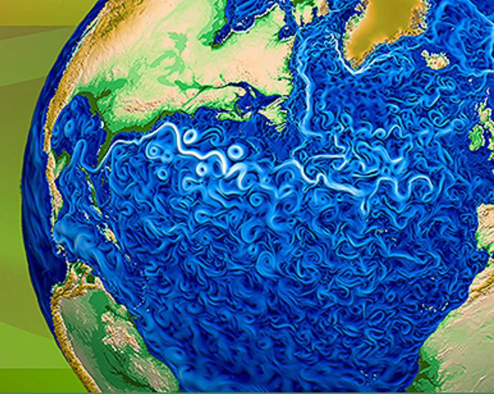

ACME
Accelerated Climate Modeling for Energy

Climate Change Science Institute
Oak Ridge National Laboratory

Quantifying the Impacts of Parametric Uncertainty on Biogeochemistry in the ACME Land Model

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ACME All-Hands, Land Group

U.S. DEPARTMENT OF ENERGY

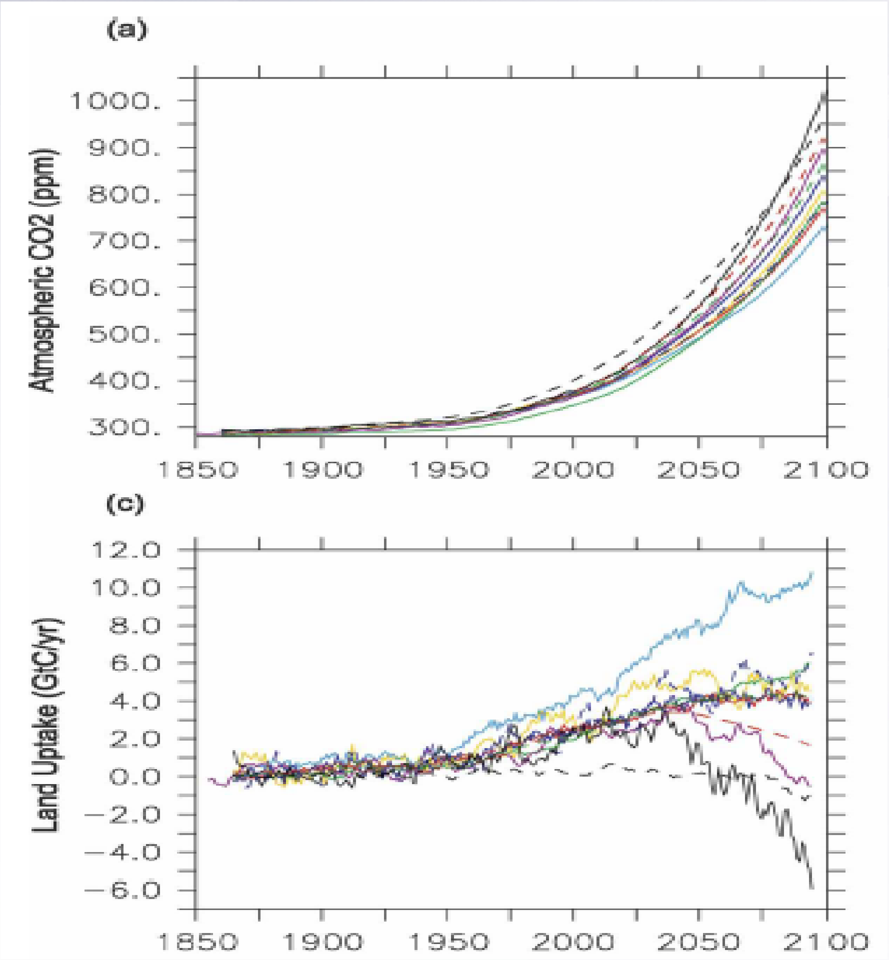
Overview and motivation

- Traditionally, uncertainty has been estimated using multi-model comparisons
- Large uncertainties about future carbon flux

Challenges:

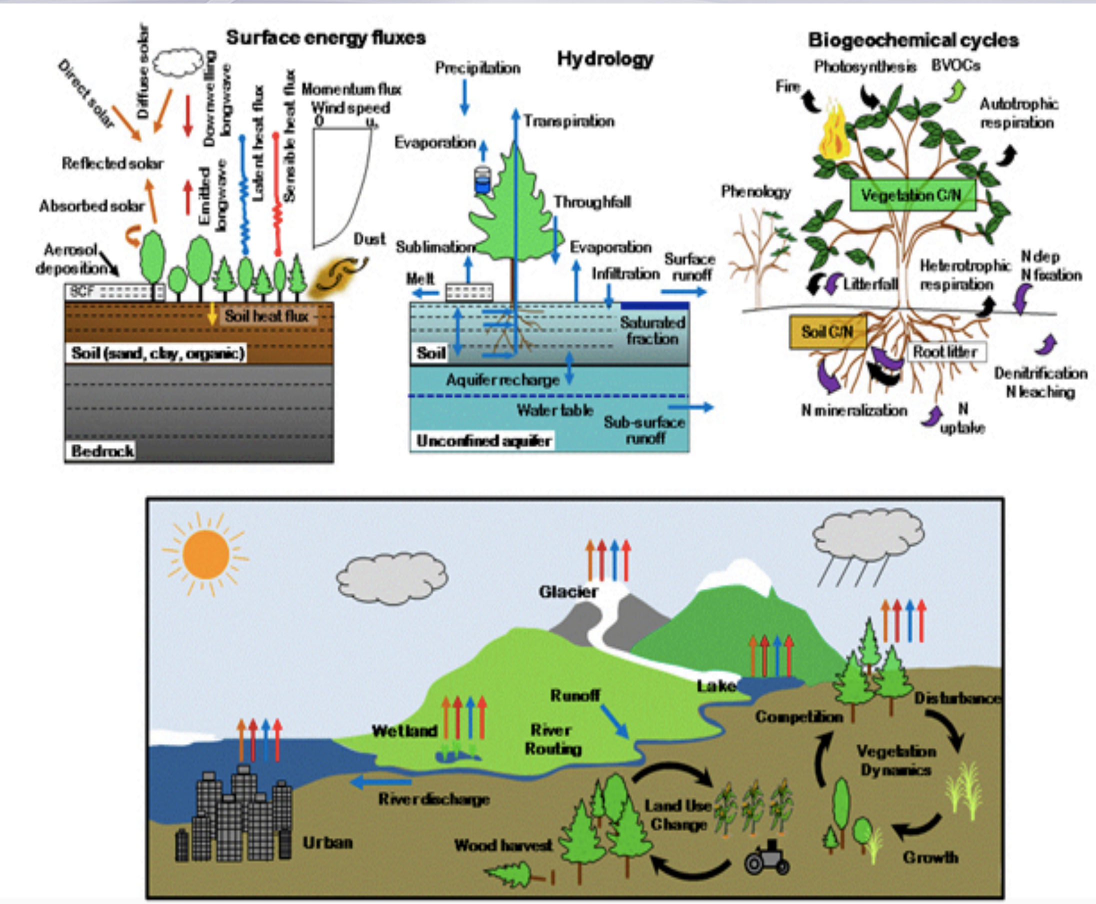
- We need to characterize within-model uncertainties better
- Understand which parameters are the key drivers of uncertainty for given outputs
- Improve model predictive skill using calibration

