Dimensionality Reduction and Global Sensitivity Analysis for the Community Land Model

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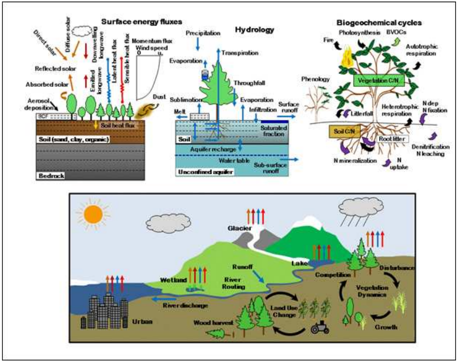
Outline

UQ Challenges in Climate Models

- Computationally expensive model simulations
- High-dimensional input parameter space
  - Physical constraints and dependencies for some input parameters
  - Uncertainties in the input parameters are not known
- Non-linear dependence of output quantities of interest on inputs

Community Land Model

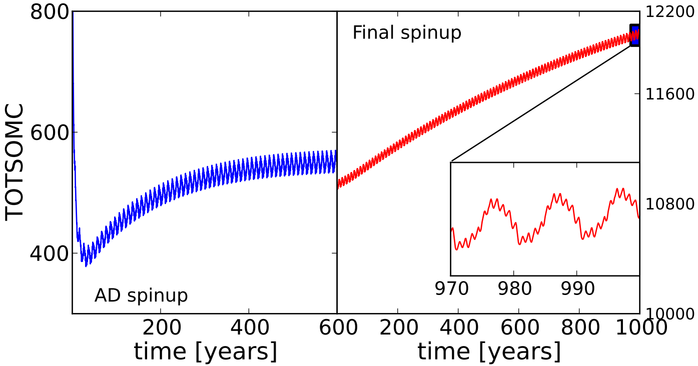


http://www.cesm.ucar.edu/models/clm/

- Nested computational grid hierarchy
- Represents spatial heterogeneity of the land surface
- A single-site, 1000-yr simulation takes ~ 10 hrs on 1 CPU
- Involves ~ 70 input parameters

Community Land Model - Typical Setup (1)

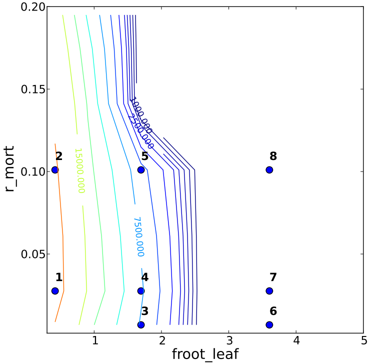
- Generate initial conditions → several spin-up stages

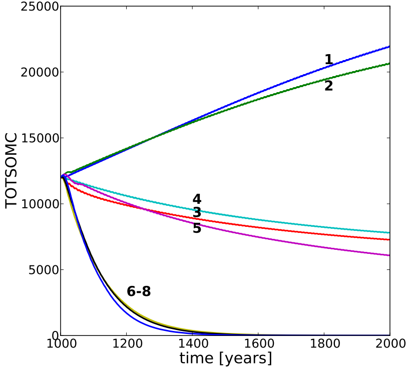


- total soil organic matter carbon $[gC/m^2]$ (*TOTSOMC*)

Community Land Model - Typical Setup (2)

- Sample the parameter space





- Left frame: Contour plot of time-averaged *TOTSOMC* values for a range of *(r_mort,froot_leaf)* values
- Right frame: Time evolution of *TOTSOMC* for select *(r_mort,froot_leaf)* values

Surrogate Models

What are surrogate models ?

- Input parameter vector $\boldsymbol{\lambda}$
- Computationally expensive model $f(\cdot)$ (e.g. CLM)
- Given a set of *training* model runs, $(\boldsymbol{\lambda}_i, f(\boldsymbol{\lambda}_i))_{i=1}^{N}$, a *surrogate* $f_s(\cdot) \approx f(\cdot)$ is a model that is cheap to evaluate and appropriately represents the underlying detailed, expensive model over a specified range of input parameters

Why do we need surrogate models ?

- Global sensitivity analysis
- Input parameter inference
- Optimization
- Forward uncertainty propagation

Polynomial Chaos Representations

To build a surrogate representation for input-output relationship, Polynomial Chaos (PC) spectral expansions are used; see Ghanem and Spanos (1991).

