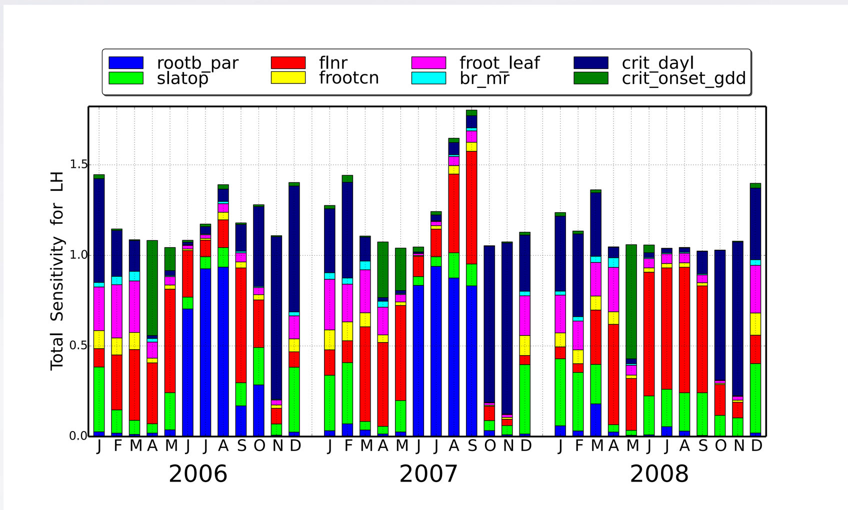
R: Forward and Inverse Uncertainty Quantification for ALM Single Point Model

Khachik Sargsyan (SNL), Daniel Ricciuto (ORNL)

Overview and Approach

Forward UQ:

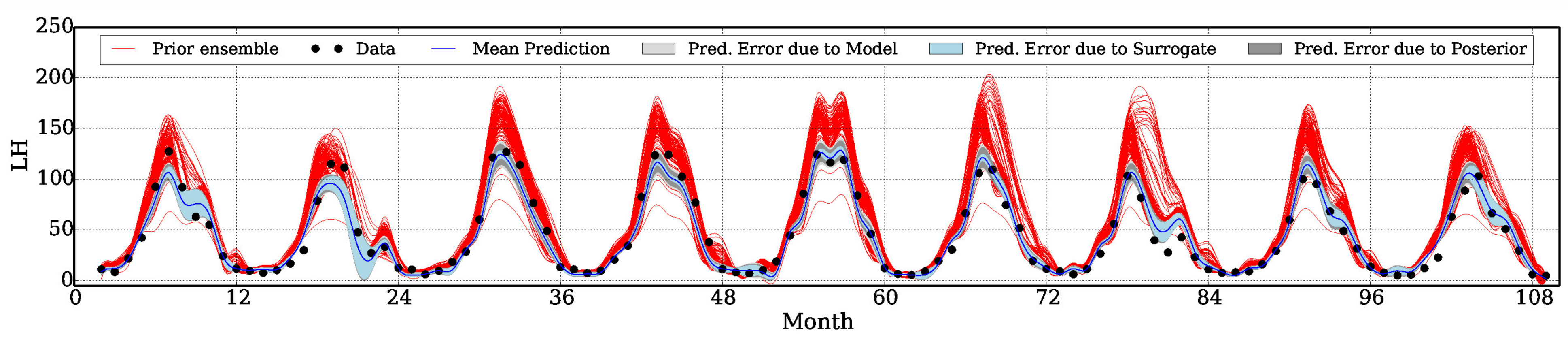
- Input parameter uncertainty propagation
- Model surrogate construction
- Global Sensitivity Analysis (GSA):
  - variance-based decomposition,
  - Sobol sensitivities
- Major challenges:
  - **Large number of input parameters (curse of dimensionality)**
  - Strong nonlinearities of input-output maps
  - **Expense of forward simulations**
- Main tools:
  - **Polynomial Chaos** surrogates are ideally fitted for parameter uncertainty propagation and surrogate construction, also providing free access to GSA
  - Weighted Iterative **Bayesian Compressive Sensing** (BCS) builds accurate surrogate models adaptively to enable forward UQ for large number of inputs and few forward simulations.



GSA for latent heat flux (LH) at the Missouri Ozark flux tower, showing monthly changes in sensitivities over a 3-year period.

