Overview of Uncertainty Quantification (UQ) Methods for Complex Models

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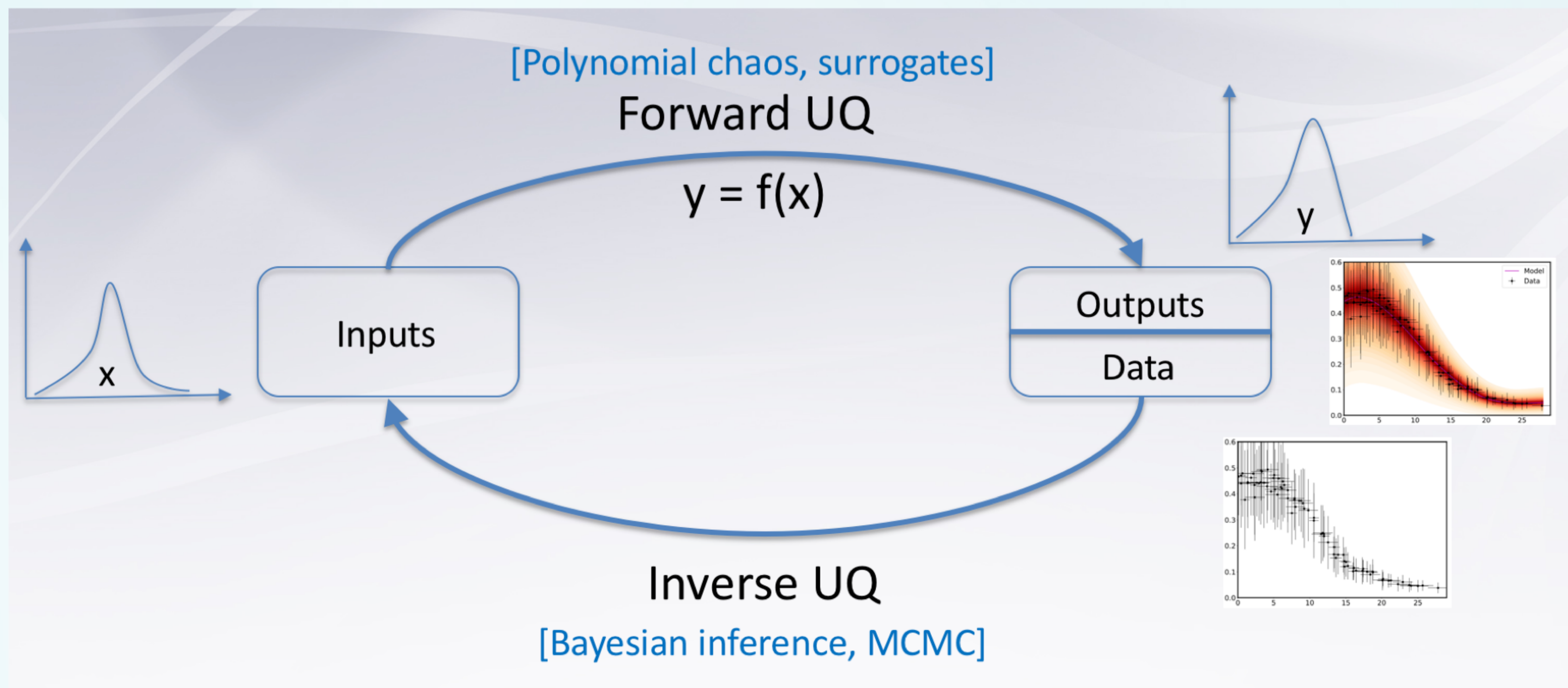
UQ Components



Forward UQ

Given input parameter uncertainty, find output QoI distributions

- Uncertainty propagation, model surrogate construction
- … otherwise called emulator, proxy, metamodel, response surface
- 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