- Interprets input parameters as random variables
- Allows propagation of input parameter uncertainties to outputs of interest
- Serves as a computationally inexpensive surrogate for calibration or optimization

Polynomial Chaos Representations

Input parameters are represented via their cumulative distribution function (CDF) $F(\cdot)$, such that, with $\eta_i \sim \mathrm{Uniform}[-1,1]$, we have:

$$\lambda_i = F^{-1}_{\lambda_i}\left(\frac{\eta_i+1}{2}\right), \qquad \text{for } i=1,2,\ldots,d.$$

If input parameters are uniform $\lambda_i \sim \mathrm{Uniform}[a_i,b_i]$, then

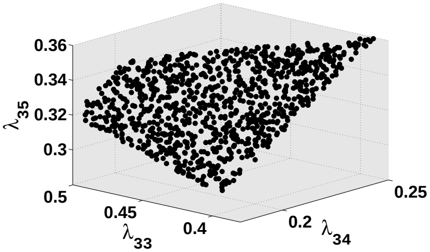
$$\lambda_i = \frac{a_i+b_i}{2} + \frac{b_i-a_i}{2}\,\eta_i.$$

Output is represented with respect to Legendre polynomials

$$f(\boldsymbol{\lambda}(\boldsymbol{\eta})) \approx y_{\mathbf{c}}(\boldsymbol{\eta}) \equiv \sum_{k=0}^{K} c_k \Psi_k(\boldsymbol{\eta}).$$

Map Constrained Parameters to Unconstrained Spaces

- Given a vector of random variables $\boldsymbol{\lambda} = (\lambda_1, \ldots, \lambda_{d'})$ with known joint cumulative distribution function (CDF) $F(\lambda_1, \ldots, \lambda_{d'})$
- Use *Rosenblatt transformation* (RT) to obtain a map $\boldsymbol{\eta} = R(\boldsymbol{\lambda})$ to a set of η_i's that are independent uniform random variables on $[-1, 1]$.



$$\begin{aligned} \lambda_{18} &< \lambda_{22}, \\ \lambda_{30} + \lambda_{31} + \lambda_{32} &= 1, \\ \lambda_{33} + \lambda_{34} + \lambda_{35} &= 1. \end{aligned}$$

Bayesian Inference of Polynomial Chaos modes

Bayesian inference of PC modes allows surrogate construction with uncertainties associated with limited sampling

- Bayes formula

$$p(\boldsymbol{c}|D) \propto L_{\mathcal{D}}(\boldsymbol{c})p(\boldsymbol{c})$$

relates the prior distribution $p(\boldsymbol{c})$ of PC modes to the posterior $p(\boldsymbol{c}|\mathcal{D})$, where the data $\mathcal{D}$ is the set of all training runs $\mathcal{D} = (\boldsymbol{\lambda}_i, f(\boldsymbol{\lambda}_i))_{i=1}^{N}$.

- The likelihood accounts for the discrepancy between the simulation data and the surrogate model (Sargsyan *et al* 2011),

$$L_{\mathcal{D}}(\boldsymbol{c}) \propto \exp\left(-\sum_{i=1}^{N}\frac{(f(\boldsymbol{\lambda}_i)-y_{\boldsymbol{c}}(\boldsymbol{\eta}_i))^2}{2\sigma^2}\right)$$

Iterative Bayesian Compressive Sensing (iBCS)

- The number of polynomial basis terms grows fast; a p-th order, d-dimensional basis has a total of $(p+d)!/(p!d!)$ terms.
- Dimensionality reduction by using hierarchical priors.

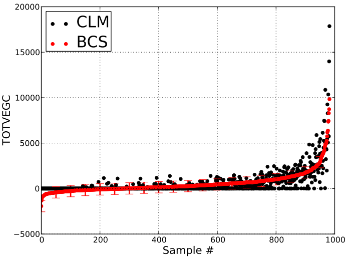
$$p(\mathbf{c}|s_k^2) \propto \prod_{k=0}^{K} \exp\left(-\frac{c_k^2}{2s_k^2}\right) \qquad p(s_k^2|\alpha) = \frac{\alpha}{2} \exp\left(-\frac{\alpha s_k^2}{2}\right)$$

- The parameter α can be further modeled hierarchically, or fixed.
- The parameters $(\sigma^2, s_0^2, \ldots, s_K^2)$ are fixed by evidence maximization, and bases corresponding to small s_i^2 are discarded (Ji *et al* 2008, Babacan *et al.*, 2010).
- *Iterative BCS*: We implement an iterative procedure that allows increasing the order for the relevant basis terms while maintaining the dimensionality reduction (Sargsyan *et al* 2011,2012).

Climate Land Model - Single site mode for Niwot Ridge

- $N = 10,000$ training runs based on uniformly LHS distributed parameter values.
- Outputs: steady-state, 10-year averages of 7 quantities

iBCS for one observable



Name	Units	Description
TOTVEGC	gC/m^2	Total vegetation carbon
TOTSOMC	gC/m^2	Total soil carbon
GPP	$gC/m^2/s$	Gross primary production
ERR	W/m^2	Energy conservation error
TLAI	none	Total leaf area index
EFLX_LH_TOT	W/m^2	Total latent heat flux
FSH	W/m^2	Sensible heat flux

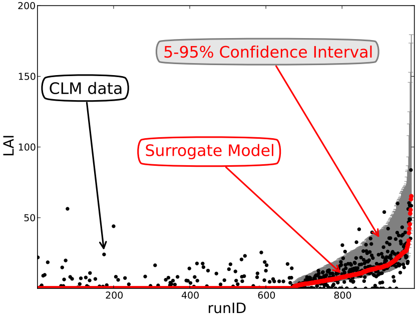
Classify Parameter Space

- Large regions of the original quasi-hypercube parameter space lead to simulations with failed vegetation.
- Partition the space using a classification algorithm
  - Classification using Random Decision Forests implemented in the AlgLib software library (http://www.alglib.net)
  - the result is the mode of the results from individual decision trees
- Calibration using 9K samples/Validation using 1K samples
- Shift accuracy from “failed vegetation” plateau to “active vegetation” regions
- Apply the iBCS algorithm on “active vegetation” results

