Bayesian inference for model error quantification and propagation with UQTk

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Sandia National Laboratories, Livermore, CA

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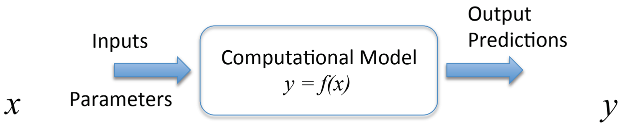
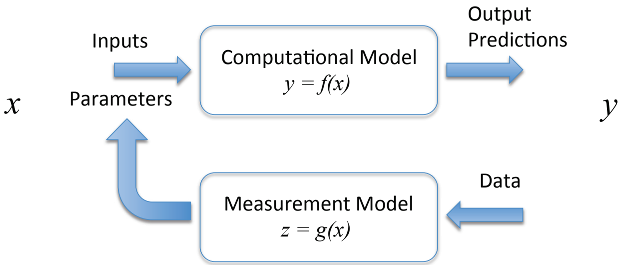
Outline

Uncertainty Quantification and Computational Science



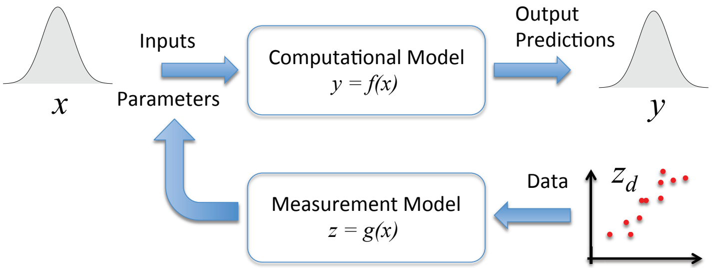
Forward problem

Uncertainty Quantification and Computational Science



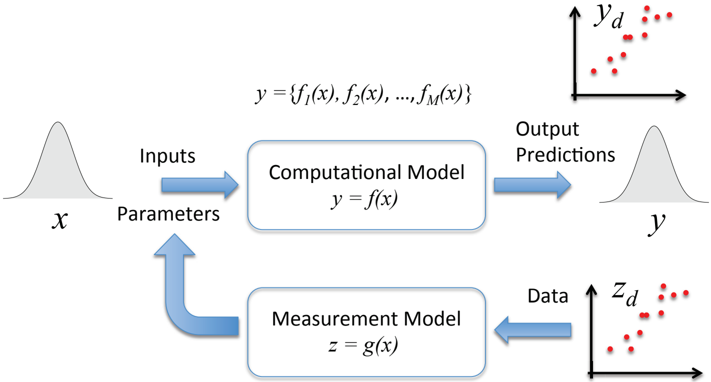
Inverse & Forward problems

Uncertainty Quantification and Computational Science



Inverse & Forward UQ

Uncertainty Quantification and Computational Science



Inverse & Forward UQ

Model validation & comparison, Hypothesis testing

The Case for Uncertainty Quantification

UQ needed for...

- Model predictions
- Model validation and comparison
- Confidence assessment
- Reliability analysis
- Dimensionality reduction
- Optimal design
- Decision support
- (Noisy) data assimilation

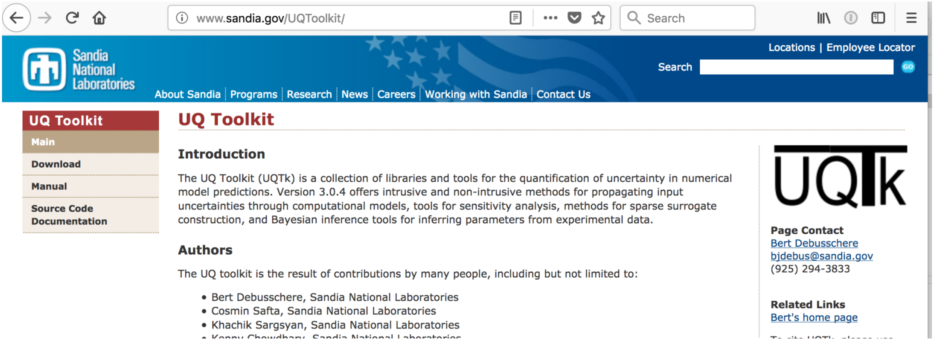
Uncertainty Sources

- Model parameters
- Initial/boundary conditions
- Model geometry/structure
- Lack of knowledge
- Data noise
- Intrinsic stochasticity
- Numerical errors, too

