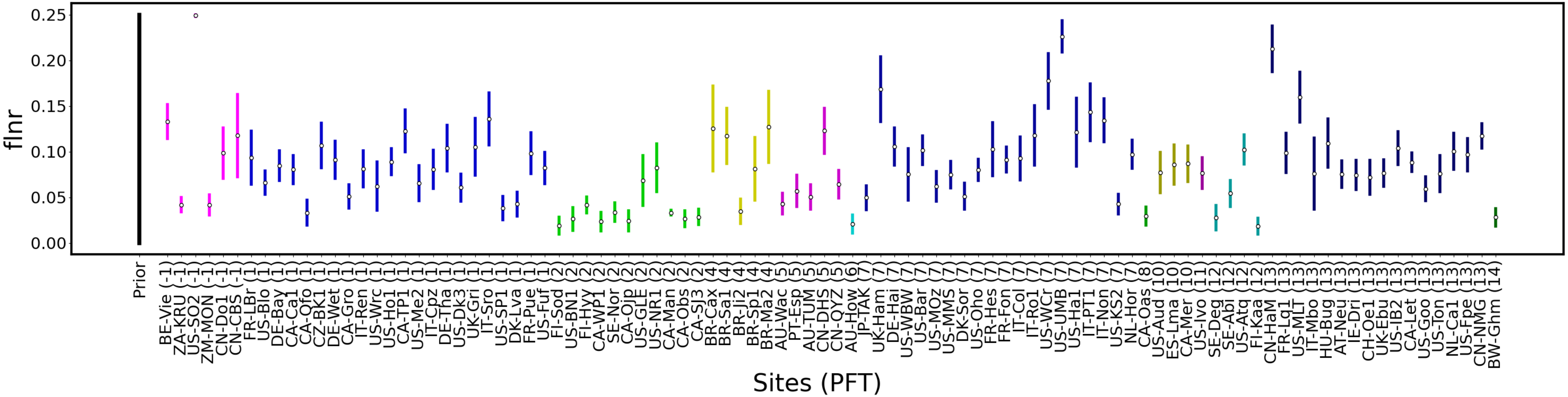

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