- Need for formal UQ methods



Friedlingstein et al 2014

Overview and motivation



- ALM is an increasingly complex model with many processes
- Slow evaluation time, poor scaling
- Large ensembles are needed for UQ
- Surrogate models can increase the efficiency of sensitivity analysis and calibration

Major 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

Black Box

$$Y = f(X)$$

Surrogate models are needed for computationally intensive tasks:

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

$$f(X) \approx f_{surr}(X)$$

Polynomial Chaos is the main workhorse

PC provides convenient means of representing model inputs and outputs in a probabilistic way.

$$X = \sum_{k=0}^{P-1} a_k \Psi_k(\xi) \qquad \boxed{Y = f(X)} \qquad Y = \sum_{k=0}^{P-1} c_k \Psi_k(\xi)$$

ξ are standard variables (uniform, normal)

$\Psi_k(\cdot)$ are standard orthogonal polynomials (Legendre, Hermite)

- Think of Fourier-type expansions, only w.r.t. polynomials.
- Uncertain inputs X and outputs Y are represented via vectors of PC modes a_k and c_k

Polynomial ~~Chaos~~ Surrogate,
a.k.a. fit the function

Simplest scenario: parameters are given up to expert-defined ranges

$$X_i \in [a_i, b_i] \qquad\qquad X_i = \frac{a_i+b_i}{2} + \frac{b_i-a_i}{2}\xi_i$$

Now ξ_i is Uniform[-1,1],

and X_i is a Legendre-Uniform PC of 1-st order,

surrogate is simply a polynomial fit

$$\boxed{Y = f(X)} \quad \approx \quad \boxed{Y = \sum_{k=0}^{P-1} c_k L_k(X)}$$

[Probabilistic interpretation remains: inputs X are uniform random variables.]

Polynomial surrogate construction

$$Y = f(X) \quad \approx \quad g_c(X) = \sum_{k=0}^{P-1} c_k L_k(X)$$

- Non-intrusive (black-box) setting: $f(X)$ is a Land Model output QoI
- Evaluate at training points $y_i = f(X_i)$, for $i=1, \ldots, N$.
- Compute c_k's using least-squares minimization
  with measurement matrix $G_{ik} = L_k(x_i)$

$$\min_c \sum_{i=1}^{N} [f(X_i) - g_c(X_i)]^2 = \min_c \| f - Gc \|$$

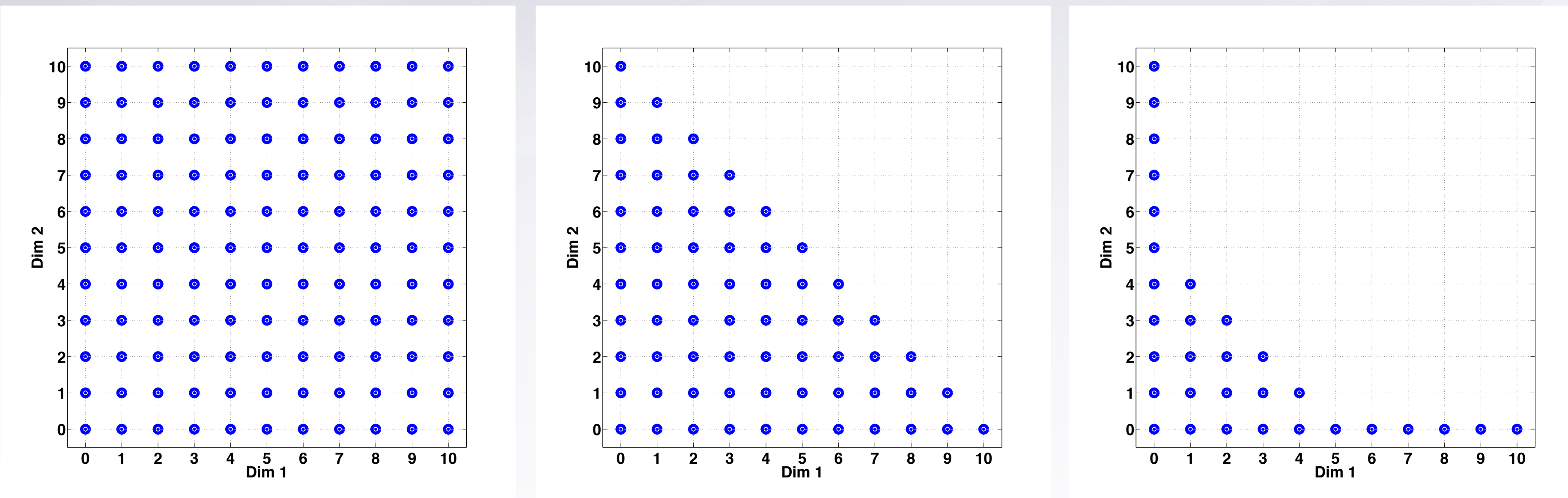
- ***Bayesian inference:*** more flexible, provides errorbars on c