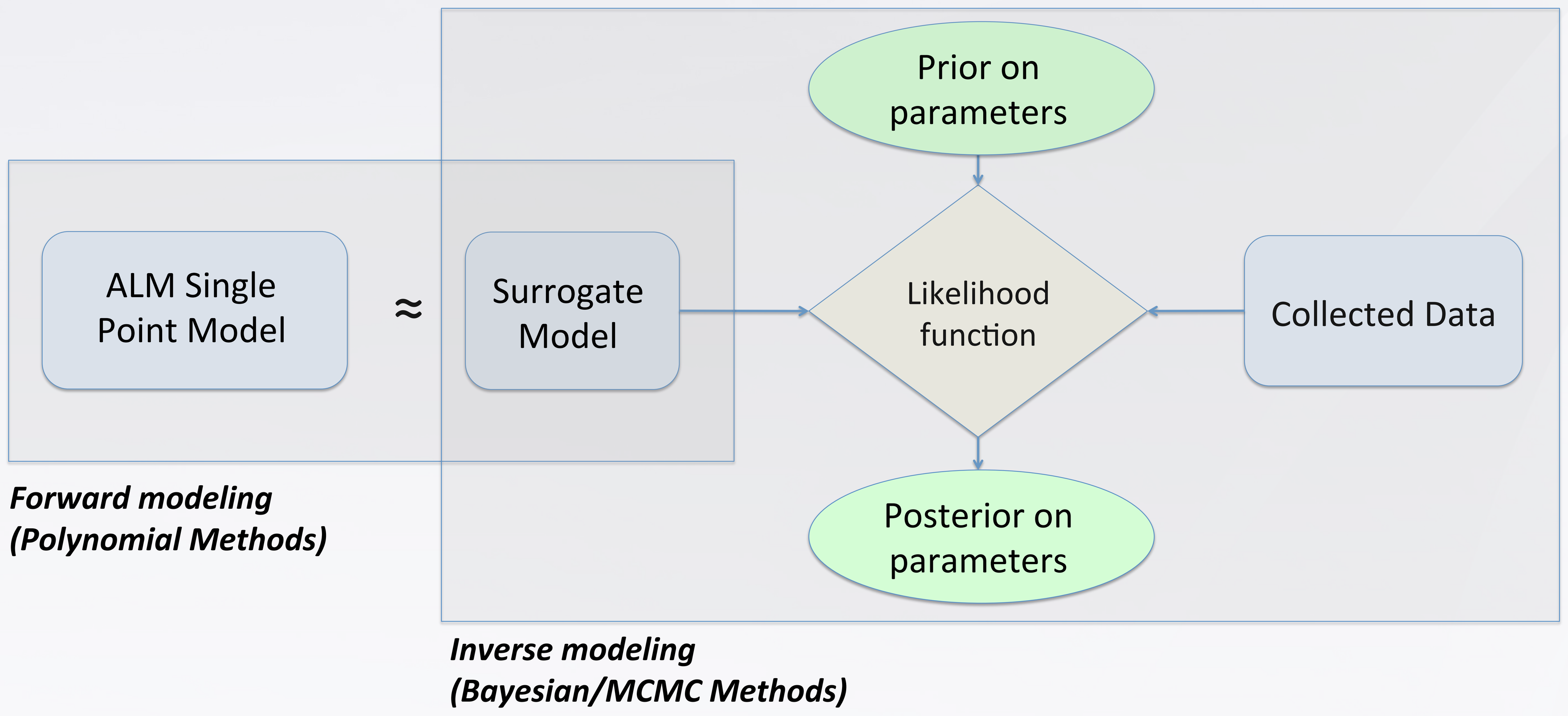
Inverse UQ:

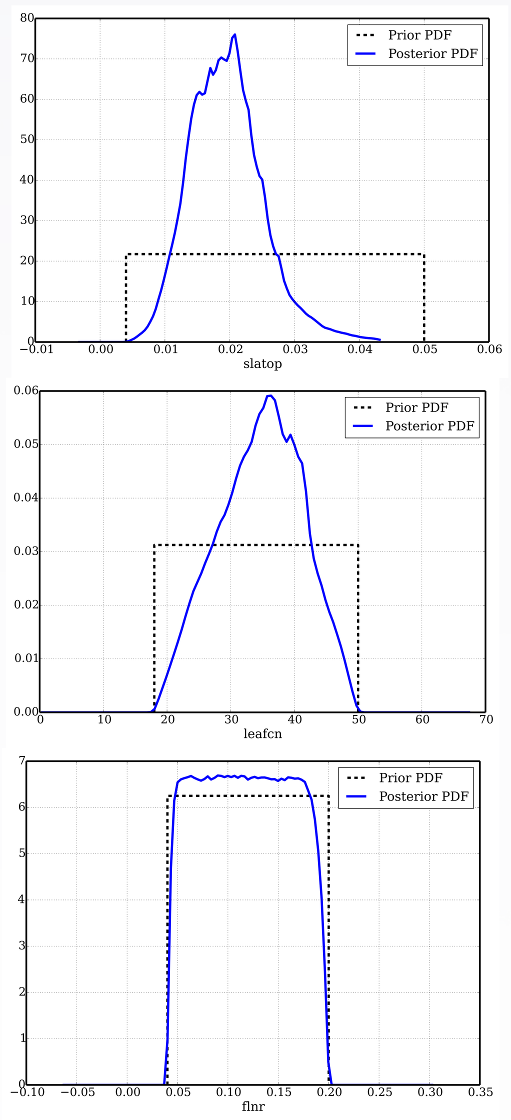
- Given experimental/observational data, find input parameter distributions
- … otherwise called calibration, tuning, parameter estimation
- Major challenges:
  - Large number of input parameters (curse of dimensionality)
  - Physical constraints, identifiability, data scarcity
  - **Model structural errors**
- Main tools:
  - **Bayesian calibration** is well-suited for accounting uncertainties from various sources, e.g. observational noise, parametric uncertainties, internal stochasticity
  - We develop and employ internal **model error embedding** approach to enable structural error representation and quantification, followed by accurate predictions (even extrapolatory!) with fair assessment of all sources of uncertainty, including structural errors