UQ Enables Predictive Simulations

- Locate all sources of (manageable) uncertainties
- Parameter selection/estimation
  - Auxilliary data collection
  - Expert opinion, physical bounds, maximum entropy
  - Submodel fitting/regression
- Forward propagation of uncertainties
  - Local SA (deterministic, error propagation)
  - Interval math, evidence theory
  - Global SA (stochastic, variance-based decomposition)
- Calibration with a separate set of data (inverse UQ)
- Model (in)validation
  - No model is perfect
  - Compare model prediction with uncertainties versus data on some QoI
  - Model comparison (Bayes Factors, Model Plausibility)

UQTk provides tools to build general UQ workflows



- Representation of random variables and stochastic processes
- Forward uncertainty propagation: Polynomial Chaos
- Inverse problems: Bayesian methods, MCMC
- Quadrature integration
- Sensitivity analysis: Sobol indices
- Dimensionality reduction: Karhunen-Loève expansions
- Gaussian Processes
- Sparse approximations: Bayesian Compressive Sensing
- Low Rank Tensors

UQTk is meant to be straightforward to download, install and use

UQTk

- Target usage:
  - Rapid prototyping of UQ workflows
  - Algorithmic research in UQ
  - Tutorials / educational
  - Expertise in UQ methods (or a desire to acquire it) helpful
- Released under the GNU Lesser General Public License
  - `http://www.sandia.gov/UQToolkit/`
  - Current version 3.0.4
  - Version 3.1.0 planned for later this year
- Download as tar file and configure with `CMake`
- No massive third party libraries to download, install, and configure

UQTk is used in a variety of applications

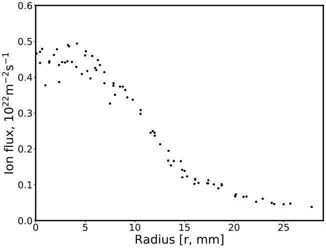
UQTk

- Direct collaborations
  - US DOE SciDAC FASTMath institute
    https://fastmath-scidac.llnl.gov/
  - Variety of US DOE SciDAC partnership projects
  - Part of US DOE BER E3SM climate model analysis tools
- Many other research groups at universities, National Labs, and industry
- Always welcome new applications / collaborations
- Mailing lists
  - uqtk-announce@software.sandia.gov
  - uqtk-users@software.sandia.gov
  - Join at http://www.sandia.gov/UQToolkit

Outline

Fitting parametric model to data: least squares

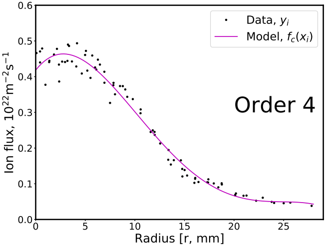
- Given data (x_i, y_i) for $i = 1, \ldots, N$



Fitting parametric model to data: least squares

- Given data (x_i, y_i) for $i = 1, \dots, N$
- Given parametrized model form $f_c(x)$
- Tune c, such that $y_i \approx f_c(x_i)$
- Least-squares

$$\underset{c}{\operatorname{argmin}} \sum_{i=1}^{N} (y_i - f_c(x_i))^2$$



- Linear parametrization (basis expansion)... $$f_c(x) = \sum_{k=0}^{K} c_k \Psi_k(x)$$
- ... allows analytical answer $c = (P^T P)^{-1} P^T y$, where $P_{ik} = \Psi_k(x_i)$

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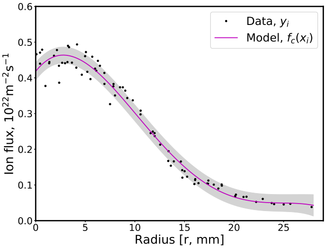

