is paper describes objective technical results and analysis. Any subjective views or opinions that might be expres
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Exploiting Model Structu for Forward Propagation of Uncertainty in Earth System Models

SAND2019-8088C

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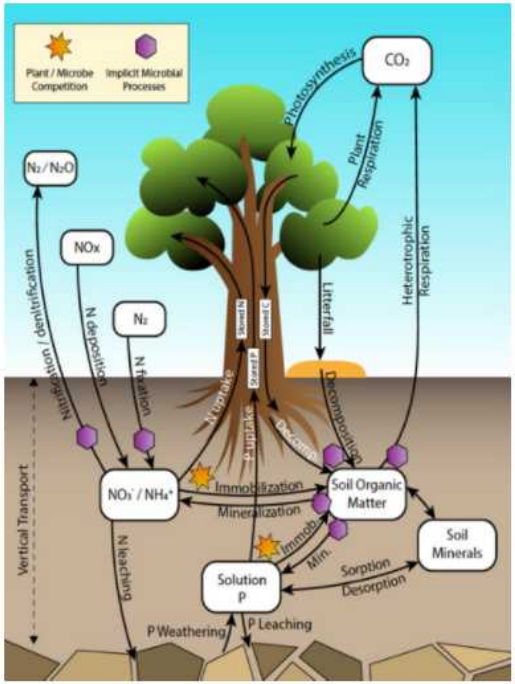
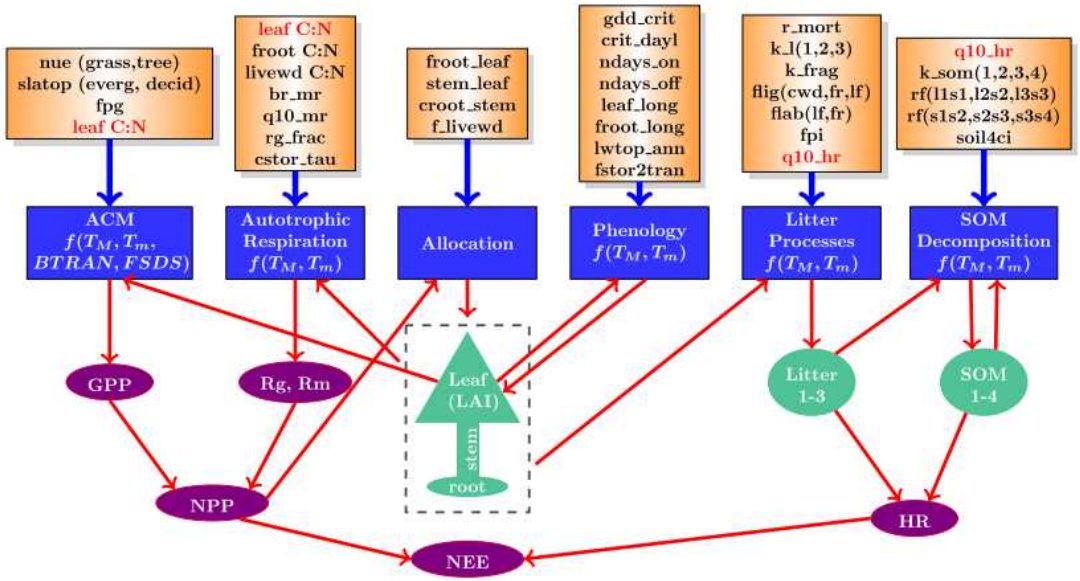
Outline

1. Motivation/Model Problem
2. Low-Rank Functional Tensor-Train Approximation
3. Earth System Model Results

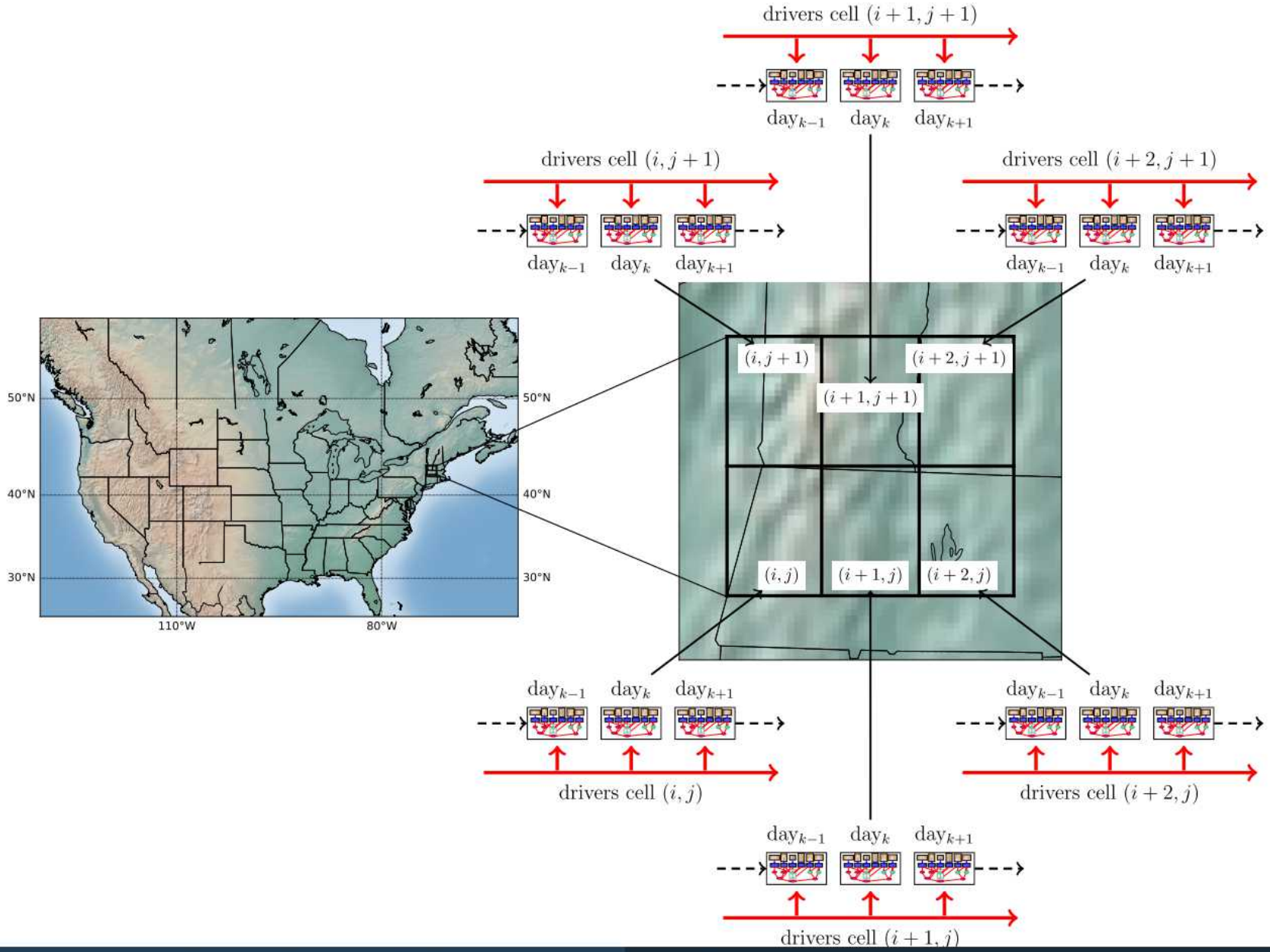
E3SM Land Model (ELM)

