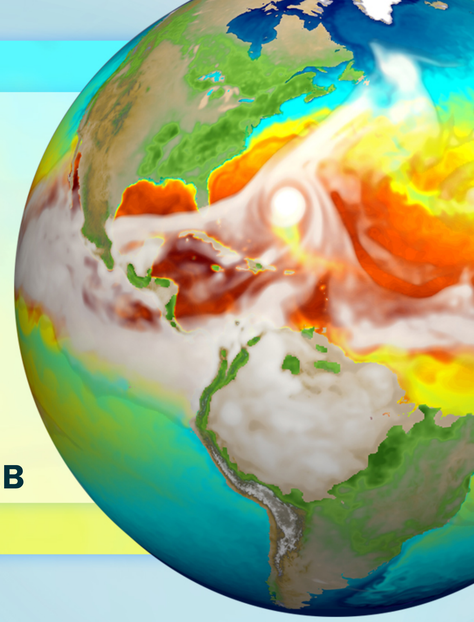
Parameter Calibration and Structural Error in Land Models

Khachik Sargsyan (SNL), Dan Ricciuto (ORNL), Jennifer Holm (LBNL)

Sandia National Laboratories

OAK RIDGE National Laboratory

BERKELEY LAB



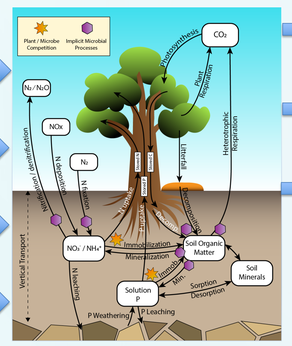
Bayesian Calibration of Land Models….

Model Input Parameters

- Critical soil water potential
- Stomatal conductance slope
- Stomatal conductance intercept
- Specific leaf area (canopy top)
- Leaf carbon:nitrogen ratio
- Fraction of leaf N in RuBisCO
- Fine root carbon:nitrogen ratio
- Fine root:leaf allocation ratio
- Critical day length for senescence
- Fraction of C storage allocated
- Bulk denitrification rate
- Base rate for plant respiration
- T sensitivity for plant respiration

...

Land Model



Model Outputs

- Gross Primary Productivity
- Leaf Area Index
- Latent Heat Flux

...

...

Posterior PDF

sampled via Markov chain Monte Carlo (MCMC)

$$p(\lambda|D) \propto p(D|\lambda)p(\lambda)$$

Bayes Formula

FLUXNET Data

…. Enabled by Surrogate Models

Key challenge:

Likelihood requires online evaluation of model at candidate values

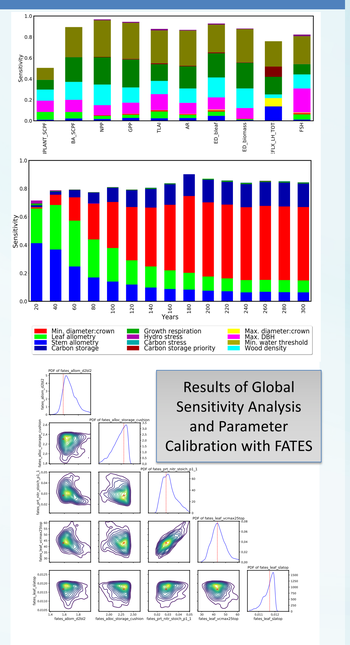
$$\log L(\lambda) \equiv \log p(D|\lambda) = -||D - f(\lambda)||^2$$

Solution:

- Construct a surrogate, inexpensive approximation of the model, otherwise called a proxy, metamodel, response surface, supervised ML

$$f(\lambda) \approx f_s(\lambda)$$

- We employ Polynomial Chaos surrogates that enable variance decomposition (global sensitivity analysis) and uncertainty propagation.
- Enables uncertainty decomposition due to model parameters, surrogate errors and data noise



Results of Global Sensitivity Analysis and Parameter Calibration with FATES

Model Structural Error

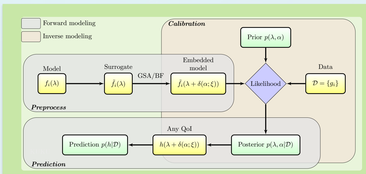
Elephant in the room

What is Model Error:

- Very loaded concept ... otherwise called (with slightly altered meanings) model discrepancy, model structural error, model inadequacy, model misspecification, model form error, model uncertainty

- Error associated with
  - Simplifying assumptions, parameterizations
  - Mathematical formulation, theoretical framework

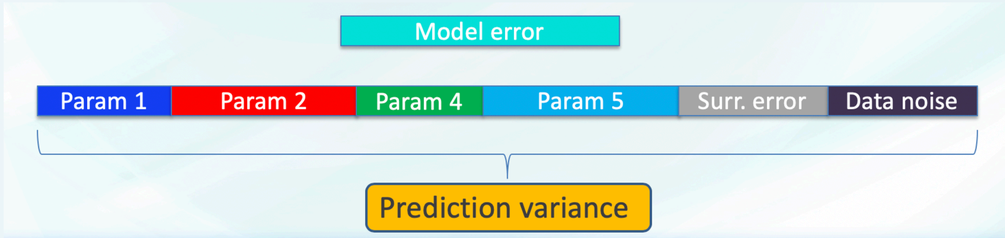
- Uncertainty decomposition of model prediction needs to account for model error – often the dominant component of the uncertainty!



UQTk workflow
https://github.com/sandialabs/UQTk

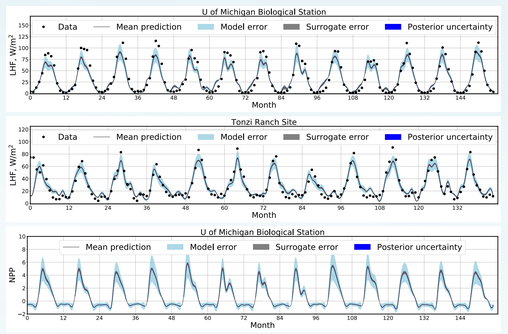
Scientific discovery and model development: "is it worth resolving details, or just parameterize empirically?"

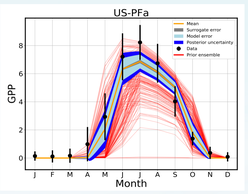
Optimal resource allocation: "do I improve my model (e.g. high-res), or run more simulations?"



Embedded (but Non-Intrusive!) Model Error approach:

- Model error correction inside the model, parameterized by ***polynomial chaos***
- ***Bayesian inference*** of physical parameters and model error parameters
- Calibrated uncertain prediction that is aware of model error
  - Physics-driven model correction
  - Meaningful extrapolation to full set of QoI predictions
  - Disambiguation between model error and data noise
  - Enables model comparison and model selection





SciDAC Project OSCM: Optimization of Sensor Networks for Improving Climate Model Predictions

- K. Sargsyan, H. Najm, R. Ghanem, "On the Statistical Calibration of Physical Models", Int. J. Chem. Kinetics, 47(4), 246-276, 2015.
- K. Sargsyan, X. Huan, H. Najm. "Embedded Model Error Representation for Bayesian Model Calibration", arXiv:1801.06768, in press, Int. J. Uncert. Quant., 2019.

E3SM Energy Exascale Earth System Model

For additional information, contact:

Khachik Sargsyan
Principal Member of Tech. Staff

Sandia National Laboratories, Livermore

(925) 294-4885
ksargsy@sandia.gov

SciDAC Scientific Discovery through Advanced Computing

FASTMATH

U.S. DEPARTMENT OF ENERGY