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- ... allows analytical answer $c = (P^T P)^{-1} P^T y$, where $P_{ik} = \Psi_k(x_i)$
- ... with covariance information $\Sigma_c \propto (P^T P)^{-1}$

Bayesian viewpoint of fitting $y_i \approx f_c(x_i)$

- Bayes' formula
$$p(\mathcal{M}|\mathcal{D}) = \frac{p(\mathcal{D}|\mathcal{M})p(\mathcal{M})}{p(\mathcal{D})}$$

- Data $\mathcal{D} = \{x_i, y_i\}_{i=1}^N$
- Model $\mathcal{M} \equiv c$
- Rewrite Bayes' formula

$$\overbrace{p(c|y)}^{\text{Posterior}} = \frac{\overbrace{p(y|c)}^{\text{Likelihood}} \quad \overbrace{p(c)}^{\text{Prior}}}{\underbrace{p(y)}_{\text{Evidence}}}$$

- Prior $p(c)$: expert knowledge, or uninformative
- Posterior $p(c|y)$: updated 'knowledge' of c, given data y
- Likelihood $L(c) = p(y|c)$: key, noise/error model, encapsulates assumptions about data collection
- Evidence $p(y)$: not important for parameter (coeff. c) estimation; crucial for model selection (e.g. poly order)

Posterior sampling via Markov chain Monte Carlo (MCMC)

$$\overbrace{p(c|y)}^{\text{Posterior}} = \frac{\overbrace{p(y|c)}^{\text{Likelihood}} \quad \overbrace{p(c)}^{\text{Prior}}}{\underbrace{p(y)}_{\text{Evidence}}}$$

- In general, when model is not linear or noise is not Gaussian, there is little alternative to MCMC
- MCMC is a search procedure in parameter space leading to a stochastic process with a stationary distribution $p(c|y)$
- Given samples from posterior, one can interrogate it further
  - Estimate PDF with KDE
  - Compute moments
  - Build functional representation, such as PC
  - Pipe it to the next model as an input

Polynomial Chaos – functional representation for RVs

$$U \simeq \sum_{k=0}^{p} u_k \psi_k(\xi)$$

- First introduced by Wiener, 1938
- Revitalized by Ghanem and Spanos, 1991
- Convergent series if U has finite variance
- Selection of order p is a modeling choice
- Describes a r.v. U with a vector of *PC modes* $(u_0, u_1, \dots, u_p)$

- Standard r.v. ξ, standard orthogonal polynomials $\psi_k(\xi)$, *i.e.*

$$\int \psi_i(\xi)\psi_j(\xi)\pi_\xi(\xi)d\xi = \delta_{ij}||\psi_i||^2$$

PC Type	Domain	Density $\pi_\xi(\xi)$	Polynomial	Free parameters
Gauss-Hermite	$(-\infty, +\infty)$	$\frac{1}{\sqrt{2\pi}} e^{-\frac{\xi^2}{2}}$	Hermite	none
Legendre-Uniform	$[-1, 1]$	$\frac{1}{2}$	Legendre	none
Gamma-Laguerre	$[0, +\infty)$	$\frac{\xi^\alpha e^{-\xi}}{\Gamma(\alpha+1)}$	Laguerre	$\alpha > -1$
Beta-Jacobi	$[-1, 1]$	$\frac{(1+\xi)^\alpha (1-\xi)^\beta}{2^{\alpha+\beta+1} B(\alpha+1,\beta+1)}$	Jacobi	$\alpha > -1, \beta > -1$

[Wiener, 1938; Ghanem & Spanos, 1991; Xiu & Karniadakis, 2002; Le Maître & Knio, 2010]

Essential use of PC in UQ $U \simeq \sum_{k=0}^{K} u_k \Psi_k(\boldsymbol{\xi})$

Strategy:

- Represent model parameters/solution as random variables
- Construct PC for uncertain parameters
- Evaluate PC for model outputs

Advantages:

- Computational efficiency
- Utility
  - Moments: $\mathbb{E}[u] = u_0, \ \mathbb{V}[u] = \sum_{k=1}^{K} u_k^2 ||\Psi_k||^2, \ \ldots$
  - Global Sensitivities – fractional variances, Sobol' indices
  - Uncertainty propagation
  - Surrogate for forward model