- US Department of Energy (DOE) sponsored Earth system model
- Land, atmosphere, ocean, ice, human system components
- High-resolution, employ DOE leadership-class computing facilities
- Some of the results are with ELM-LF: a lower-fidelity, python version





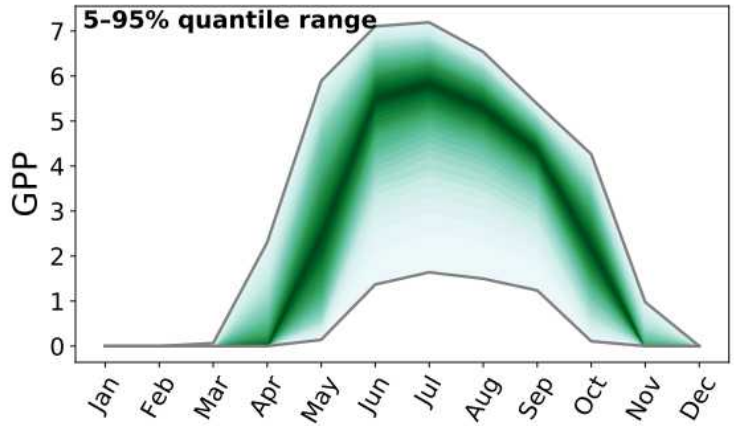
ELM-LF: Model Workflow

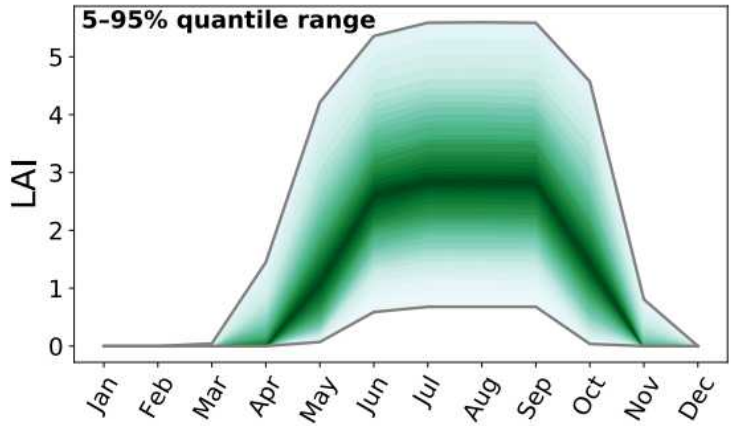


ELM-LF: Pushed-forward Prior Distributions

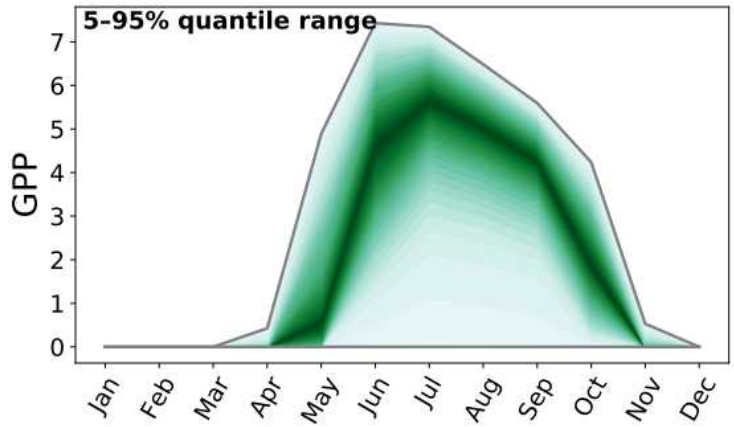
- Uniform priors for all model parameters
  - bounds set based on physical constraints and/or information from subject matter experts

