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UQTk

The UQTk C++/Python Toolkit for Uncertainty Quantification: Overview and Applications

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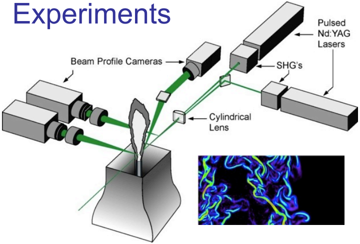
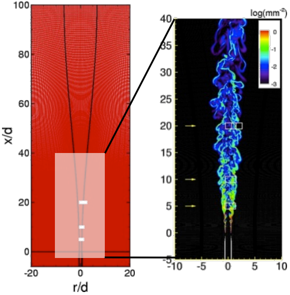
Outline

UQ is about enabling predictive simulations

Experiments



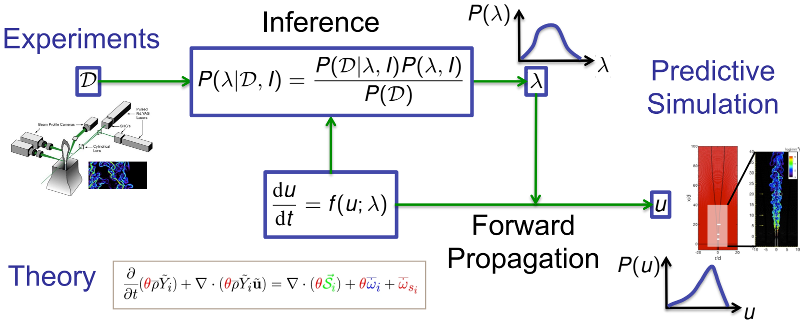
Predictive Simulation



$$\frac{\partial}{\partial t}(\theta\bar{\rho}\tilde{Y}_i) + \nabla\cdot(\theta\bar{\rho}\tilde{Y}_i\tilde{\mathbf{u}}) = \nabla\cdot(\theta\vec{\tilde{S}}_i) + \theta\bar{\dot{\omega}}_i + \bar{\dot{\omega}}_{s_i}$$

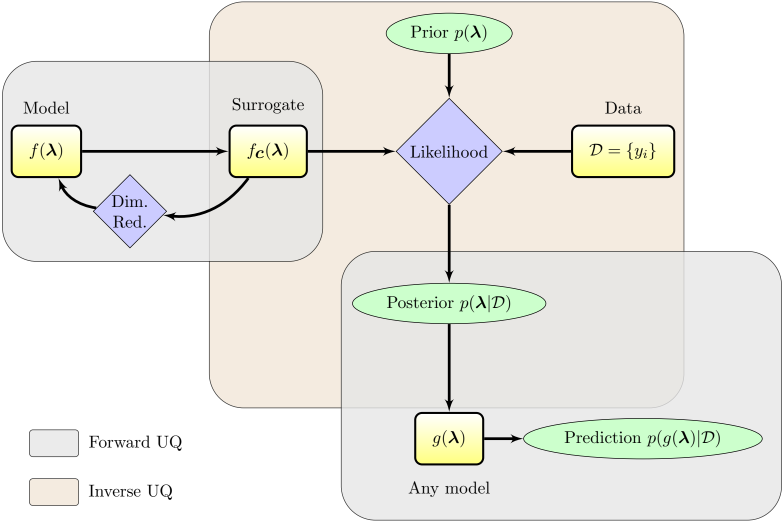
Theory

UQ methods extract information from all sources to enable predictive simulation



- UQ not just about propagating uncertainties
- The term UQ covers a wide range of methods

An example UQTk workflow



UQTk provides tools to build a general UQ workflow

- Tools for
  - Representation of random variables and stochastic processes
  - Forward uncertainty propagation
  - Inverse problems / Model calibration
  - Embedded model error
  - Global Sensitivity Analysis
  - Dimensionality reduction
  - Bayesian Compressive Sensing
  - Low Rank Tensors
  - Gaussian Processes
  - ...
- Tools can be used stand-alone or combined into a general workflow