Multivariate polynomial basis

$$g_c(X) = \sum_{k=0}^{P-1} c_k L_k(X) \qquad L_k(X_1, X_2, \ldots, X_d) = L_{p_1}(X_1) L_{p_2}(X_2) \cdots L_{p_d}(X_d)$$

Key challenge: how to truncate polynomial expansion?

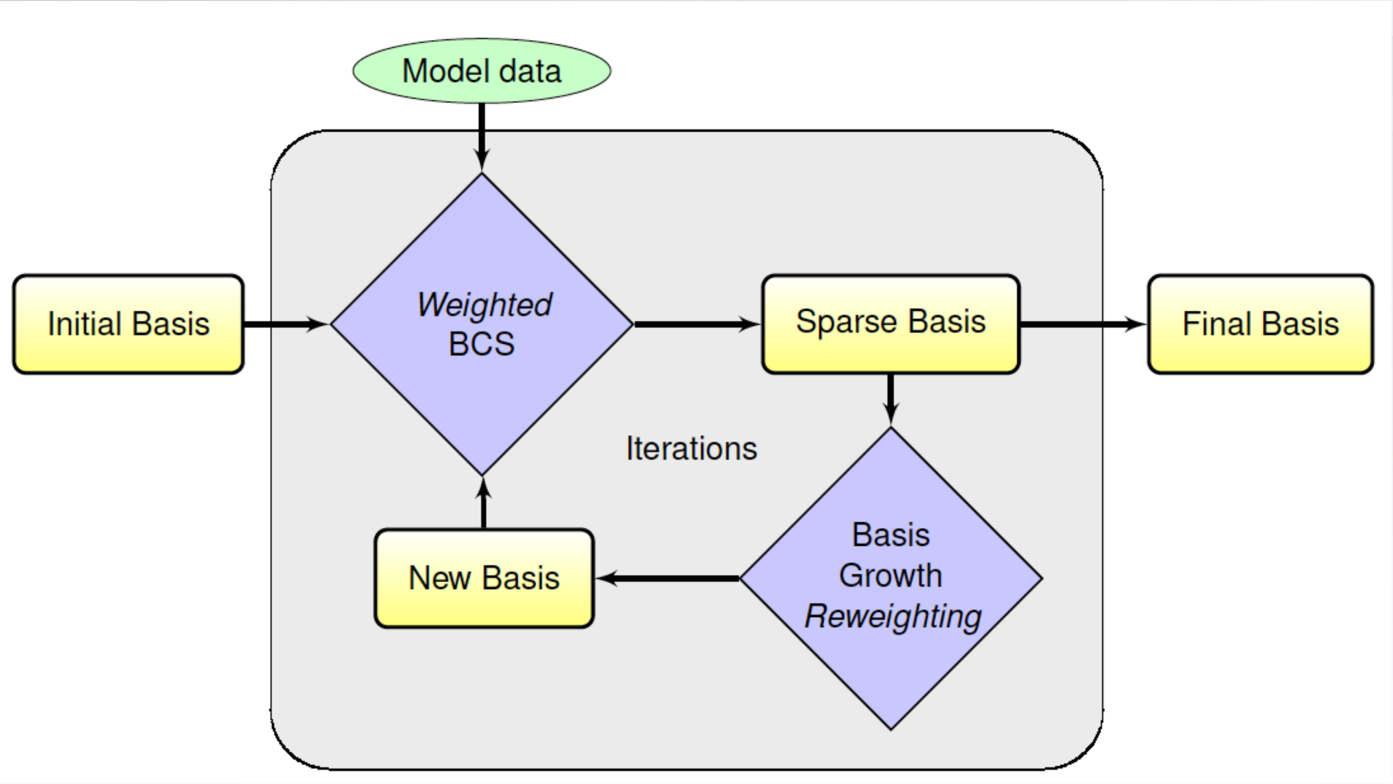
in high-dimensional cases, often *N*<*P*.



(Bayesian) Compressed Sensing helps find the sparsest signal,
***i.e.* selects as few polynomial terms as possible.**