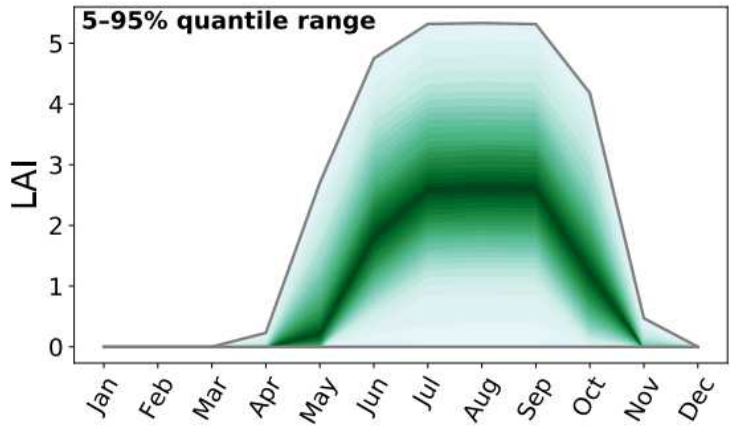
Harvard Forest EMS Tower (42.5° *N*,75.2° *W*)





University of Michigan Biological Station (45.6° *N*,84.7° *W*)



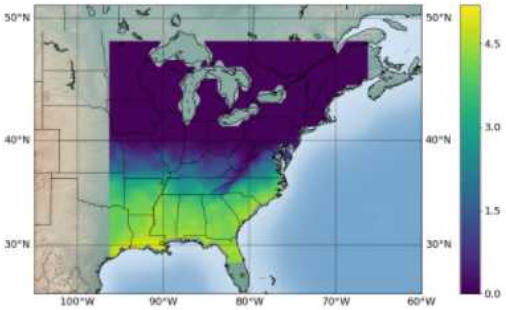


ELM-LF: Sample Spatial Patterns

Gross Primary Production (GPP)

- spatio-temporal patterns for one parameter sample

April



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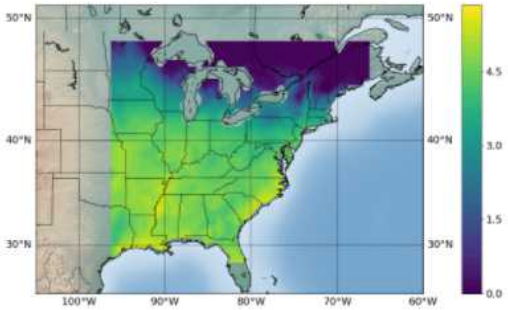
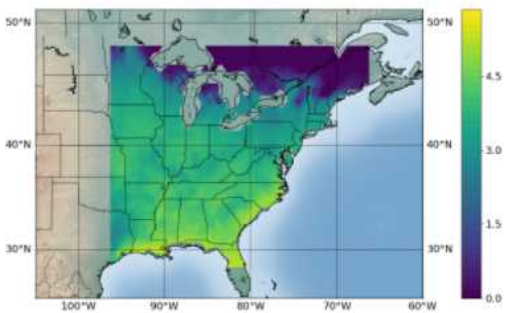
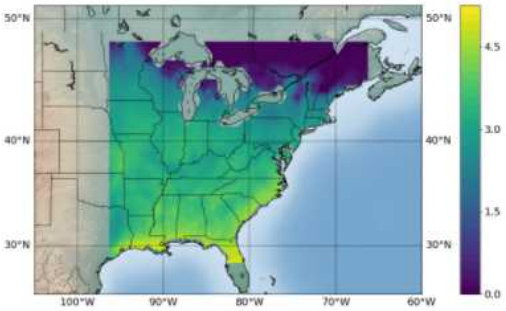


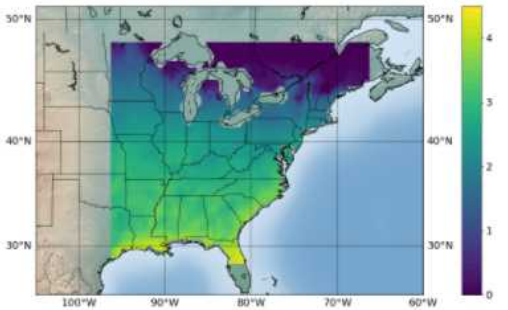
August



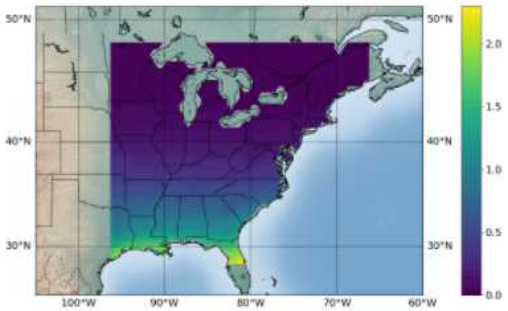
September



October



November



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Surrogates via Low-Rank Tensor Train Models

Tackle high-dimensionality and computational expense in Earth System Models via Global Sensitivity Analysis

- Explore Model Structure
- Seek efficient surrogate models for subsequent analysis of E3SM model components.

The low-rank functional tensor-train representation employs a set of matrix-valued functions in a tensor-train format to reveal couplings in high-dimensional models

- Subsequent Global Sensitivity Analysis results reveal that only a small number of parameters are driving the variability in output Quantities of Interest (QoIs).
- furthermore, spatial and temporal proximity results in correlated model behaviors.