UQTk is geared towards research, education, prototyping

- 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 BSD 3-Clause License
  - `https://github.com/sandialabs/UQTk`
  - Current version 3.1.4
- Some dependencies included with UQTk. Others (Sundials) downloaded by CMake build system as needed

UQTk supports a wide variety of Polynomial Chaos Expansions (PCEs) operations

- Standard PC Basis types supported:
  - Gauss – Hermite
  - Uniform – Legendre
  - Gamma – Laguerre
  - Beta – Jacobi
- Also support for custom orthogonal polynomials
  - Defined by user-provided three-term recurrence formula
- Both intrusive and non-intrusive PC tools provided
  - Primarily Galerkin projection methods
  - Some regression approaches offered through Bayesian Compressed Sensing module
  - See also Debusschere, *et al.* 2004; Sargsyan, *et al.* 2014

UQTk uses a combination of C++ and Python

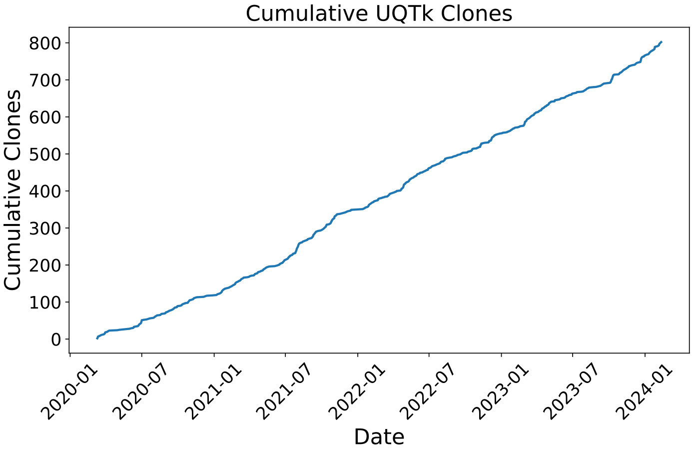
- Main libraries in C++
  - `PCBasis` and `PCSet` classes: PC tools (intrusive and non-intrusive)
  - `Quad` class: quadrature rules (full tensor and sparse tensor product rules)
  - `MCMC, Gproc,...`
- Functionality available via
  - Direct linking of C++ code
  - Standalone apps
  - Python interface using pybind11
- Examples of common workflows provided

Recent Features in UQTk 3.1.x

- New functionality (UQTk 3.1.0)
  - Canonical Low Rank Tensor (LRT) Representations
  - Data Free Inference (DFI) Library
  - tempered MCMC (tMCMC)
  - Basis adaptation
- Improved software engineering
  - Refactored MCMC Class (UQTk 3.1.1)
  - Interface to Python moved from swig to pybind11 (UQTk 3.1.2)
- Miscellaneous improvements
  - New DFI app, compatibility with Sundials 6.x, expanded Python pce_tools (UQTk 3.1.3)
  - UM-Bridge example, upgraded BCS interface (UQTk 3.1.4)
- Watch the UQTk repo and discussion at

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

UQTk Github Repo Clones



- Clones from `https://github.com/sandialabs/UQTk/`
- $\approx$ 200 clones per year

UQTk is used in a variety of applications

- Direct collaborations
  - US DOE SciDAC FASTMath Inst. `https://scidac5-fastmath.lbl.gov/`
  - Variety of US DOE SciDAC partnership projects
  - DOE BER E3SM climate model analysis
- Many other groups at universities, National Labs, and industry
- Common uses: Surrogate Construction, Global Sensitivity Analysis, Bayesian Inference, Forward UQ
- Always welcome new applications / collaborations

Outline

1. UQTk Overview
2. Bayesian Compressed Sensing Illustration
3. Future Developments
4. Summary
5. References
6. Extra Material
7. Bayesian Model Inference and Comparison
8. SciDAC: Application in Climate Modeling