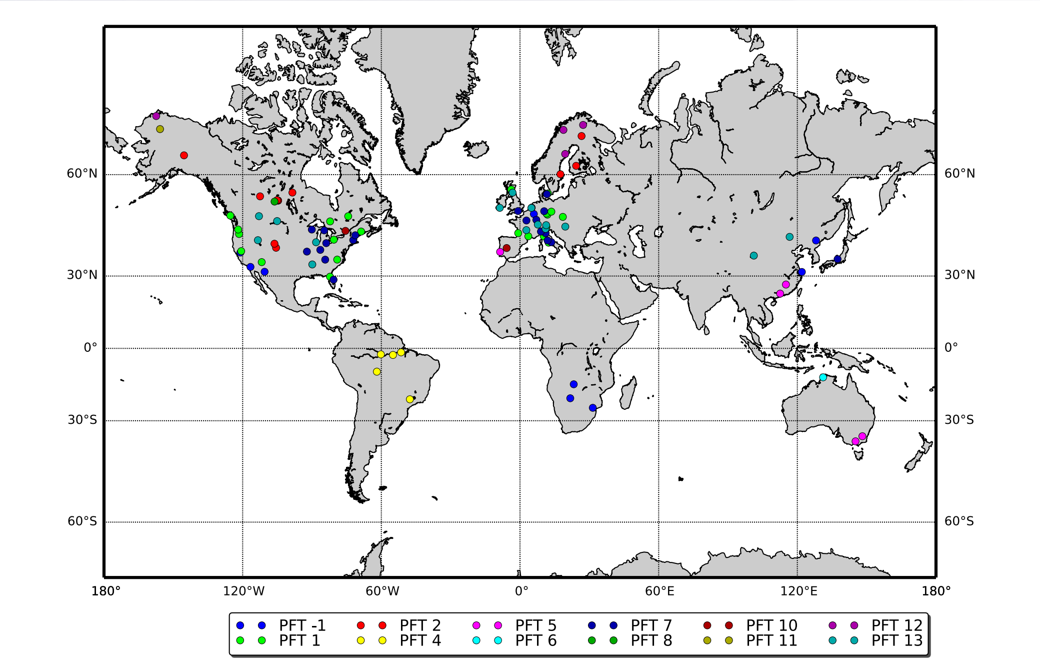
Major UQ challenge: High-dimensionality

… so we start from a smaller basis and iteratively grow it [Sargsyan et al., 2014].



FLUXNET sensitivity analysis: ALM-CN

- 96 FLUXNET sites covering major biomes and plant functional types
- 68 input parameters varied over uniform prior ranges
- 3000 simulations on Titan
- Surrogate construction and sensitivity analysis with Bayesian Compressive Sensing (Sargsyan et al., 2014)
- Site-specific PFT, but reanalysis forcings/soil properties



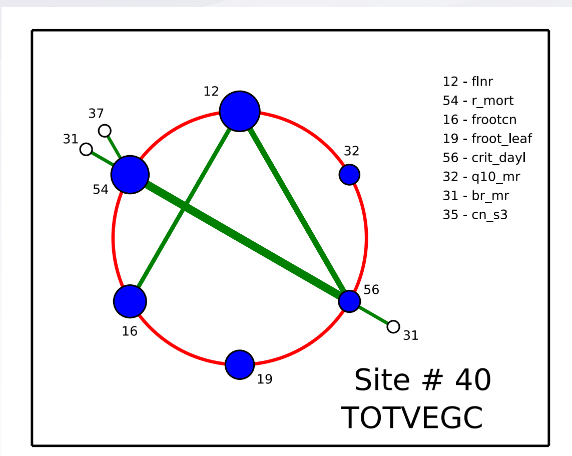
- Ensemble of 3000 runs in 68-dimensions is extremely scarce information
- BCS leads to polynomial fits with only 200 terms
- Surrogate is not too accurate, but sensitivity analysis is meaningful

Output uncertainty decomposition

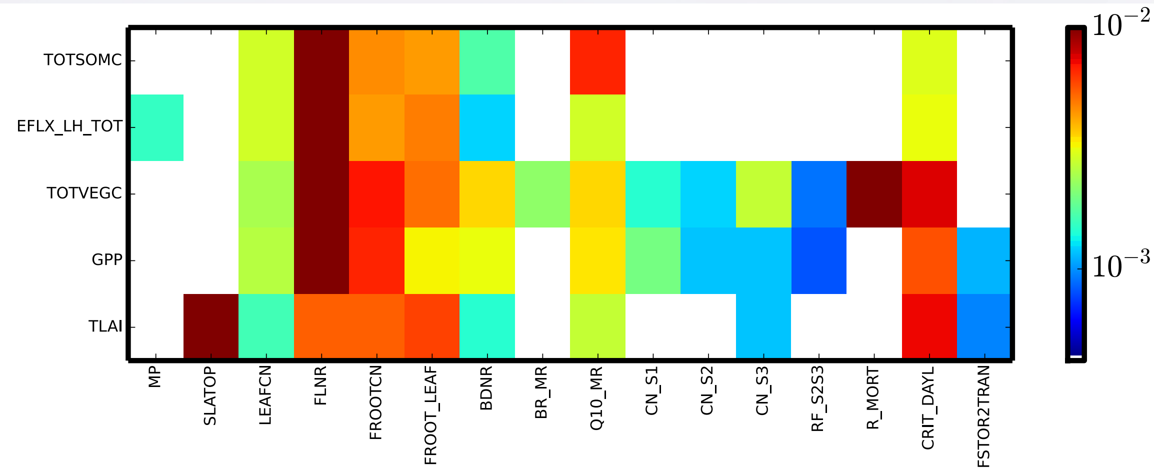
… otherwise called

- Global Sensitivity Analysis (GSA)
- Sobol sensitivity indices
- Variance-based decomposition
- similar to ANOVA-decomposition

PC surrogate gives easy access for fractional variance contributions to output uncertainties.



