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# Exploiting Low-Rank Structures for Sensitivity Analysis in Earth System Models

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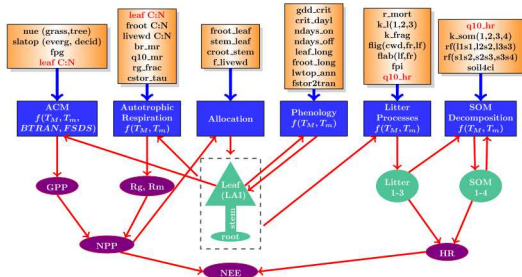
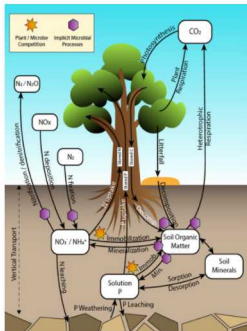
# Outline

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

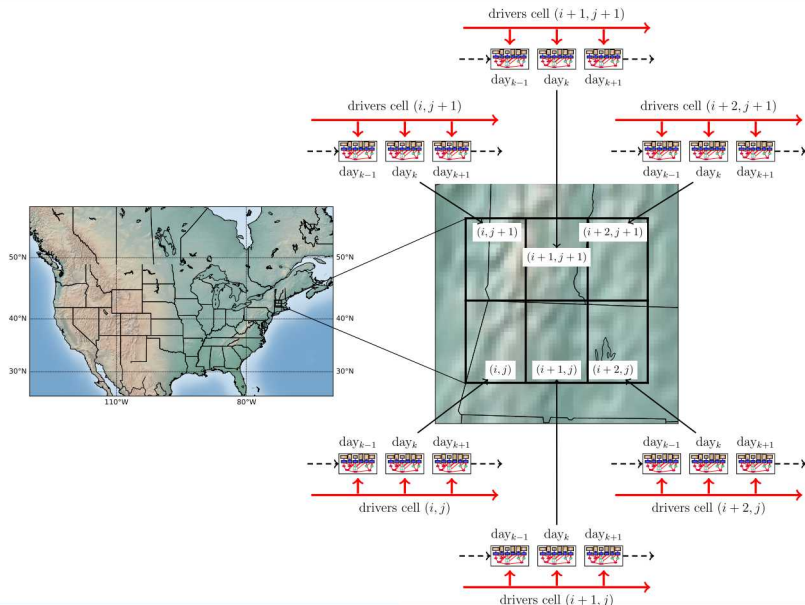
# E3SM Land Model (ELM)



- 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



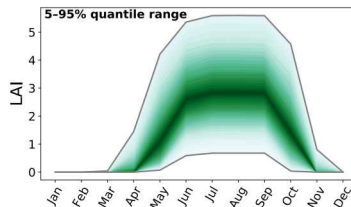
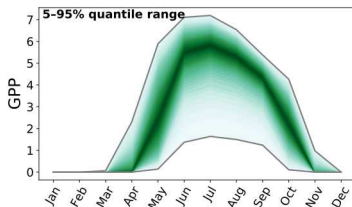
# ELM-LF: Model Workflow



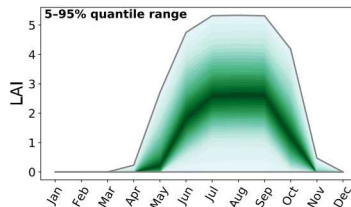
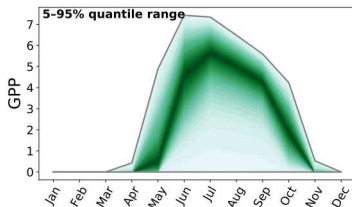
# ELM-LF: Prior Predictive Distributions

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

Harvard Forest EMS Tower ( $42.5^{\circ}\text{N}, 75.2^{\circ}\text{W}$ )



University of Michigan Biological Station ( $45.6^{\circ}\text{N}, 84.7^{\circ}\text{W}$ )