Compressed Sensing addresses sparsity in samples

Sparse regression (Compressive Sensing):

$$\begin{aligned} \boldsymbol{c}^{CS} &= \arg\min_{\boldsymbol{c}} \sum_{i=1}^{m} \left(f(\boldsymbol{x}(\boldsymbol{\xi}^{(i)})) - \sum_{\boldsymbol{\alpha}\in\mathcal{I}} c_{\boldsymbol{\alpha}} \Psi_{\boldsymbol{\alpha}}(\boldsymbol{\xi}^{(i)}) \right)^2 + \lambda \sum_{\boldsymbol{\alpha}\in\mathcal{I}} |\boldsymbol{c}_{\boldsymbol{\alpha}}| \\ &= \arg\min_{\boldsymbol{c}} \left[||\boldsymbol{f} - \boldsymbol{\Psi}\boldsymbol{c}||_2^2 + \lambda ||\boldsymbol{c}||_1 \right] \end{aligned}$$

. . . and in a Bayesian framework → Bayesian Compressive Sensing [Sargsyan, et al., 2014]:

$$\overbrace{p(\boldsymbol{c}|\mathcal{D})}^{\text{Posterior}} \propto \overbrace{p(\mathcal{D}|\boldsymbol{c})}^{\text{Likelihood}} \overbrace{p(\boldsymbol{c})}^{\text{Prior}} \longrightarrow \boldsymbol{c}^{MAP} = \arg\max_{\boldsymbol{c}} \log p(\boldsymbol{c}|\mathcal{D}) = \arg\max_{\boldsymbol{c}} \left[\log L_{\mathcal{D}}(\boldsymbol{c}) + \log p(\boldsymbol{c})\right]$$

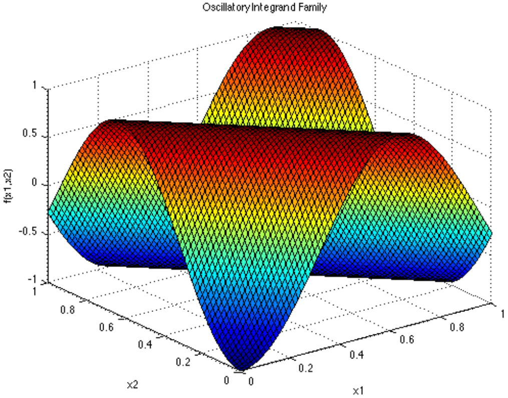
with Laplace sparsifying prior

$$p(\boldsymbol{c}) = \left(\frac{\lambda}{2}\right)^K \exp\left(-\lambda \sum_{\boldsymbol{\alpha}\in\mathcal{I}} |\boldsymbol{c}_{\boldsymbol{\alpha}}|\right)$$

UQTk BCS Function Call

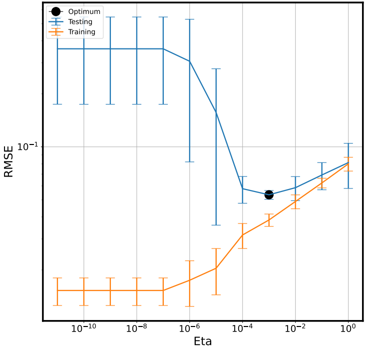
```
def UQTkBCS(pc_begin, xdata, ydata, eta=1.e-3, niter=1,\
            mindex_growth=None, ntry=1, eta_folds=5,\
            eta_growth=False, eta_plot = False,\
            regparams=None, sigma2=1e-8, npccut=None,\
            pcf_thr=None, verbose=0, return_sigma2=False):

Inputs:
pc_begin:   PC object with information about the starting basis
xdata:      Sampled input values [#samples, #dimensions]
ydata:      Function evaluations (QoIs)
eta:        NumPy array, list, or float with the threshold for
            stopping the evidence maximization algorithm.
niter:      Number of iterations for order growth
ntry:       Number of folds cross-validation of the retained basis

Outputs:
pc_model_final: PC object with retained basis terms
cfs_final:      Corresponding PC coefficients
```

Genz Oscillatory Function Test Case



- $f(x) = cos\left(\sum_{i=1}^{d} a_i x_i\right)$
- $d = 4, a_i = 2.0/i^2, \sigma_{data} = 0.05, nTrain = 100$
- `https://www.sfu.ca/~ssurjano/oscil.html`