Requirements:

- Finite variances (not a handicap in practice)
- Smooth forward functions

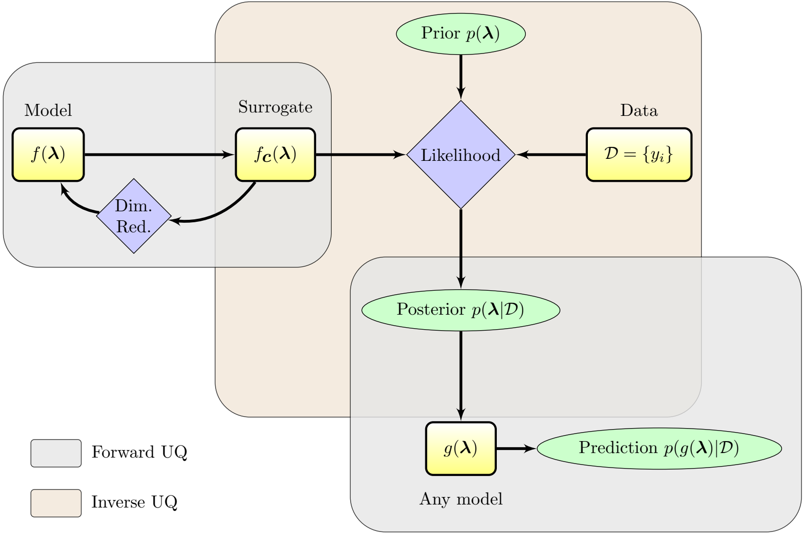
PC features: uncertainty propagation

$$U \simeq \sum_{k=0}^{K} u_k \Psi_k(\boldsymbol{\xi})$$

$$Z = f(U) \simeq \sum_{k=0}^{K} c_k \Psi_k(\boldsymbol{\xi})$$

- Basic task: given PC for inputs, find PC for outputs.
- Input-output map can also be defined implicitly, via governing equations $G(Z, U) = 0$.
- Two approaches
  - Intrusive: project governing equations
    - Results in set of equations for the PC modes
    - Requires redesign of computer code
    - PCEs for all uncertain variables in system
  - Non-intrusive: project outputs of interest
    - Sampling to evaluate projection operator
    - Can use existing code as black box
    - Only computes PCEs for quantities of interest

An example UQTk workflow (UQTk version 3.0)

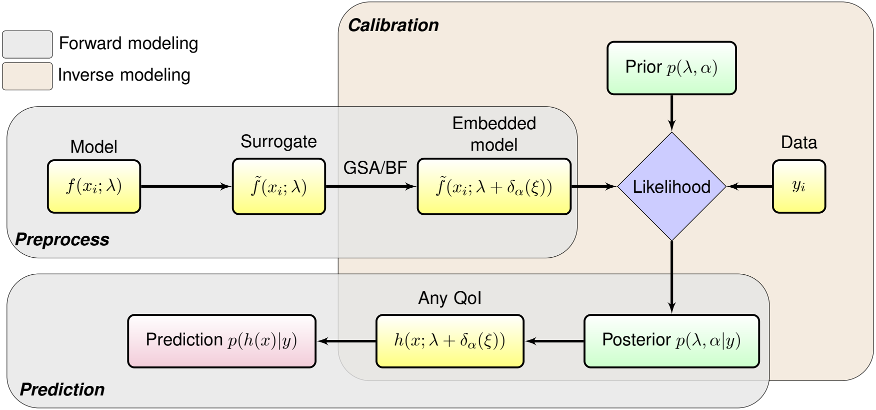


Model Error: Quantification of Structural Error

Model error = deviation from ‘truth’, or from a higher-fidelity model

- Represent and estimate the error associated with
  - Simplifying assumptions, parameterizations
  - Mathematical formulation, theoretical framework
  - Numerical discretization
- ...will be useful for
  - Model validation
  - Model comparison
  - Scientific discovery and model improvement
  - Reliable computational predictions
- Inverse modeling context
  - Given experimental or higher-fidelity model data, estimate the model error