Parameter down-selection (68 to 10-20)

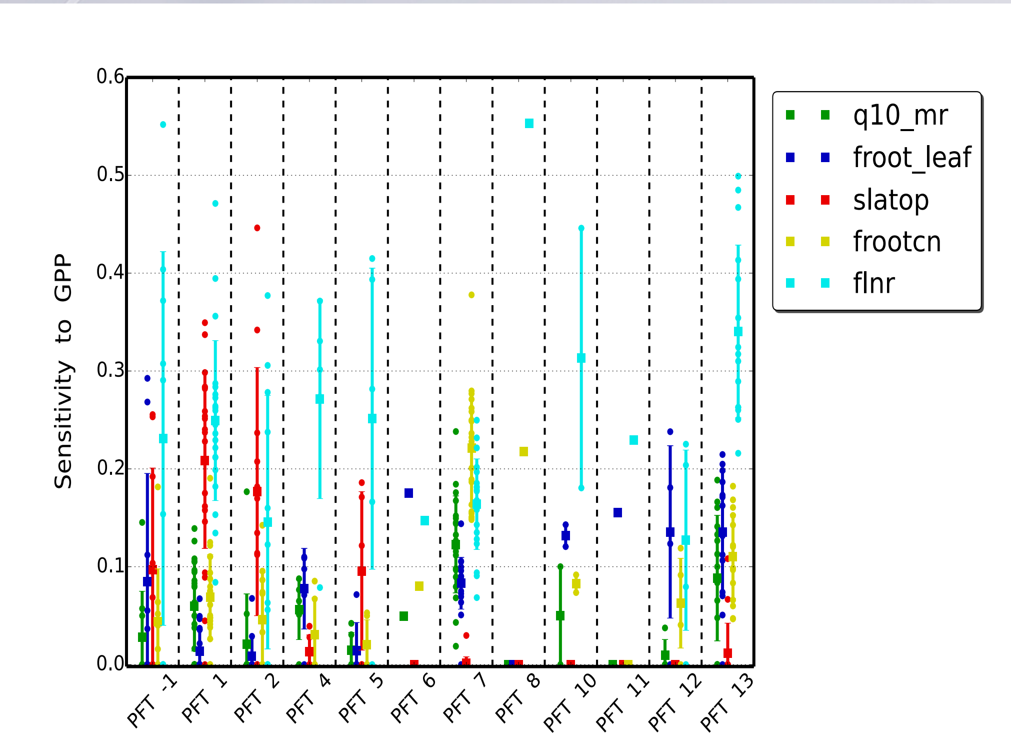


Site #40, Harvard Forest, US

Forward UQ Summary

- Global parametric surrogate is not very accurate (~30%), but that is as good as one can hope with a 65-d space and 3K runs
- It is still good enough to extract the major players, i.e. the highest main and joint sensitivities
- Paper in preparation on the Weighted Iterative Bayesian Compressive Sensing + Multisite Surrogate/Sensitivity Analsys
- For calibration purposes, one needs to have adaptive, localized surrogates that are more accurate
- Multi-output (site, QoI) forward UQ implemented in python scripts employing UQTk (www.sandia.gov/uqtoolkit)
- Git repository ACME/Uncertainty-Quantification
- Hackathon this Friday!

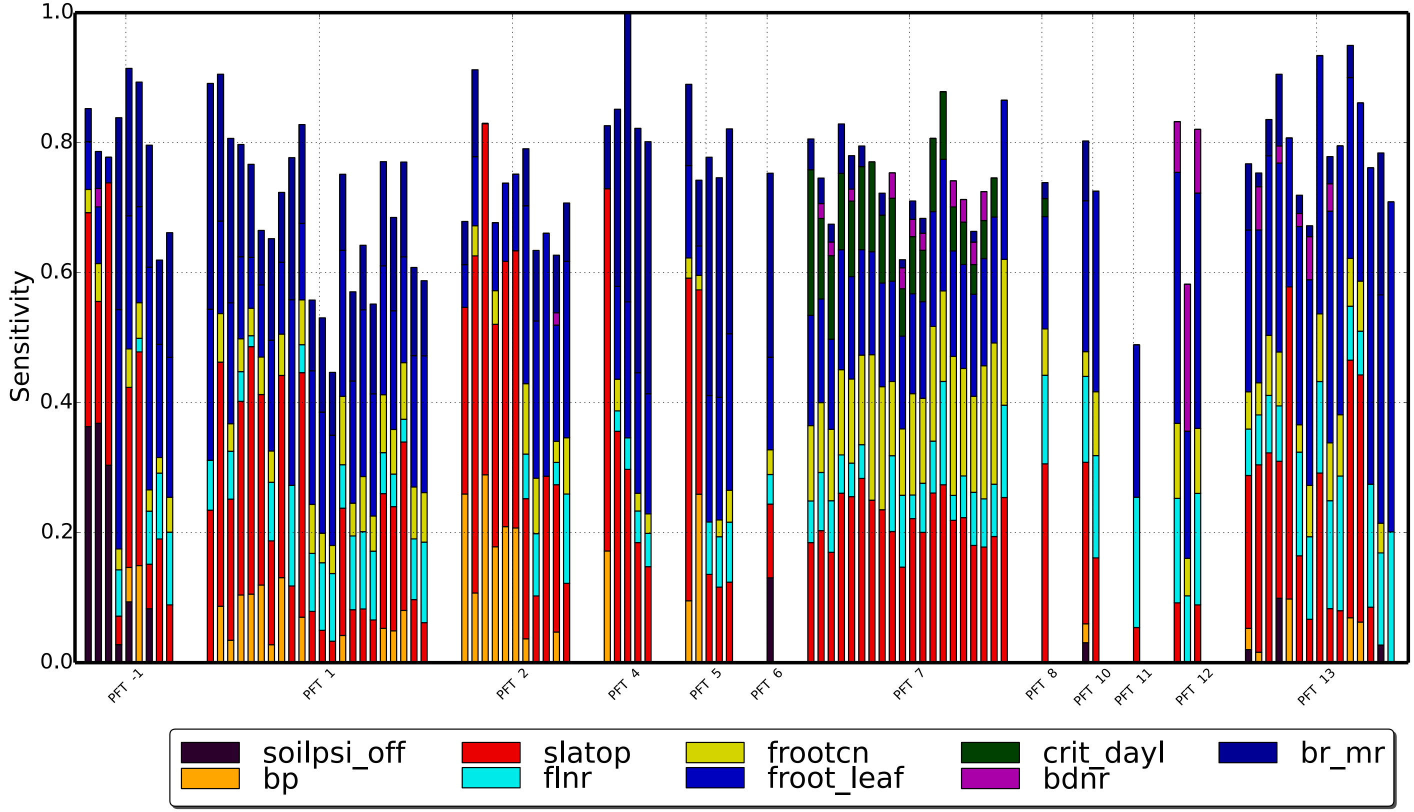
Sensitivity analysis: Interpreting the results