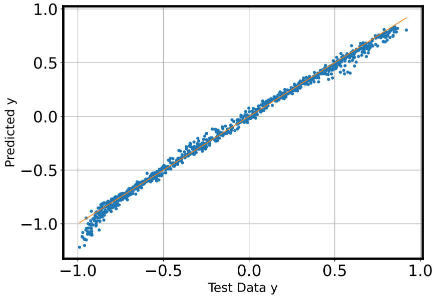
Cross-validation identifies the optimal stop criterion




```
import PyUQTk.pce as uqtkpce
import PyUQTk.PyPCE.pce_tools as pce_tools
nord = 4; ndim = 4; type = "LU"; alpha = 0.0; beta = 1.0
pc_begin = uqtkpce.PCSet("NISPnoq", nord, ndim, type, alpha, beta)
eta_range = 1/np.power(10,[i for i in range(0,12)])
pc_final, c_k = pcetools.UQTkBCS(pc_begin,xdata,ydata,eta=eta_range)
```

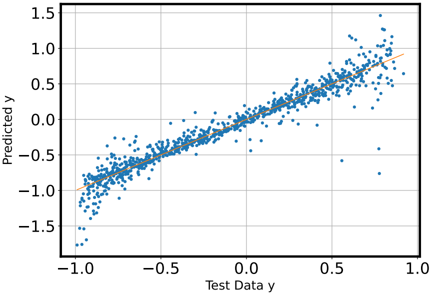
BCS approximates the Genz function quite well using only 10 basis terms

```
=====================================================
multi-indices(i,j), with i = 0 ... P, j = 1 ... nDim
with P = 9, and nDim = 4
-----------------------------------------------------
i\j | 1  2  3  4
------------------
0   | 1  0  0  0
1   | 0  1  0  0
2   | 0  0  0  0
3   | 2  2  0  0
4   | 0  0  1  0
5   | 2  0  0  1
6   | 2  0  1  0
7   | 3  0  0  0
8   | 0  0  0  1
9   | 0  0  0  2
```



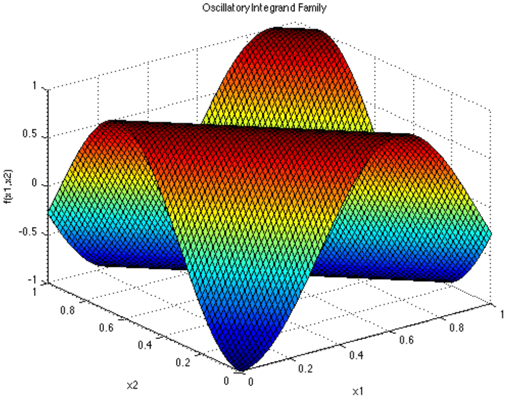
- Original full PCE has 70 terms
- Lower dimensions show up with highest order

Regression with full basis set has larger testing error



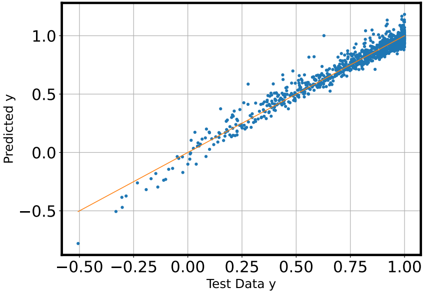
- Full PCE basis with 70 terms leads to overfitting

Higher-Dimensional Genz Oscillatory Function



- $f(x) = cos\left(\sum_{i=1}^{d} a_i x_i\right)$
- $d = 10, a_i = 2.0/i, \sigma_{data} = 0.05, nTrain = 400$
- `https://www.sfu.ca/~ssurjano/oscil.html`

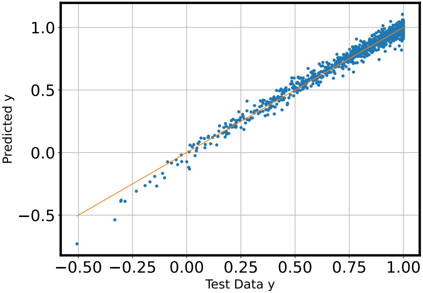
Compressed sensing on full basis is challenging



- Selects 31 basis terms out of a total of 1001
- Agreement is OK, but not stellar