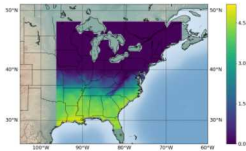


# ELM-LF: Sample Spatial Patterns

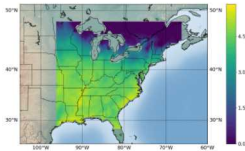
## Gross Primary Production (GPP)

- spatio-temporal patterns for one parameter sample

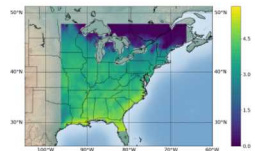
April



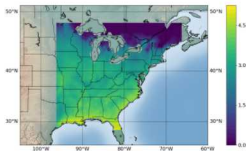
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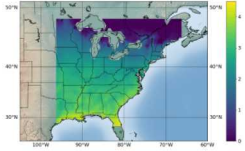
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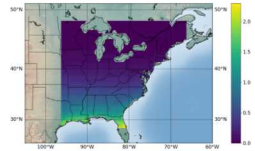
September



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 analogous to low-rank tensor decompositions:

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

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

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

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

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

# 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  $\xi_k$ ,

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

and can be 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  $\xi_k$ ,  $\pi(\xi_k) = 1/2$  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  $\mathbf{y}$  corresponding to a set of choices  $\mathbf{x}$  for the model inputs.

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

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

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

- Quasi-Newton method using L-BBFGS

C<sup>3</sup>: Compressed Continuous Computation library

<https://github.com/goroda/Compressed-Continuous-Computation>

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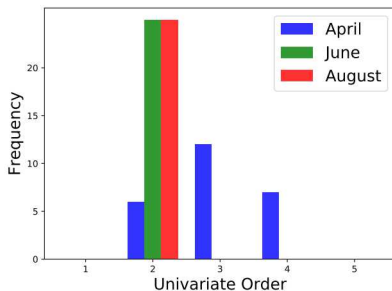
# Sequence of Tests

- 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 → 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) Partitioned into training and testing sets
  - K-fold cross-validation (4 folds)
- Global Sensitivity Sensitivity Analysis Results
  - ELM-LF monthly averages for select Qols: LAI & GPP

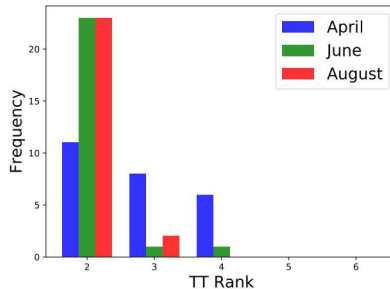
# LRFTT Cross-validation: Ranks and Polynomial Orders

*Leaf Area Index (LAI)*

Polynomial Orders

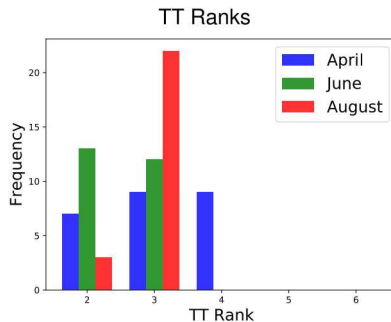
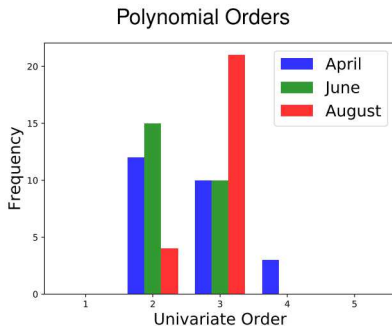


TT Ranks



# LRFTT Cross-validation: Ranks and Polynomial Orders

## *Gross Primary Production (GPP)*





# LRFTT vs Sparse Polynomial Chaos Expansions

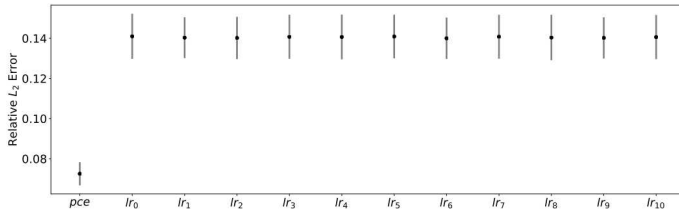
LRFTT: parameter ordering matters → explore several permutations

Name	Sequence of processes
$lr_0$ :	<b>acm, ar, alloc, phen, litter, decomp</b>
$lr_1$ :	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
...	...