Low-Rank Tensor-Train

Employ an approach analoguous to low-rank tensor decompositions:

$$f(x_1, x_2, \ldots x_d) = \sum_{i_0=1}^{r_0} \sum_{i_1=1}^{r_1} \cdots \sum_{i_d=1}^{r_d} f_1^{(i_0 i_1)}(x_1) f_2^{(i_1 i_2)}(x_2) \cdots f_d^{(i_{d-1} i_d)}(x_d)$$

A compact expression can be assembled using a set of products of matrix-valued functions

$$f(x_1, x_2, \ldots x_d) = \mathcal{F}_1(x_1)\mathcal{F}_2(x_2) \cdots \mathcal{F}_d(x_d)$$

Each matrix-valued function $\mathcal{F}_k(x_k)$ is a collection of univariate functions

$$\mathcal{F}_i(x_i) = \begin{bmatrix} f_k^{(11)}(x_k) & f_k^{(12)}(x_k) & \ldots & f_k^{(1 r_k)}(x_k) \\ f_k^{(21)}(x_k) & f_k^{(22)}(x_k) & \ldots & f_k^{(2 r_k)}(x_k) \\ \vdots & \vdots & \ddots & \vdots \\ f_k^{(r_{i-1} 1)}(x_k) & f_k^{(r_{i-1} 2)}(x_k) & \ldots & f_k^{(r_{i-1} r_k)}(x_k) \end{bmatrix}$$

Low-Rank Tensor-Train – Univariate Functions

The univariate function $f_k^{(ij)}(x_k)$ can be viewed as a random variable induced by the uniform random input ξ_k,

$$\xi_k \to x_k \to f_k^{(ij)}(x_k(\xi_k))$$

and can written as a Polynomial Chaos Expansion with respect to standard polynomials $\Psi_\alpha(\xi_k)$,

$$f_k^{(ij)}(x_k(\xi_k)) \approx \sum_{l=0}^{p_k} \theta_{ijkl} \Psi_l^{(ijk)}(\xi_k),$$

where p_k is the number of basis terms chosen to approximate $f_k^{(ij)}(x_k(\xi_k))$.

- Legendre polynomials are orthogonal with respect to uniform measure of ξ_k, $\pi(\xi_k) = 1/2$ in $[-1, 1]$

$$\langle \Psi_\alpha(\xi_k)\Psi_{\alpha'}(\xi_k)\rangle \equiv \int_{-1}^{1} \Psi_\alpha(\xi_k)\Psi_{\alpha'}(\xi_k)\pi(\xi_k)d\xi_k = \delta_{\alpha\alpha'}\langle \Psi_\alpha(\xi_k)^2\rangle$$

- Other polynomials are available depending on the expected behavior of the QoIs.

Low-Rank Tensor-Train – Optimization

- Consider a number of ELM-LF model results **y** corresponding to a set of choices **x** for the model inputs.

$$\text{argmin}_{\boldsymbol{\theta}} ||\boldsymbol{y} - \boldsymbol{f}||_2^2 + \Omega[\boldsymbol{f}]$$

- A penalty term is added to minimize the norm of the functions in the matrix-valued $\mathcal{F}_k(x_k)$

$$\Omega[\boldsymbol{f}] = \lambda \sum_{k=1}^{d} \sum_{i=1}^{r_{k-1}} \sum_{j=1}^{r_k} ||f_k^{ij}||^2$$

- Quasi-Newton method using L-BBFGS

C^3: Compressed Continuous Computation library
`https://github.com/goroda/Compressed-Continuous-Computation`

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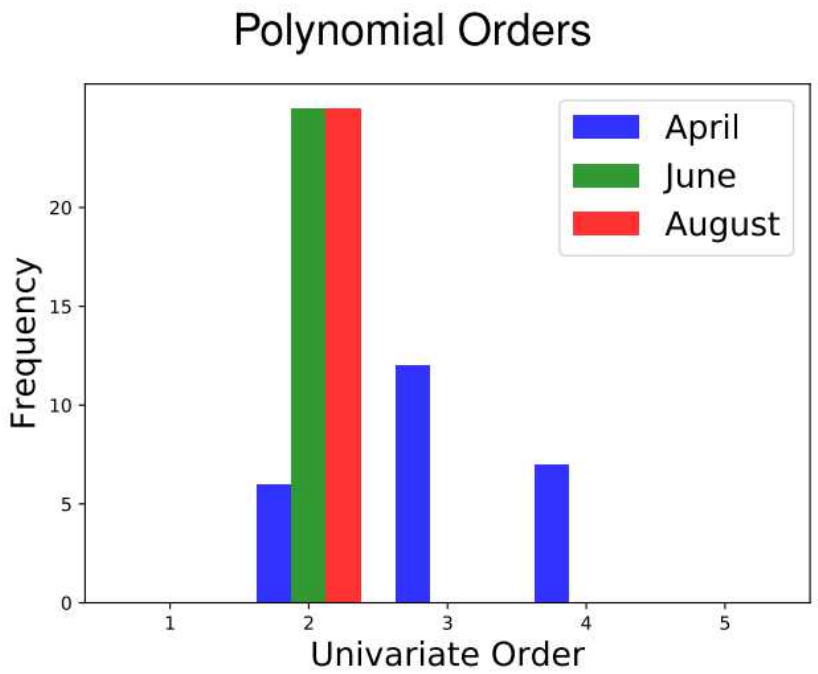
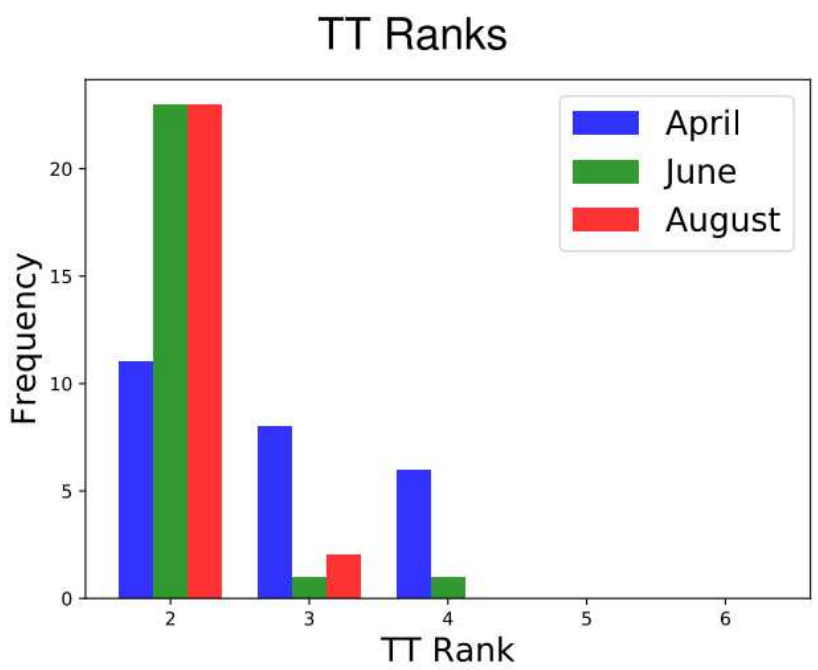
Sequence of Tests