Inverse UQ

Given experimental/observational data, find input parameter distributions

- … otherwise called calibration, tuning, parameter estimation

Major challenges

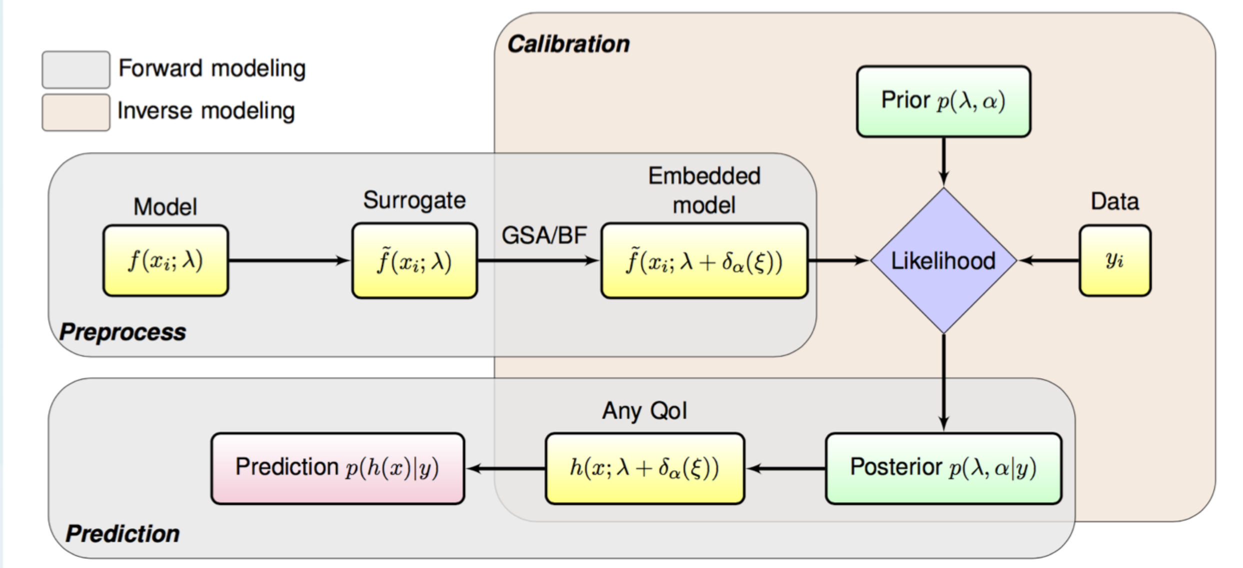
- Large number of input parameters (curse of dimensionality)
- Physical constraints, identifiability, data scarcity
- **Model structural errors**

Main tools

- **Bayesian calibration** is well-suited for accounting uncertainties from various sources, e.g. observational noise, parametric uncertainties, internal stochasticity
- 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

UQ Workflow

1. **Surrogate construction**
   - Perturbed parameter ensemble
   - Prior predictive distribution
   - Global sensitivity analysis
   - Dimensionality reduction
2. **Model structural error embedding**
   - Model correction
   - Can be non-intrusive!
   - Respects physics
   - Disambiguated with data error
3. **Calibration/tuning**
   - Bayesian inference
   - Adaptive Markov chain Monte Carlo
   - Posterior analysis and model selection
4. **Prediction**
   - Posterior predictive
   - Output uncertainty decomposition