Iterative basis growth better captures important terms

```
==== BCS with multiindex of size 66 ====
BCS has selected 53 basis terms out of 66
==== BCS with multiindex of size 267 ====
BCS has selected 37 basis terms out of 267
==== BCS with multiindex of size 222 ====
BCS has selected 65 basis terms out of 222
```




```
import PyUQTk.pce as uqtkpce
import PyUQTk.PyPCE.pce_tools as pce_tools
nord = 4; ndim = 4; type = "LU"; alpha = 0.0; beta = 1.0; n_it = 3
pc_begin = uqtkpce.PCSet("NISPnoq", nord, ndim, type, alpha, beta)
eta_r = 1/np.power(10,[i for i in range(0,12)])
pc_final,c_k = pcetools.UQTkBCS(pc_begin,xdata,ydata,
               mindex_growth='nonconservative',eta=eta_r,niter=n_it)
```

Outline

A Python-only implementation will provide more flexibility

- Current mix of C++ and Python is main source of install problems
- Original C++ data structures limit new developments (mixed PC bases) and make coupling to other packages challenging
- Original implementation pre-dates github development tools
- Some (large) Third Party Libraries (TPLs) support only legacy functionality (intrusive UQ)
- Plan to take main Python functionality into standalone Python Toolkit for UQ
    - Installation via pip install
    - Documentation directly into github pages

General Python Surrogate Modeling Interface

- There are many Python UQ tools and libraries in the community
- Most of them have different implementations of commonly used UQ operations
  - Surrogate models
  - Global Sensivity Analysis
  - Bayesian Inference
- Can we develop general interfaces to some of these operations?
  - Start with surrogate modeling interface
  - Avoid duplication and allow codes like DAKOTA to call surrogate models implemented by multitude of Python UQ toolboxes

Surrogate Modeling Interface Specifications

- Python class
  - Allow scalar and multivariate Quantities of Interest (QoIs)
  - Provide option to return derivatives?
  - Provide option to return Sobol' indices?
  - Provide option for adaptive refinement?
- Illustrative examples:
  - SMT: Surrogate Modeling Toolbox (`https://smt.readthedocs.io/`)
  - Others?
- Other suggestions?
- Input welcome at `bjdebus@sandia.gov`

Summary

- 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 through pybind11
- Available at `https://github.com/sandialabs/UQTk`
- Suggestions and questions welcome at `https://github.com/sandialabs/UQTk/discussions`
- Python-only version with general surrogate modeling interface in the planning stages

References

- B. Debusschere, H. Najm, P. Pébay, O. Knio, R. Ghanem and O. Le Maître, "Numerical Challenges in the Use of Polynomial Chaos Representations for Stochastic Processes", *SIAM J. Sci. Comp.*, 26:2, 2004.
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- K. Sargsyan, X. Huan, and H. Najm. "Embedded Model Error Representation for Model Calibration", in press, *International Journal for Uncertainty Quantification*, 2019.

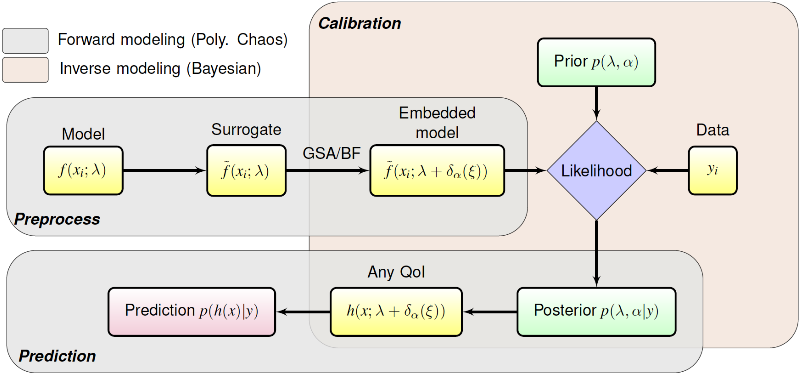
Outline

DAKOTA and UQTk implement similar methods but are geared towards different user groups.