- Summary of Low-Rank Function Tensor Train (LRFTT) Approximation Model Fits
  - select polynomial orders (same for all univariate functions), TT rank, and regularization constant through cross-validation $\rightarrow$ explore a 3D grid of choices
- Comparison with Polynomial Chaos Models (PCE) via Sparse Regression
  - . . . via Bayesian Compressive Sensing
  - `https://www.sandia.gov/UQToolkit`
- 1000-2000 model simulations
  - (Randomized) Partioned into training and testing sets
  - K-fold cross-validation (4 folds)
- Global Sensitivity Sensitivity Analysis Results
  - ELM-LF monthly averages for select QoIs: LAI & GPP

LRFTT Cross-validation: Ranks and Polynomial Orders

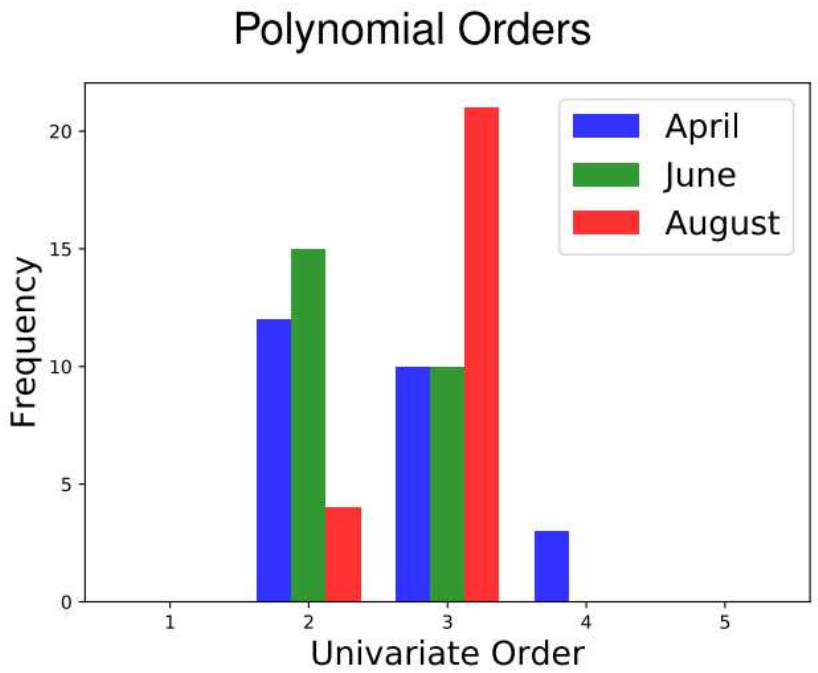
Leaf Area Index (LAI)

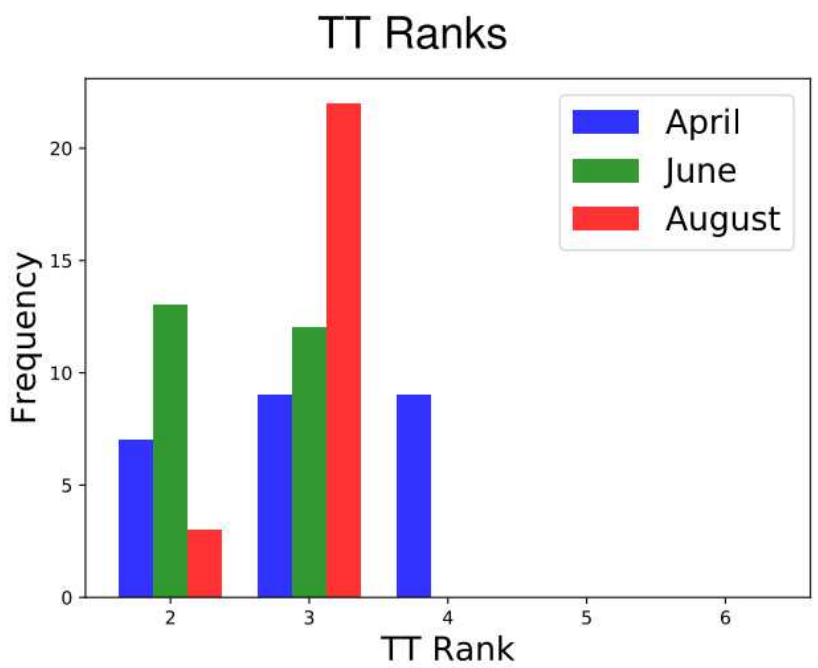




LRFTT Cross-validation: Ranks and Polynomial Orders

Gross Primary Production (GPP)