Results from a calibration of monthly latent heat flux data at the Missouri Ozark flux. This calibration method partitions posterior uncertainties into errors from the surrogate model representation, posterior uncertainty and model error.

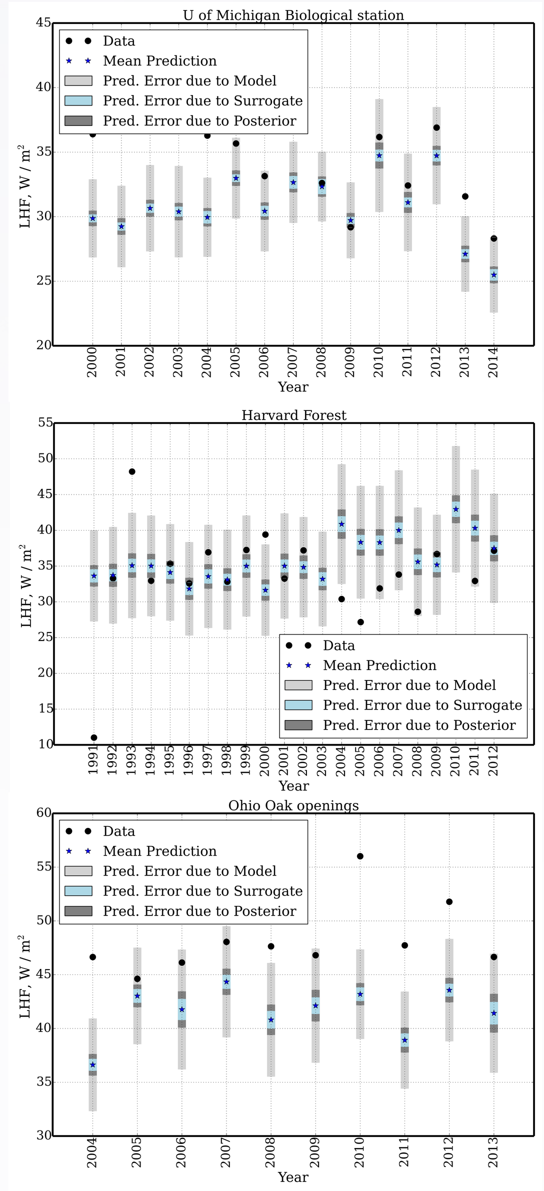
Early Results





Demo Case Study

- Three sensitive inputs
- Three sites, annual FLUXNET data and model simulations
- Calibration reveals that *flnr* is not constrained by data (posterior = prior)
- Prediction variance is composed of surrogate error, posterior uncertainty and model structural error
- Structural error is the highest contributor – no surprise!
- Allows meaningful and robust extrapolation to QoIs and sites outside the calibration set



References

- D. Ricciuto, K. Sargsyan, P. Thornton, The impact of parametric uncertainties on biogeochemistry in the ACME land model. J. Advances in Modeling Earth Systems, in review.
- K. Sargsyan, H. N. Najm, R. Ghanem, On the Statistical Calibration of Physical Models, International Journal for Chemical Kinetics, Vol. 47, No. 4, p.246–276, 2015.
- 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, Vol. 4, No. 1, p.63-93, 2014.

- *git clone git@github.com:ACME-Climate/Uncertainty-Quantification.git*
- Python interface to UQTk v3.0 (www.sandia.gov/uqtoolkit)
- Full workflow is non-intrusive, i.e. model runs as a black-box

For additional information, contact:
Khachik Sargsyan
Principal Member of Technical Staff
Sandia National Laboratories
(925) 294-4885
ksargsy@sandia.gov