Model error embedding – workflow



- Predictive uncertainty decomposition: Total Variance =

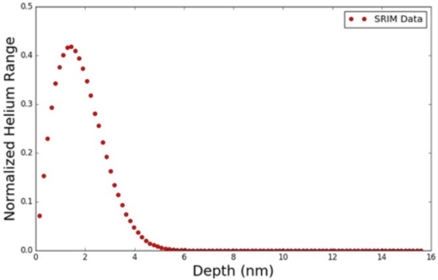
  Posterior uncertainty + Data noise + Model error + Surrogate error

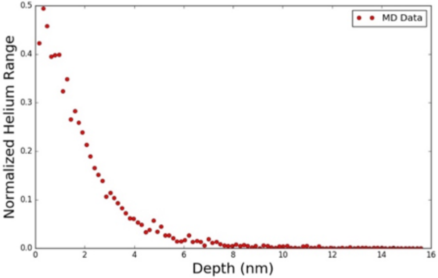
Outline

UQ in PSI – Xolotl: overview

Normalized helium range as a function of tungsten depth obtained by

- Stopping and Range of Ions in Matter (SRIM), or
- Molecular Dynamics (MD).



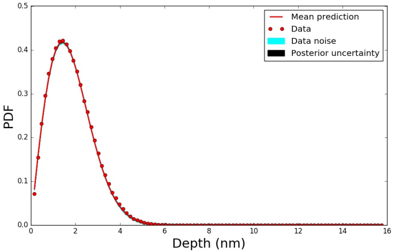


Main targets:

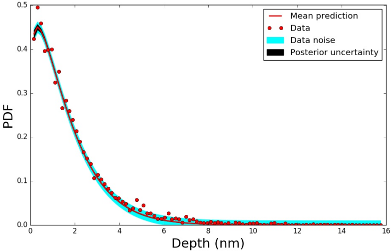
- fit a probability density function (PDF) to this data
- incorporate all uncertainty sources
- propagate through Xolotl (Plasma Surface Interactions Simulator)

UQ in PSI – Conventional calibration: no model error

SRIM only

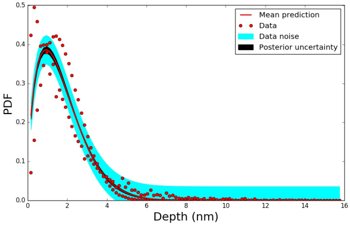


MD only



- Fit a Weibull PDF
  $$f(x;\lambda_1,\lambda_2) = \frac{\lambda_2}{\lambda_1}\left(\frac{x}{\lambda_1}\right)^{\lambda_2-1} e^{-\left(\frac{x}{\lambda_1}\right)^{\lambda_2}}$$
- Given data $y(x_i)$, apply Bayes' theorem
  $$p(\lambda|y) \propto p(y|\lambda)p(\lambda)$$
- Classical Bayesian Likelihood (generalized least-squares)
  $$\ln p(y|\lambda) = \text{const} - \sum_i \frac{(y(x_i) - f(x_i;\lambda))^2}{2\sigma^2}$$

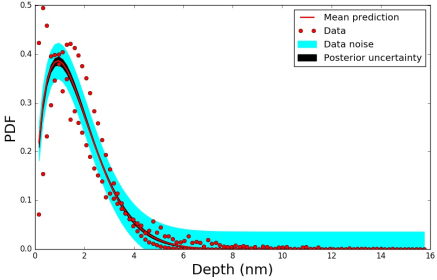
SRIM and MD



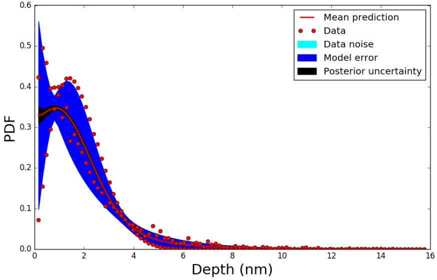
Embedded model error: captures modeling discrepancies