- Some parameters are sensitive everywhere (flnr)
- Maintenance respiration base rate (br_mr) is critically important in tropical rainforests but not in other ecosystems.
- Relative consistence within PFTs

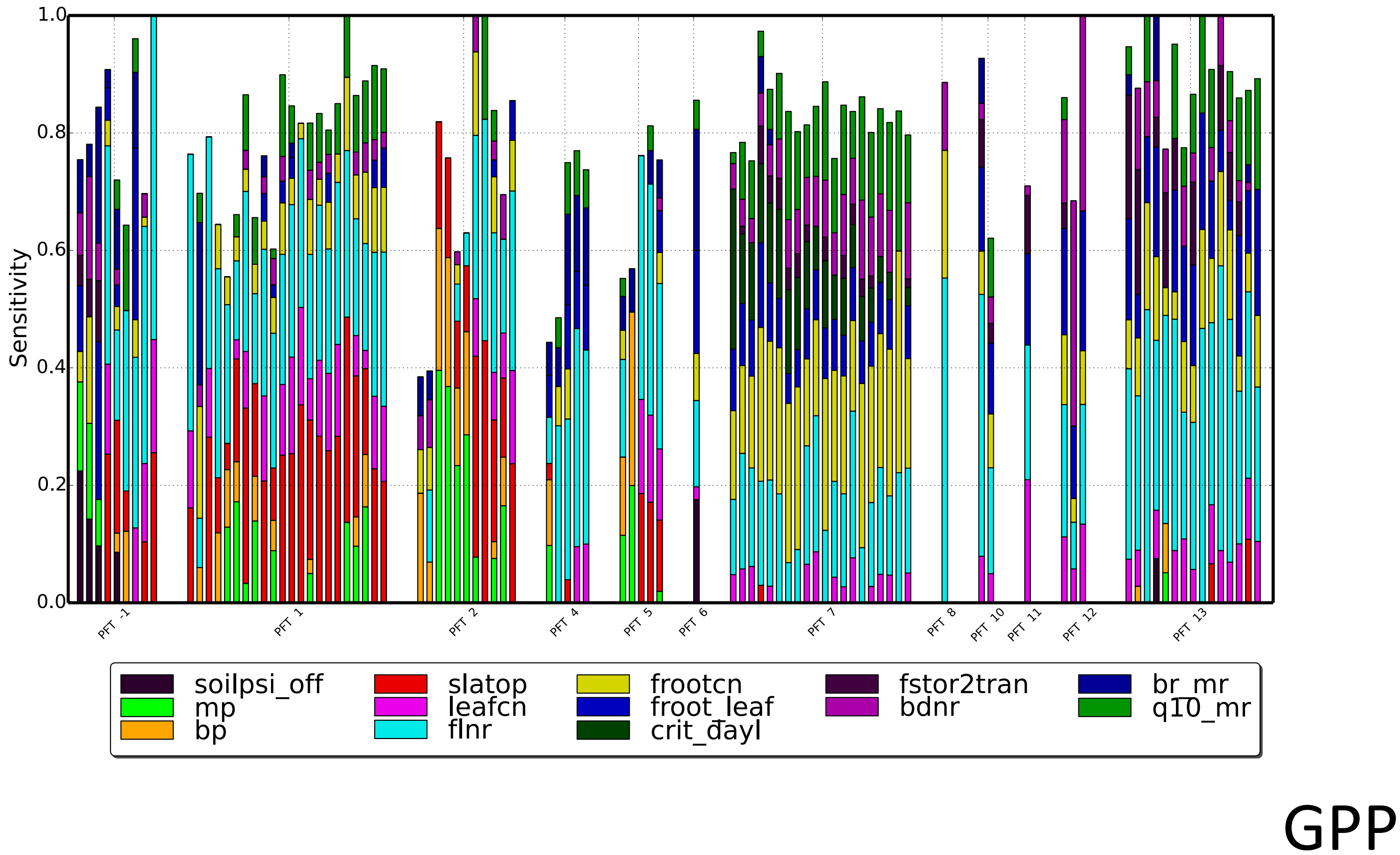
- Can provide guidance about where specific measurements or data are more valuable
- Reduction of parameter space for optimization