LRFTT vs Sparse Polynomial Chaos Expansions

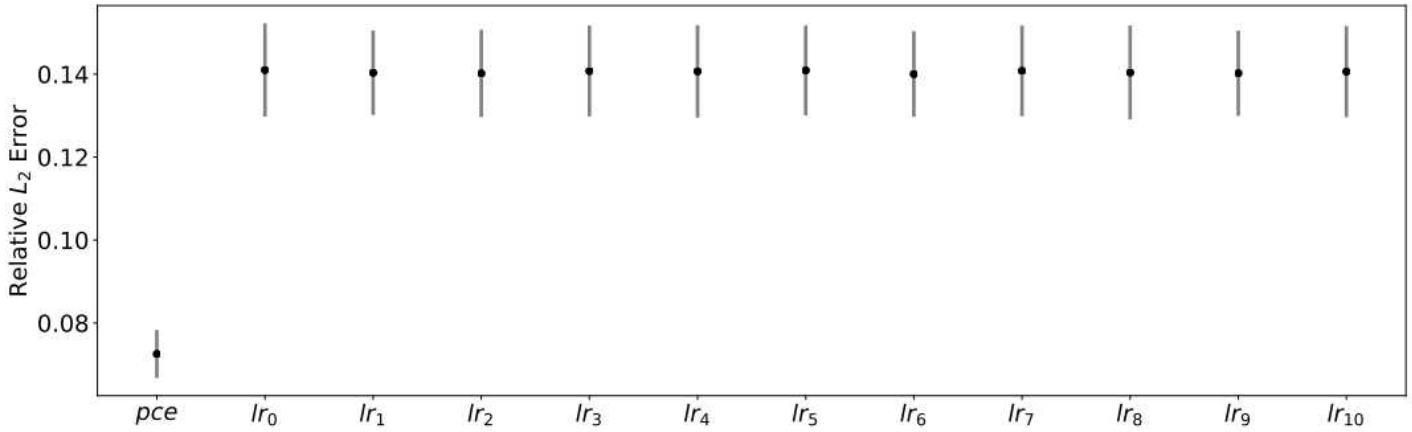
LRFTT: parameter ordering matters $\rightarrow$ explore several permutations

Name	Sequence of processes
lr_0:	**acm, ar, alloc, phen, litter, decomp**
lr_1:	decomp, alloc, acm, ar, phen, litter
lr_2:	phen, decomp, ar, litter, alloc, acm
...	...
lr_5:	alloc, phen, ar, decomp, acm, litter
...	...
lr_8:	ar, alloc, decomp, litter, acm, phen
...	...