- Allow variability in λ: cast it as a random variable $\lambda(\alpha)$
- Deterministic model $f(x;\lambda) \Rightarrow$ Stochastic model $f(x;\lambda)$ with mean $\mu(x;\alpha)$ and variance $\sigma^2(x;\alpha)$
- Infer α instead of λ
- Likelihood function $\ln p(y|\alpha) = \mathrm{const} - \sum_i \frac{(y(x_i)-\mu(x_i;\alpha))^2}{2\sigma^2(x_i;\alpha)}$

No model error



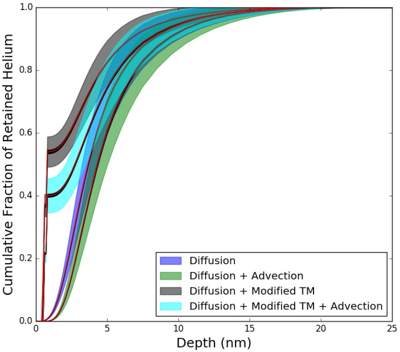
Model error



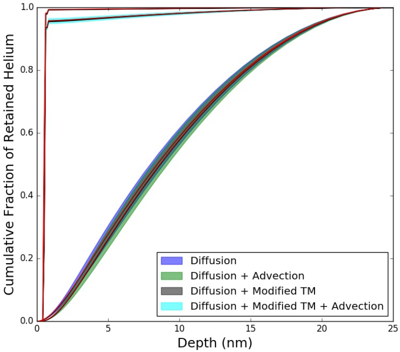
Propagate all sources of uncertainty through Xolotl

- Propagate further in the pipeline with uncertainties
- Two values of nominal flux F_N

$F_N = 4 \times 10^{25}$ He m^{-2}s^{-1}



$F_N = 4 \times 10^{22}$ He m^{-2}s^{-1}



Cumulative Fraction of Helium Retention vs. Depth

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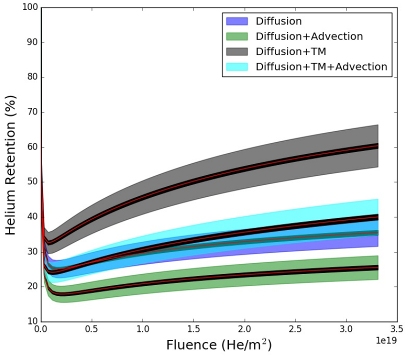

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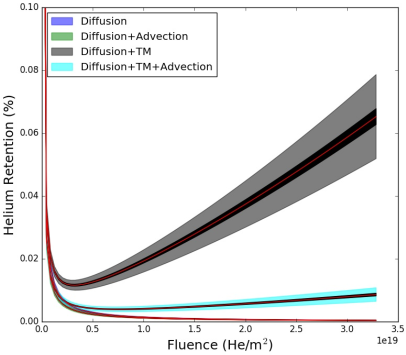
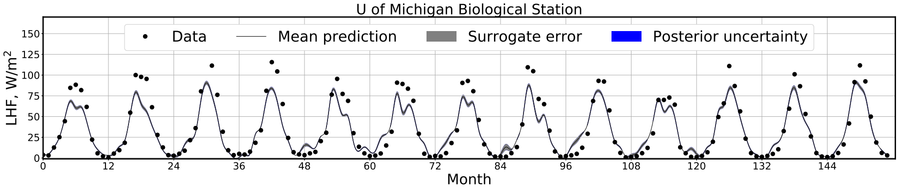


Helium Retention vs. Fluence

E3SM Land Model (ELM)

- US Department of Energy (DOE) sponsored Earth system model
- Land, atmosphere, ocean, ice, human system components
- High-resolution, employ DOE leadership-class computing facilities



- Conventional calibration without model error

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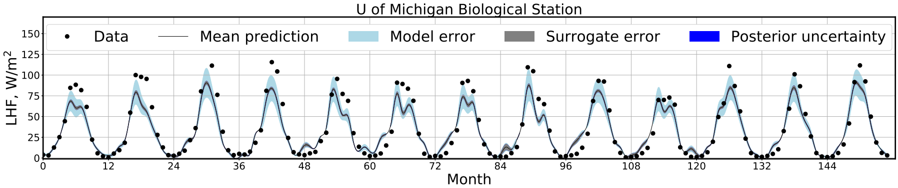

