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Weighted Iterative Bayesian Compressive Sensing (WIBCS) for High Dimensional Polynomial Surrogate Construction

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Goal: Parametric Uncertainty Quantification

Quantify uncertainties due to parameter variability in high-dimensional, computationally expensive physical models.

Key: Build a Surrogate Model

$G(x) \approx g_c(x)$ **... otherwise called metamodel, proxy, response surface, emulator.**

- Surrogate approximation to input-output map
- Computationally inexpensive to evaluate
- Replaces the model in forward UQ (parametric UQ, global sensitivity analysis) and inverse UQ (calibration, optimization, tuning)

Polynomial chaos (PC) as a surrogate model.

- Interprets input parameters as random variables
- Propagates input uncertainties to outputs of interest, e.g.,

$$x_i \sim \text{Uniform}[a_i, b_i] \quad \Rightarrow \quad x_i = \frac{a_i + b_i}{2} + \frac{b_i - a_i}{2}\xi_i.$$

Output is represented with respect to Legendre polynomials of standard input $\xi_i \sim \text{Uniform}[-1, 1]$

$$G(x(\xi)) \approx g_c(\xi) \equiv \sum_{k=0}^{K} c_k \Psi_k(\xi).$$

Challenge: High Dimensionality

- Large number of input parameters, $x \in \mathbb{R}^d$ with $d \sim 30$ or above
- Model is expensive; $N \gg 1$ simulations of $G(x)$ are required
- Truncation of PC is challenging; too many basis terms $K > N$

- **Compressive sensing** allows learning sparse polynomial expansion and deals with high-dimensionality
- **Bayesian inference** works with any number of model simulations and constructs uncertain surrogate

Weighted Iterative Bayesian Compressive Sensing

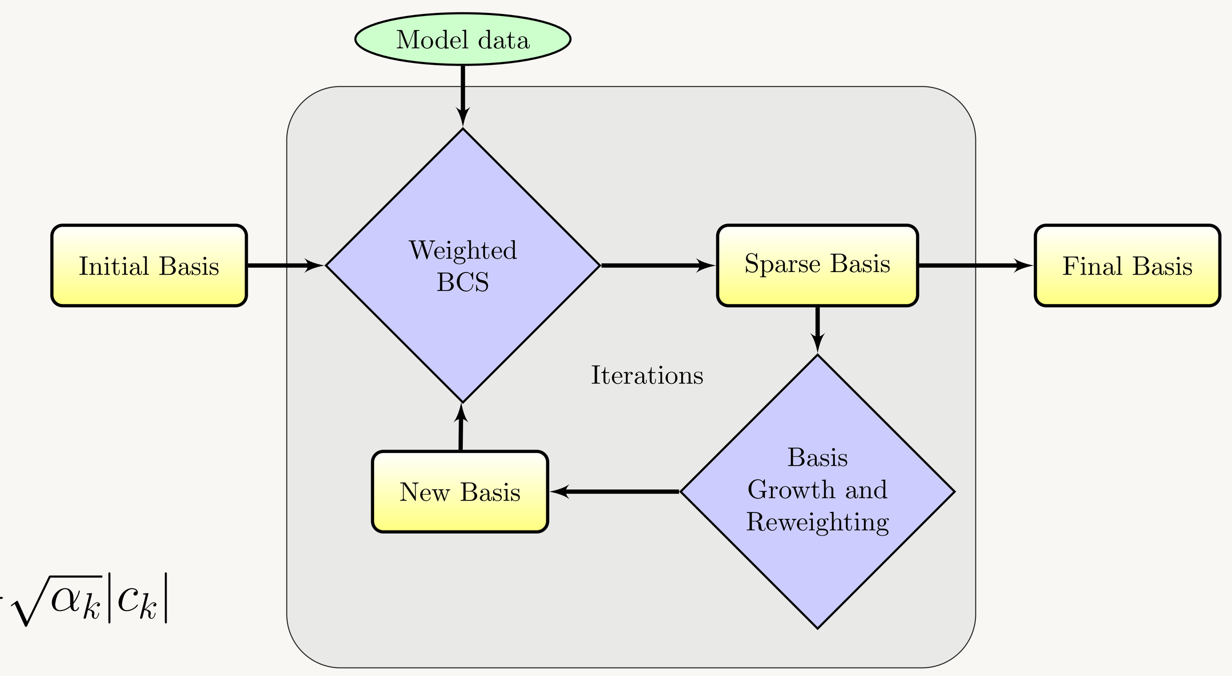
Bayesian inference of PC coefficients: $\underbrace{p(c|\mathcal{D})}_{\text{Posterior}} \propto \underbrace{L_{\mathcal{D}}(c)}_{\text{Likelihood}} \underbrace{p(c)}_{\text{Prior}}$