Multisite analysis

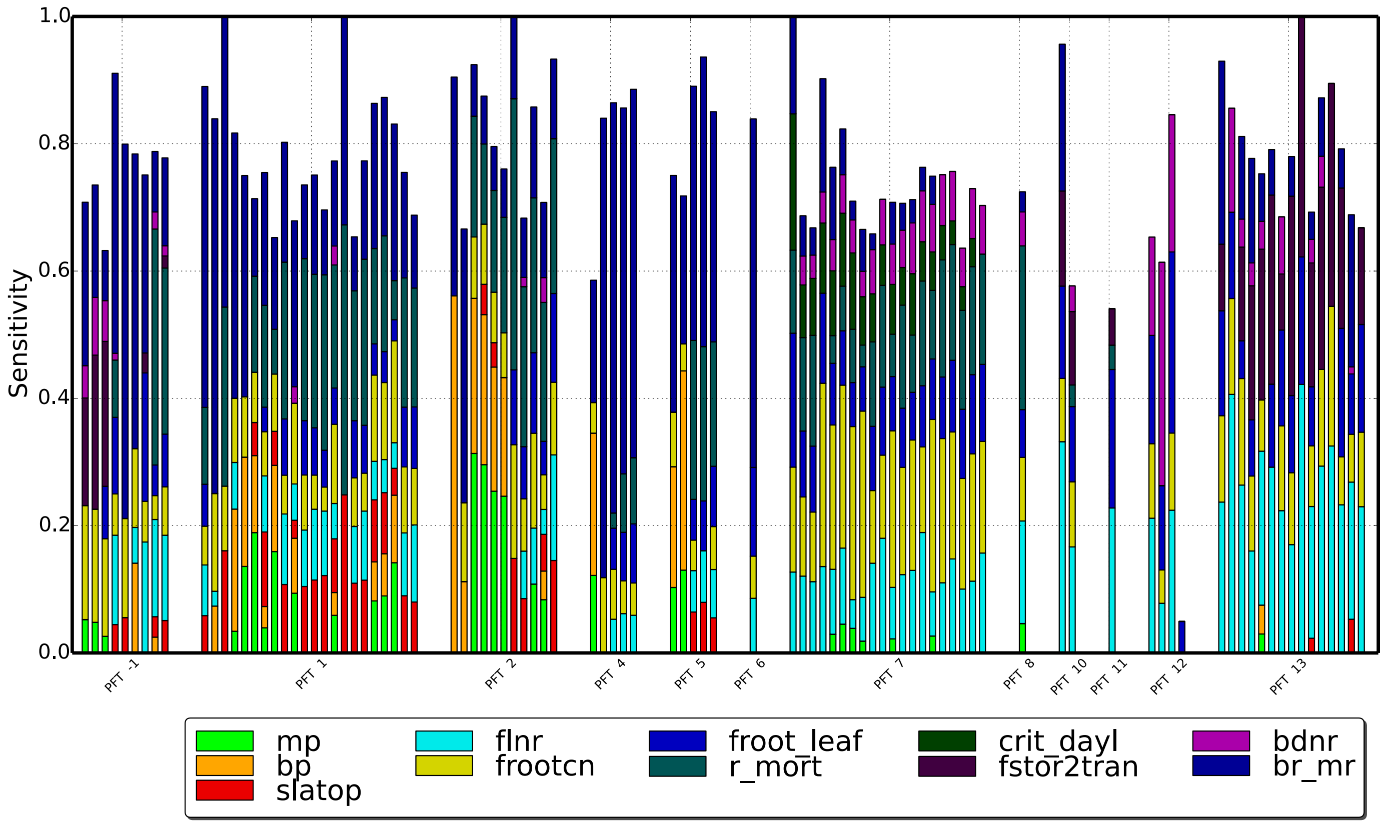


TLAI

Multisite analysis

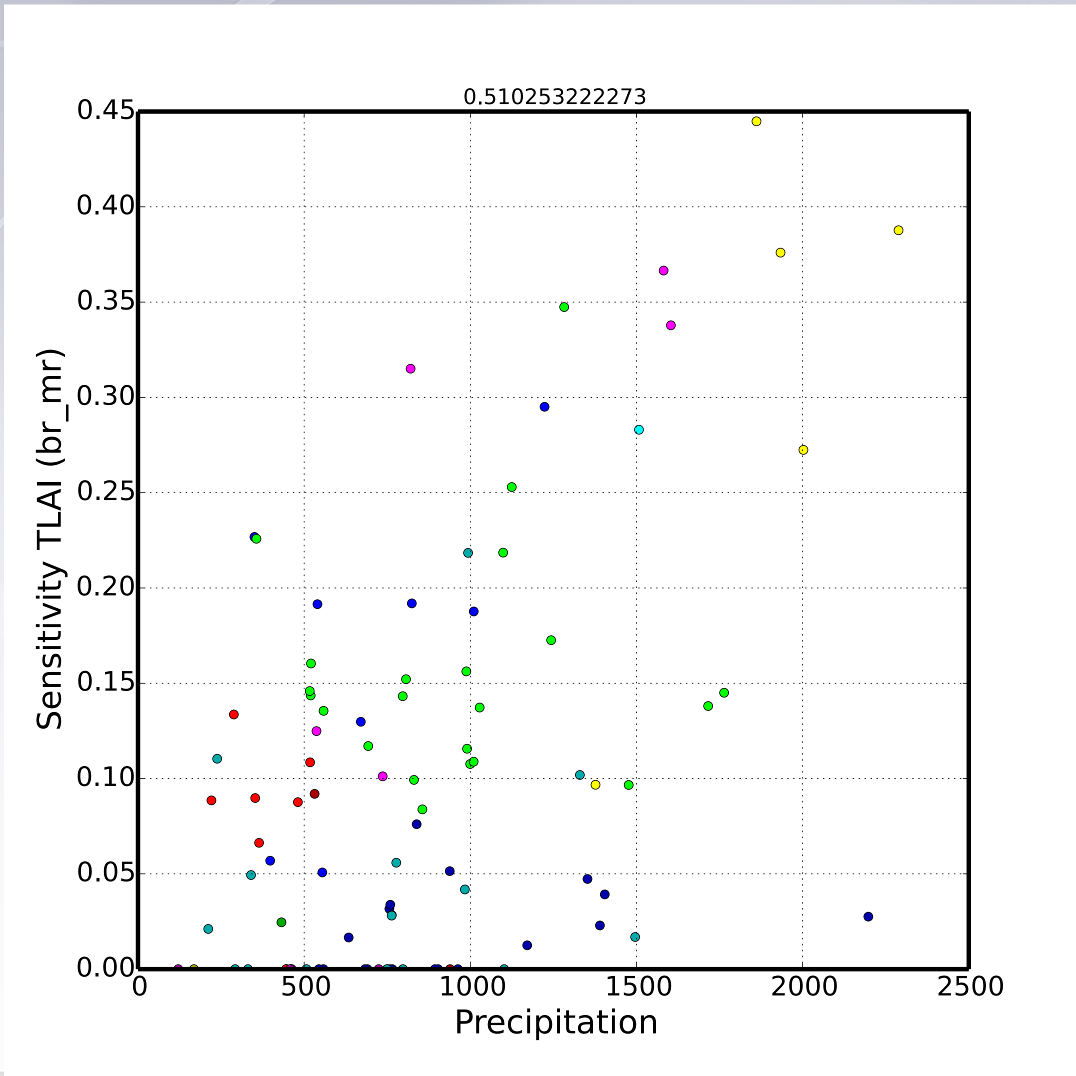


Multisite analysis



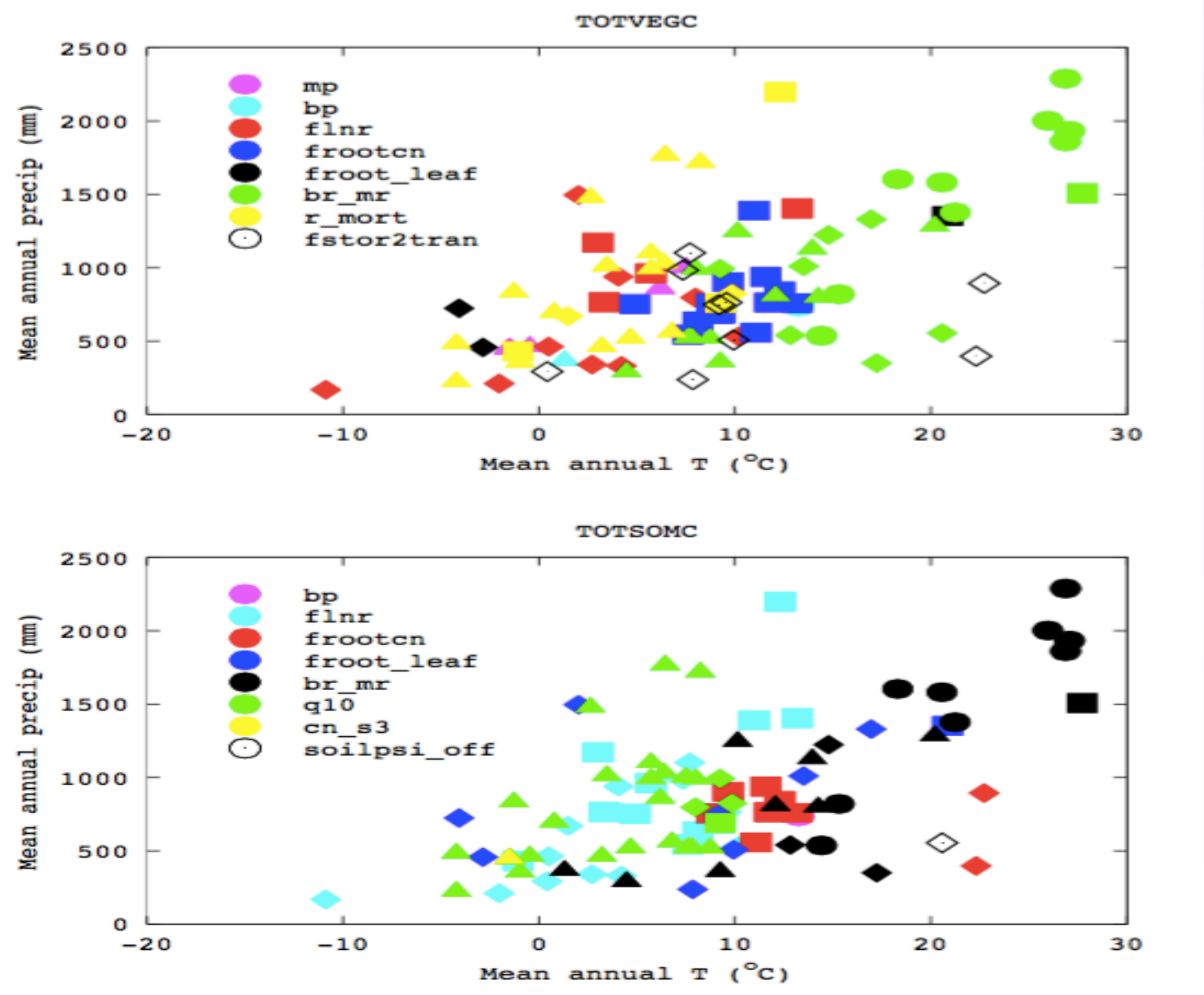
TOTVEGC

Correlations with climate variables



- The sensitivity of some parameters is correlated with climate variables
- Illustrates how some mechanisms are relatively more important in specific conditions
- Example: sensitivity of maintenance respiration base rate to mean annual precipitation

Parameter sensitivity in climate space



UQ, optimization and benchmarking

- Sensitivity analysis: Determining which model parameters are sensitive for given QoIs, timescales
  - Examining coherence of sensitivity within and among PFTs
  - Using trait databases to guide model experiments
  - Dependence on model structure (testing model versions)
- Ensemble benchmarking
  - Consider parameter, driver, and structural uncertainty (compare PDFs of scores rather than individual numbers)
- Model calibration: Improving predictions
  - Multivariate optimization, use of emergent constraints
  - Independent data must be reserved for validation/benchmarking
  - Complex LSMs require sophisticated approaches
  - Opportunity for standardization of workflows