- Predictive variance decomposition with model-error component
- ... with predictive uncertainty that captures model error

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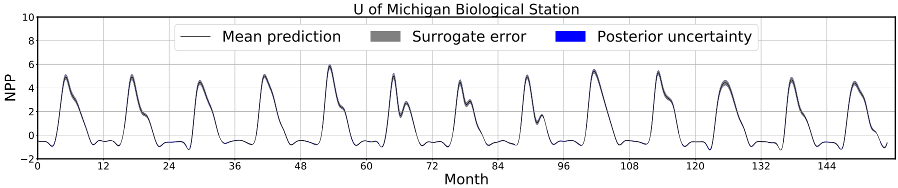

- Predictive variance decomposition with model-error component
- Allows meaningful prediction of other QoIs
  (e.g. no data/observable)

E3SM Land Model (ELM)

E3SM Energy Exascale Earth System Model

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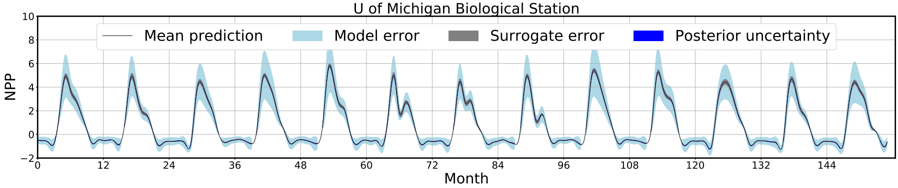

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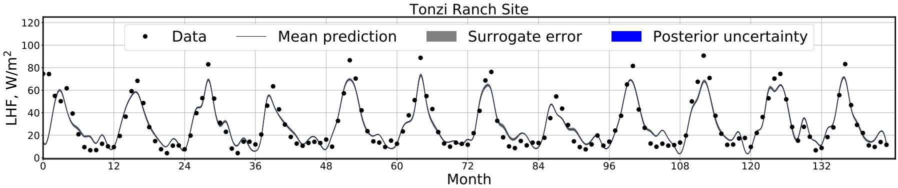

- Predictive variance decomposition with model-error component
- Allows (a more dangerous) extrapolation to other sites

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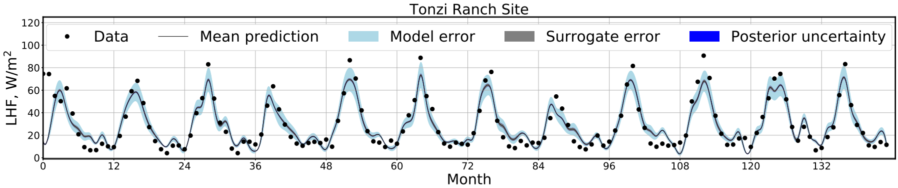

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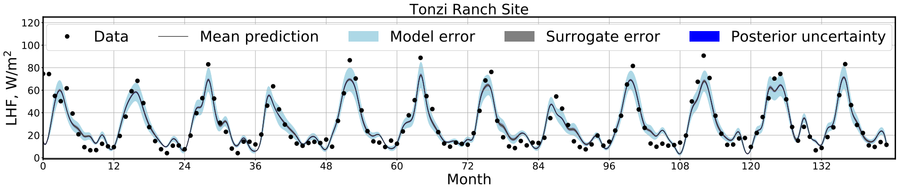

Outline

1. Uncertainty Quantification
   - Intro
   - UQ Toolkit
2. Workflows
   - Inverse UQ: Bayesian Inference, Model Calibration
   - Forward UQ: Surrogate Modeling, Uncertainty Propagation
   - Model Structural Error
3. Applications in SciDAC
   - Plasma Surface Interactions
   - Land Model
4. Summary

Wrap-up

- UQTk provides a powerful set of tools for building general UQ workflows
- Multiple ways to access functionality
  - Direct linking of C++ code
  - Standalone apps
  - Python interface based on Swig
- Available at `http://www.sandia.gov/UQToolkit`
- Suggestions for improvements welcome!
- Do not hesitate to contact us
  `uqtk-users@software.sandia.gov`

Literature

Thank you!

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