Classification+iBCS

- Clustering/classification-based piecewise Polynomial Chaos construction to accommodate non-smooth transition between dead and live vegetation regions

- Classification errors are approximately 10-15%
- Posterior predictive distribution of the surrogate model output covers the spread of simulation data



Climate Land Model - Global Sensitivity Analysis

- Ranking of the most influential input parameters for each output of interest

$$S_i = \frac{\sum_{k\in\mathbb{I}_i} c_k^2 ||\Psi_k||^2}{\sum_{k>0} c_k^2 ||\Psi_k||^2}$$

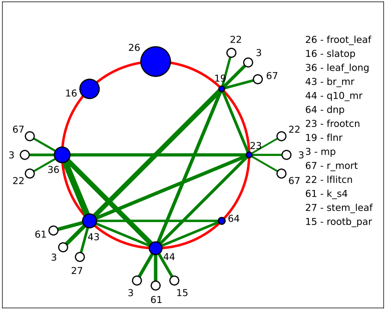
rank	TOTVEGC	TOTSOMC	GPP
1	r_mort	q10_mr	leafcn
2	q10_mr	leafcn	k_s4
3	froot_leaf	froot_leaf	froot_leaf
4	br_mr	br_mr	flnr
5	q10_hr	fflnr	q10_mr
6	leafcn	dnp	q10_hr
7	k_s4	q10_hr	dnp
8	stem_leaf	leaf_long	rf_s3s4
9	flnr	k_s4	leaf_long
10	dnp	frootcn	br_mr

Climate Land Model - Global Sensitivity Analysis

- Most influential input parameter couplings for each output - energy contained in each parameter pair
- Results below correspond to Leaf Area Index *(LAI)*

$$S_{ij} = \frac{\sum_{k\in\mathbb{I}_{ij}} c_k^2 ||\Psi_k||^2}{\sum_{k>0} c_k^2 ||\Psi_k||^2}$$

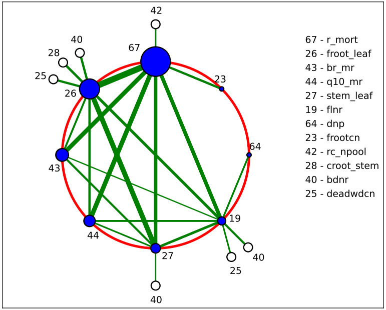
- Blue discs sizes are proportional to S_i
- Thickness of green lines is proportional to S_{ij}



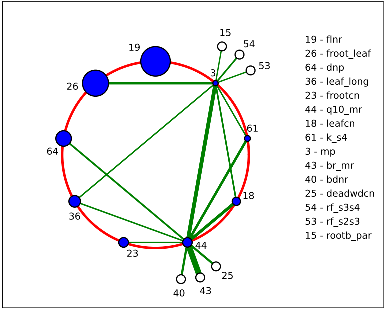
Climate Land Model - Global Sensitivity Analysis

- Most influential input parameter couplings for each output - energy contained in each parameter pair

TOTVEGC

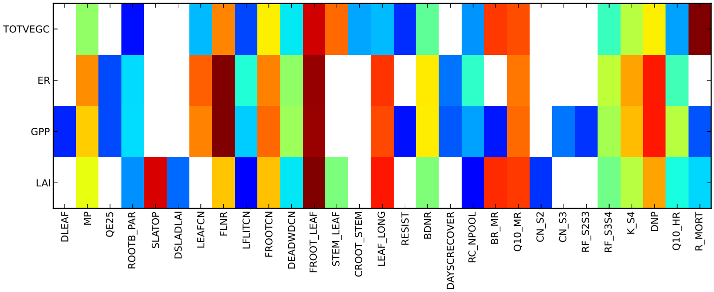


GPP



Climate Land Model - Global Sensitivity Analysis

- Sensitivity indices used to discard unimportant parameters
- Combine analysis for several outputs of interest, {TOTVEGC,LAI,ER,GPP}, to arrive to a reduced input parameter space.



Summary

- *Sensitivity analysis for complex, expensive, climate models is enabled by cheap surrogate models*
  - Polynomial Chaos surrogate model is constructed using Bayesian techniques
  - Constrained/dependent input parameters are mapped to an unconstrained input set via Rosenblatt transformation
  - High-dimensionality is tackled by iterative Bayesian compressive sensing algorithm
  - Classification for efficient domain decomposition to relieve the non-linear effects
- Future plans include running CLM ensembles on lower-dimensional parameter spaces.
  - Goal is to increase predictive fidelity of the CLM surrogate, for reliable *parameter calibration*.