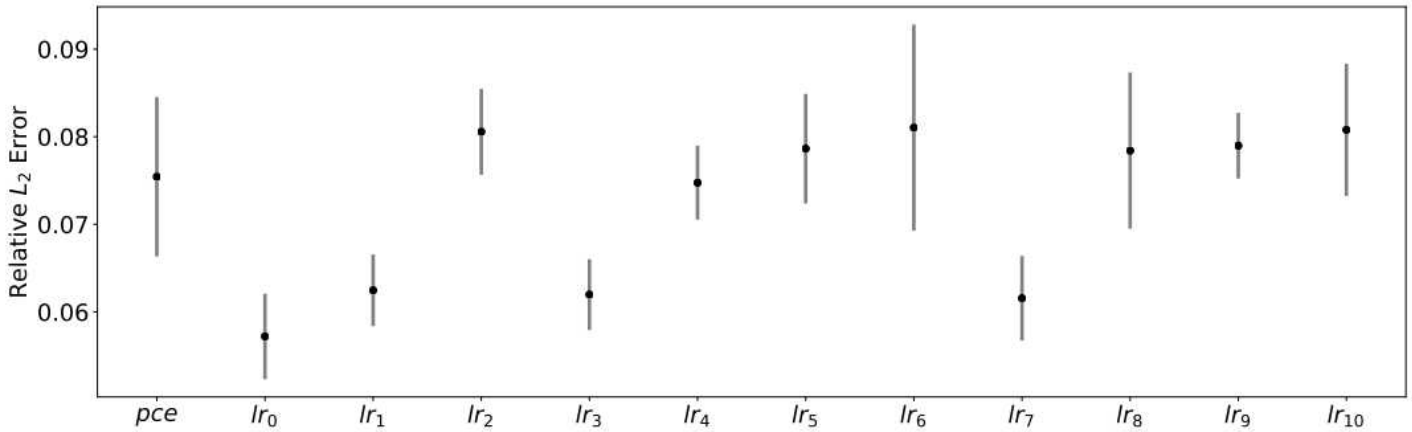
Sparse PCE results denoted as *pce*

GPP Accuracy: LRFTT vs Sparse PCE

April @ US-Ha1

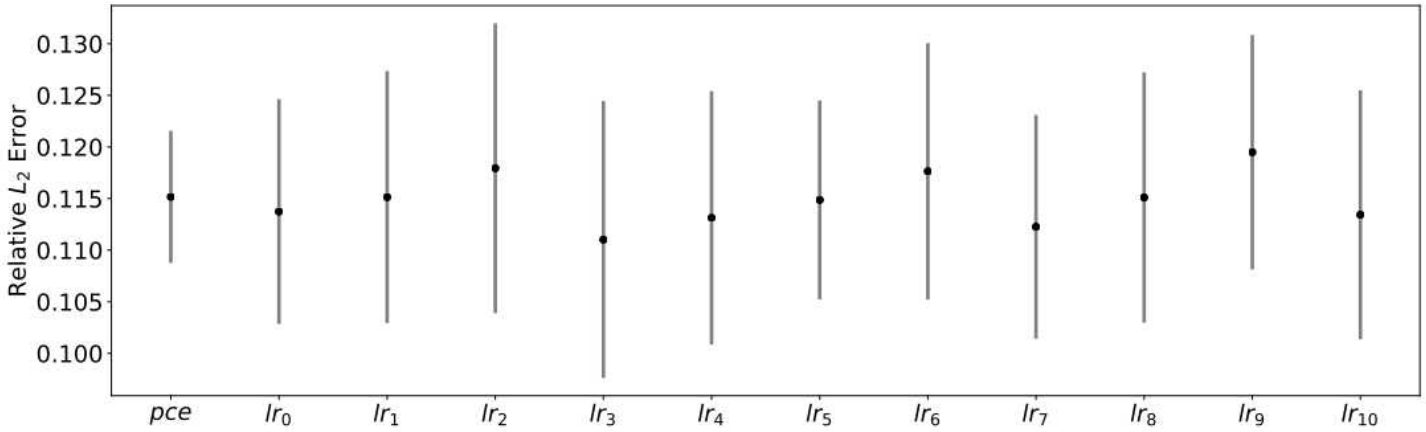


June @ US-Ha1

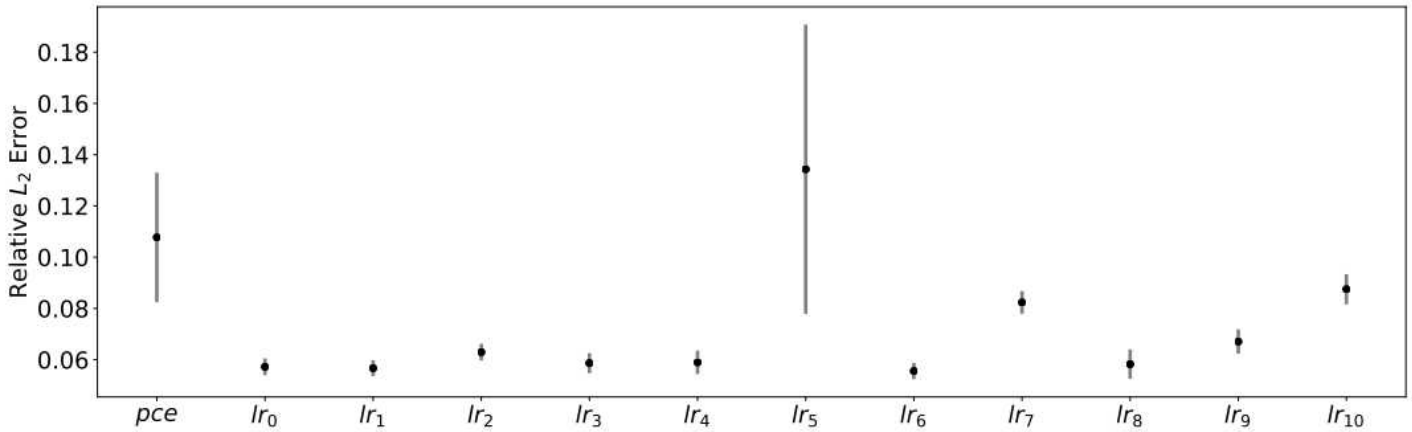


LAI Accuracy: LRFTT vs Sparse PCE

April @ US-Ha1

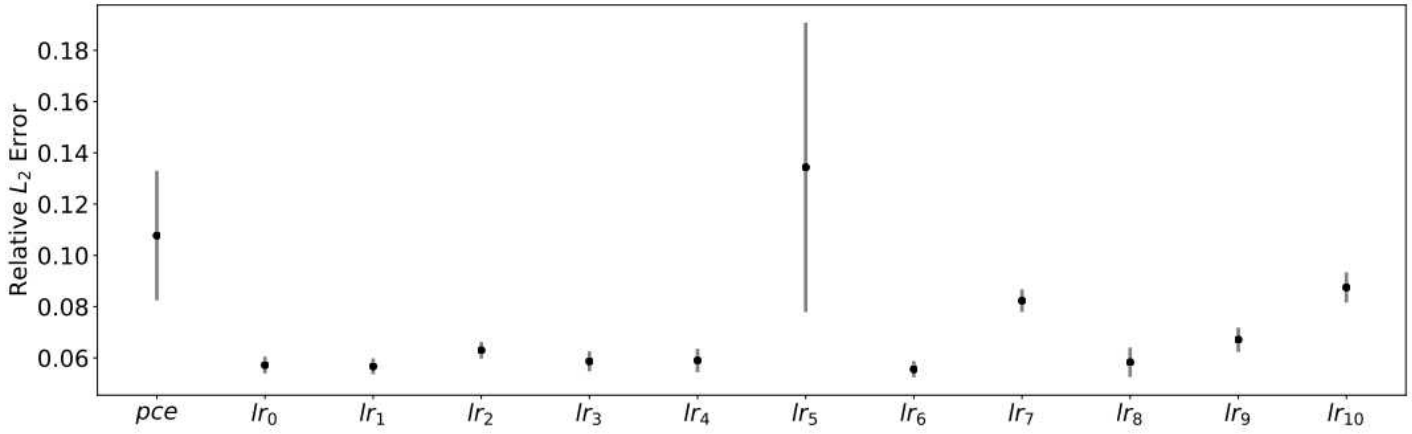


June @ US-Ha1

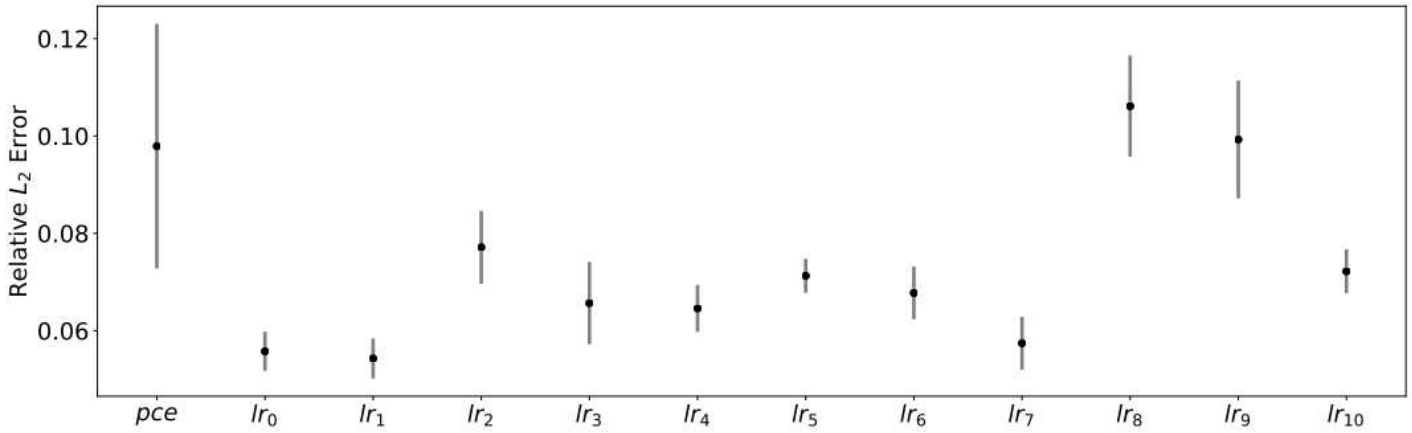


LAI Accuracy: LRFTT vs Sparse PCE

June @ US-Ha1



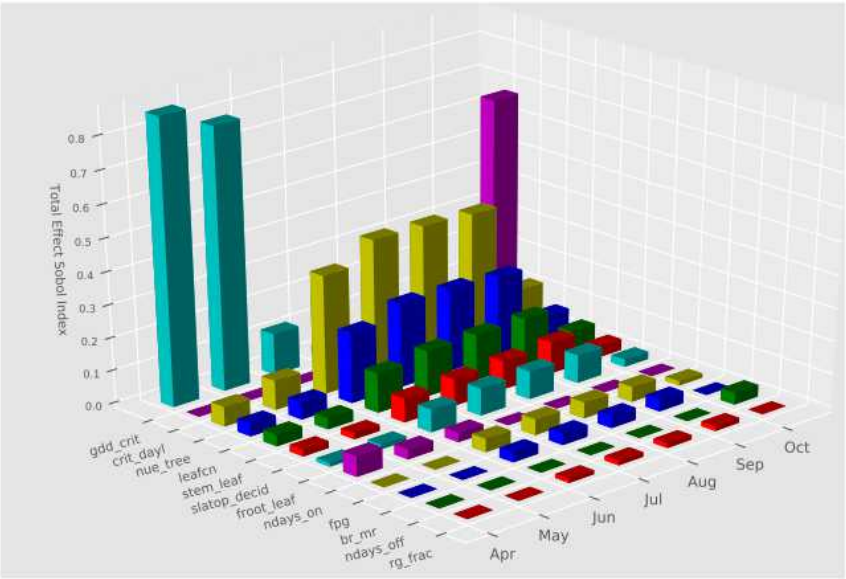
August @ US-Ha1



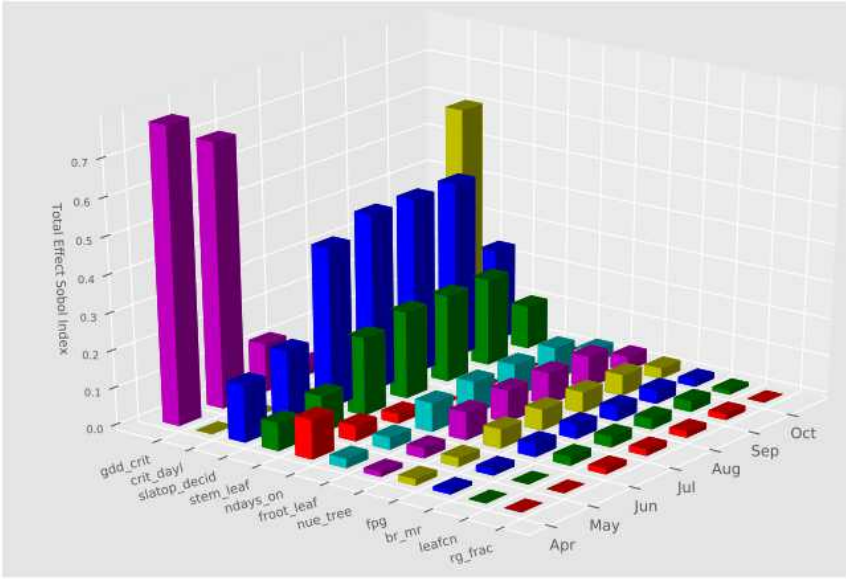
GSA - Total Effect Sobol Indices

- Results corresponding to US-Ha1 site
- Sobol indices correspond to monthly QoI averages over 1980-2009
- Temporal trends match subject matter expert intuition for relevant processes controling GPP and LAI.

GPP



LAI



Summary and Future Work

- Functional low-rank approximations proved efficient in capturing input-output dependencies imposed by land model processes.
    - Land Model is amenable to surrogate modeling via low-rank interactions.
    - For this set of models the low-rank functional approximation performs slightly better compared to a sparse regression polynomial chaos fit.
    - Identified a set of 10-12 parameters (out of 47) which are driving the variance in the selected QoIs.
- Exploring techniques for discovering and folding spatial dependencies (space/time) into the low-rank approximation.