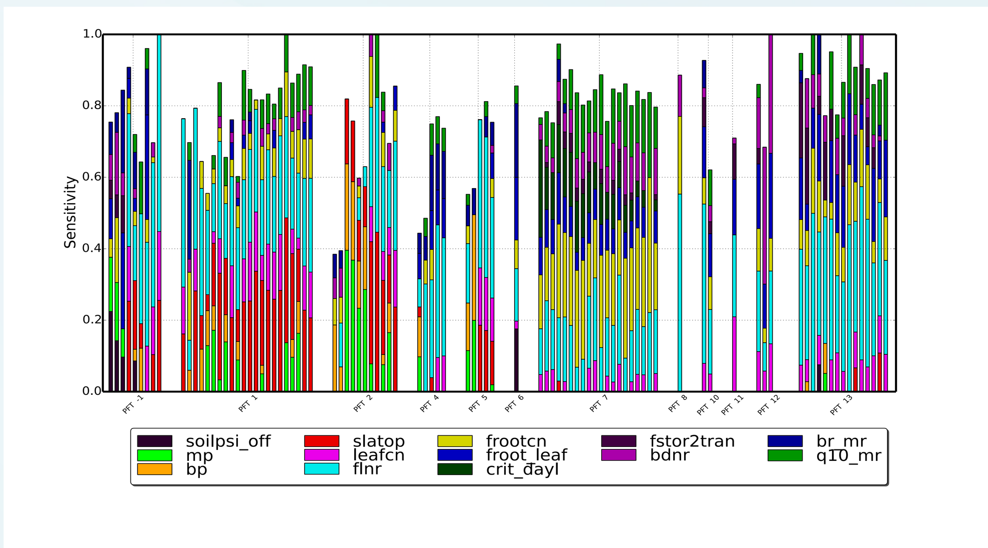


Predictive uncertainty decomposition: Total Variance =

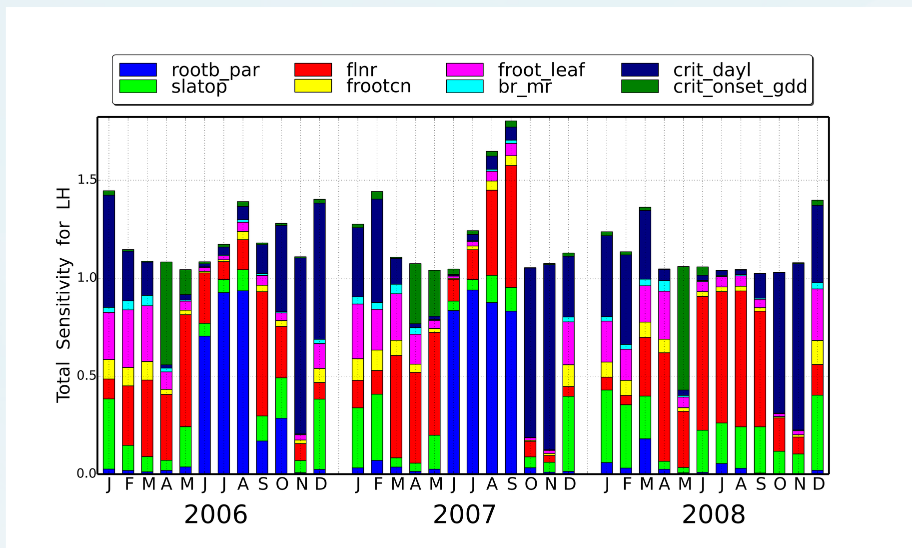
Parametric uncertainty + Data noise + Model error + Surrogate error

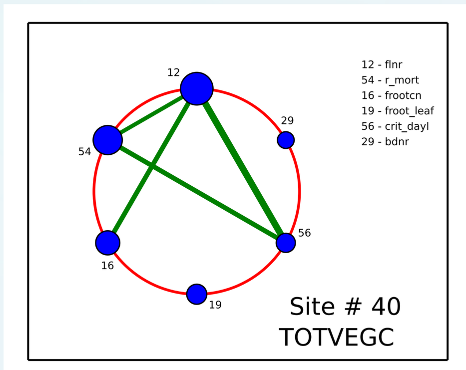
Selected ELM Results

GSA for gross primary productivity (GPP) at 96 FLUXNET sites, grouped by PFTs

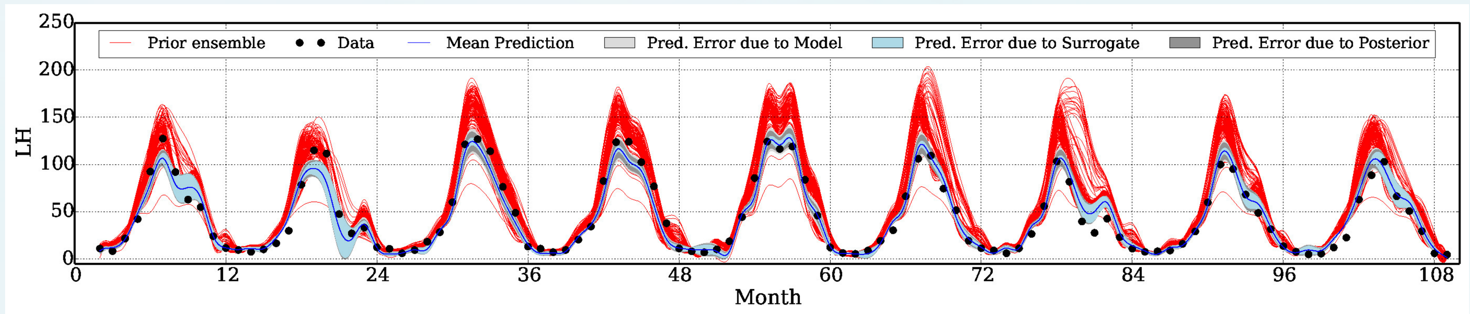


GSA for latent heat flux (LH) at the Missouri Ozark flux tower, showing monthly changes in sensitivities over a 3-year period





Main and joint sensitivities for Harvard Forest site



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.

Software

- *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

UQTk

References

- D. Ricciuto, K. Sargsyan, P. Thornton, The impact of parametric uncertainties on biogeochemistry in the ACME land model. Journal of Advances in Modeling Earth Systems, 10(2), p. 297-319, 2018.
- K. Sargsyan, H. N. Najm, R. Ghanem, On the statistical calibration of physical models, International Journal for Chemical Kinetics, 47(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 for Uncertainty Quantification, 4(1), p.63-93, 2014.

E3SM Energy Exascale Earth System Model
e3sm.org

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