- Gaussian likelihood:

$$L_{\mathcal{D}}(c) = \prod_{i=1}^{N} \frac{1}{\sqrt{2\pi}s} \exp\left(-\frac{(G(x_i) - g_c(\xi_i))^2}{2s^2}\right)$$

- Hierarchical Laplace prior:

$$p_\alpha(c) = \int \prod_{k=0}^{K-1} \underbrace{p(c_k|\sigma_k^2)}_{\text{Gaussian}} \underbrace{p_\alpha(\sigma_k^2)}_{\text{Gamma}} d\sigma_k^2 = \prod_{k=0}^{K-1} \frac{\sqrt{\alpha_k}}{2} e^{-\sqrt{\alpha_k}|c_k|}$$



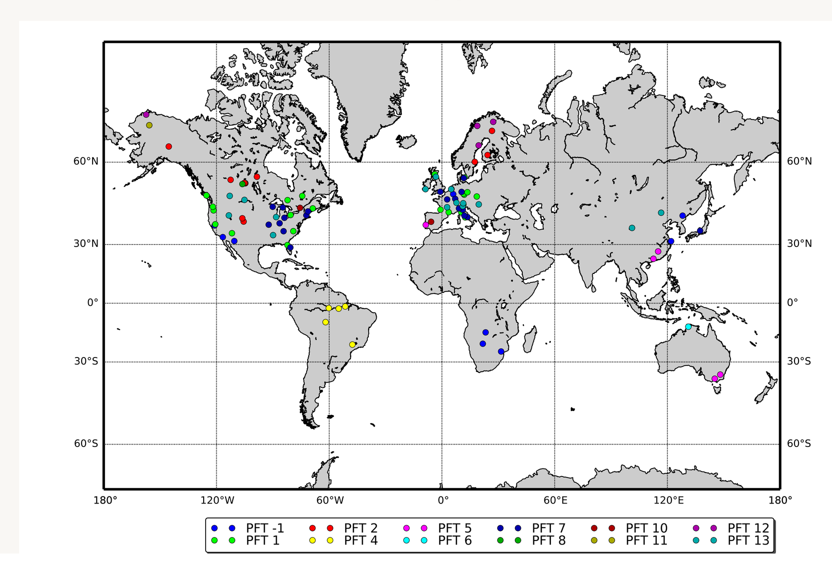
- **Weighted** Laplace prior, hyperparameter vector α_k
- **Iterative growth** of polynomial bases to capture high order terms
- Implemented in **UQTk** software library (www.sandia.gov/uqtoolkit)

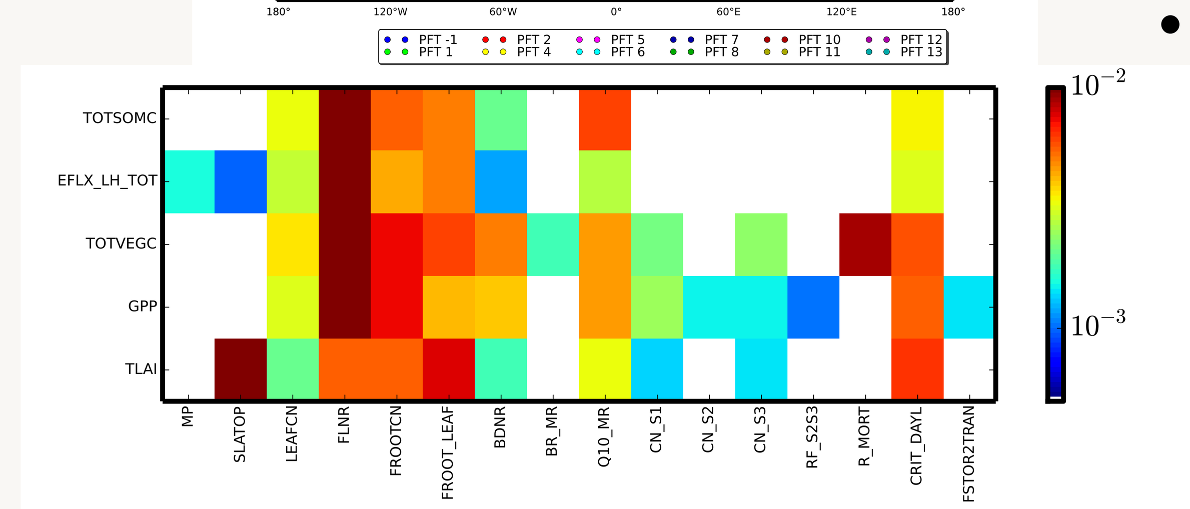
K. Sargsyan, C. Safta, H. Najm, B. Debusschere, D. Ricciuto, P. Thornton, "Dimensionality Reduction for Complex Models via Bayesian Compressive Sensing", *International Journal of Uncertainty Quantification*, 4(1), pp. 63-93, 2014.