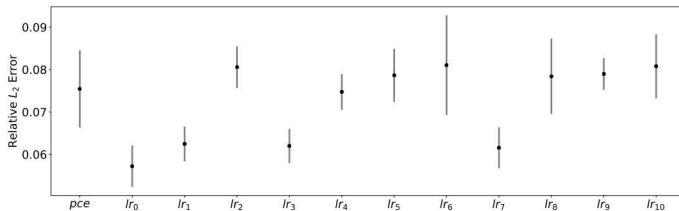
Sparse PCE results denoted as *pce*

# GPP Accuracy: Sparse PCE vs LRFTT

April @ US-Ha1

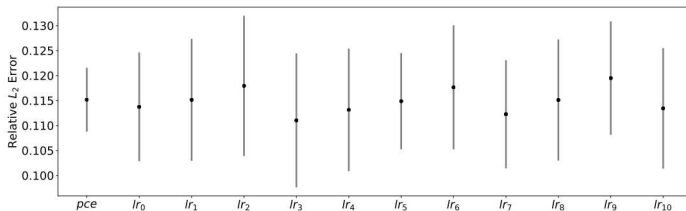


June @ US-Ha1

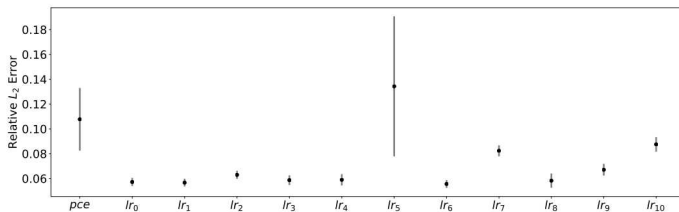


# LAI Accuracy: Sparse PCE vs LRFTT

April @ US-Ha1

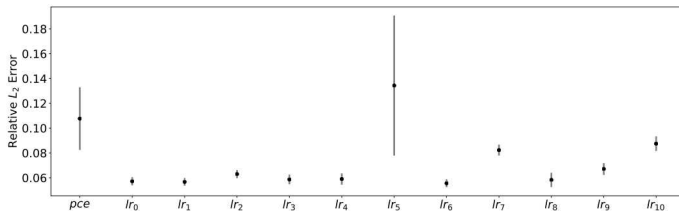


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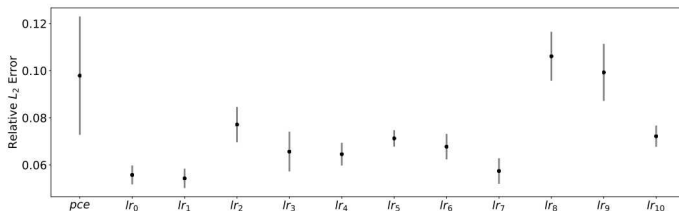


# LAI Accuracy: Sparse PCE vs LRFTT

June @ US-Ha1



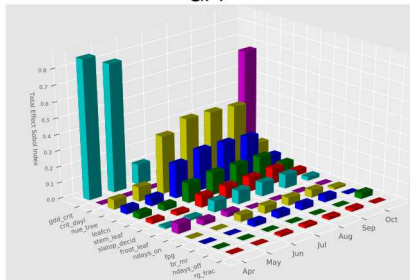
August @ US-Ha1



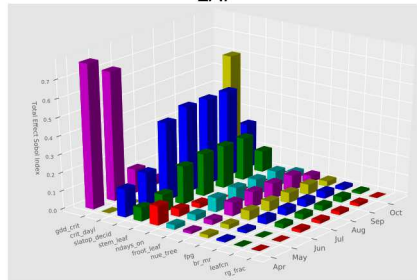
# GSA - Total Effect Sobol Indices

- 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 controlling 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.