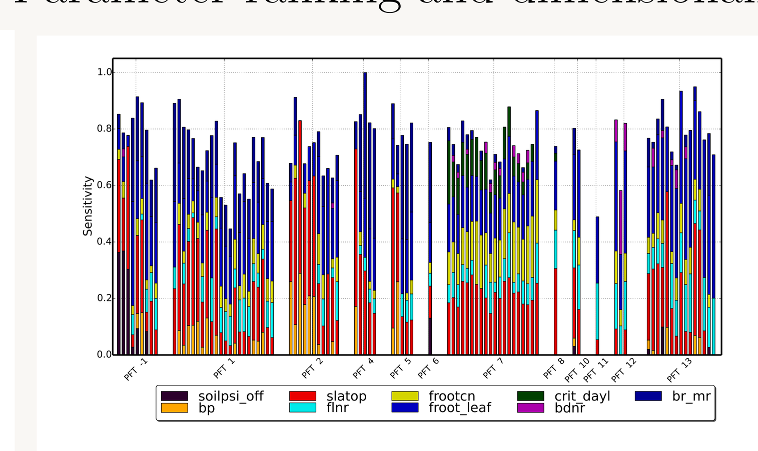
Application: ACME Land Model

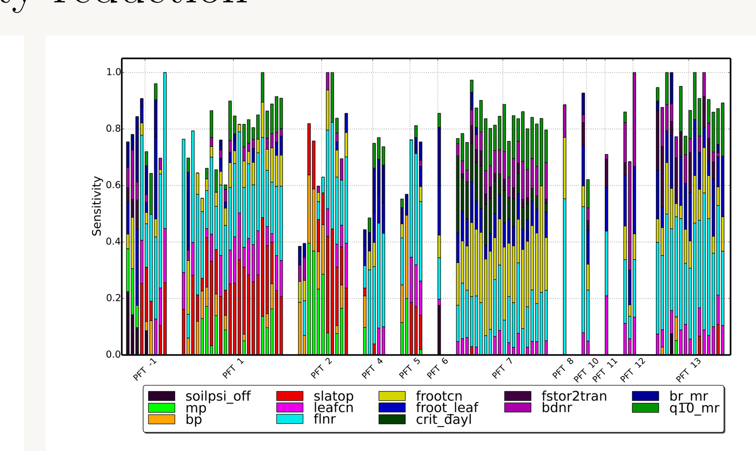
ACME Accelerated Climate Modeling for Energy

- Study 5 steady state outputs for 96 FLUXNET sites:
  - Gross primary productivity (GPP)
  - Total leaf area index (TLAI)
  - Total vegetation carbon (TOTVEGC)
  - Total soil organic matter carbon (TOTSOMC)
  - Latent heat flux (EFLX_LH_TOT)
- Vary 68 input parameters over selected ranges
- Built surrogate model approximations (per site, per output) w.r.t 68 inputs using 3000 ensemble simulations
- Performed variance-based decomposition
- Sensitivities grouped according to Plant Functional Types (PFTs)
- Only ∼15 (out of 68) parameters have significant impact to overall uncertainty
- Parameter ranking and dimensionality reduction









D. Ricciuto, K. Sargsyan, P. Thornton, "The Impact of Parametric Uncertainties on Biogeochemistry for ACME Land Model", *in prep.*, 2016.

U.S. DEPARTMENT OF ENERGY

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