- DAKOTA:
  - Geared towards end-user, analyst
  - Fully packaged, parallel workflow
- UQTk:
  - Geared towards developers, students, researchers
  - Components to build a workflow with
  - More lightweight and easier to get “under the hood”

There are plans to couple DAKOTA and UQTk through sharing libraries

General Uncertainty Quantification Workflow



- Predictive uncertainty decomposition: Total Variance =

Parametric uncertainty + Data noise + Model error + Surrogate error

Many flavors of MCMC are available

- Single Site MCMC (ssMCMC)
- Adaptive MCMC (aMCMC)
- Metropolis-adjusted Langevin algorithm (MALA) or Langevin sampling
- Tempered MCMC (tMCMC)

Surrogate models reduce the cost of computing Sobol' indices.

Variance-based decomposition:

$$f(x_1, x_2, \ldots, x_d) = f_0 + \sum_{1\leq i\leq d} f_i(x_i) + \sum_{1\leq i<j\leq d} f_{i,j}(x_i, x_j) + \sum_{1\leq i<j<k\leq d} f_{i,j,k}(x_i, x_j, x_k) + \ldots$$

- f_i, $f_{i,j}$, $f_{i,j,k}$, $\ldots$ are mutually orthogonal

Sobol' sensitivity indices measure fractional contributions of each parameter or group of parameters towards the total variance of selected QoIs

$$S_i = \frac{\mathrm{V}_{\boldsymbol{x}_i}\left[\mathrm{E}_{\boldsymbol{x}_{-i}}[f(\boldsymbol{x})]\,|\boldsymbol{x}_i]\right.}{\mathrm{V}\,[f(\boldsymbol{x})]}\ \text{(main)}, \quad S_i^T = \frac{\mathrm{E}_{\boldsymbol{x}_{-i}}\left[\mathrm{V}_{\boldsymbol{x}_i}[f(\boldsymbol{x})|\boldsymbol{x}_{-i}]\right]}{\mathrm{V}\,[f(\boldsymbol{x})]}\ \text{(total)}$$

- joint (most of the time between two variables) can also be informative

Sobol' indices estimates:

- Random Sampling → need computationally cheap (surrogate) models & slow to converge
- Polynomial Chaos Expansions → exploit orthogonality of basis terms

Compressed Sensing addresses sparsity in samples.

f (ELM-LF) is high-dimensional (47 input parameters)

- standard regression approaches are underdetermined $\rightarrow$

Sparse regression (Compressive Sensing):

$$\begin{aligned} \boldsymbol{c}^{CS} &= \arg\min_{\boldsymbol{c}} \sum_{i=1}^{m} \left(f(\boldsymbol{x}(\boldsymbol{\xi}^{(i)})) - \sum_{\boldsymbol{\alpha}\in\mathcal{I}} c_{\boldsymbol{\alpha}} \Psi_{\boldsymbol{\alpha}}(\boldsymbol{\xi}^{(i)}) \right)^2 + \lambda \sum_{\boldsymbol{\alpha}\in\mathcal{I}} |\boldsymbol{c}_{\boldsymbol{\alpha}}| \\ &= \arg\min_{\boldsymbol{c}} \left[||\boldsymbol{f} - \boldsymbol{\Psi}\boldsymbol{c}||_2^2 + \lambda ||\boldsymbol{c}||_1 \right] \end{aligned}$$

. . . and in a Bayesian framework $\rightarrow$ Bayesian Compressive Sensing [Sargsyan, et al., 2014]:

$$\overbrace{p(\boldsymbol{c}|\mathcal{D})}^{\text{Posterior}} \propto \overbrace{p(\mathcal{D}|\boldsymbol{c})}^{\text{Likelihood}} \overbrace{p(\boldsymbol{c})}^{\text{Prior}} \longrightarrow \boldsymbol{c}^{MAP} = \arg\max_{\boldsymbol{c}} \log p(\boldsymbol{c}|\mathcal{D}) = \arg\max_{\boldsymbol{c}} \left[\log L_{\mathcal{D}}(\boldsymbol{c}) + \log p(\boldsymbol{c})\right]$$

with Laplace sparsifying prior

$$p(\boldsymbol{c}) = \left(\frac{\lambda}{2}\right)^K \exp\left(-\lambda \sum_{\boldsymbol{\alpha}\in\mathcal{I}} |\boldsymbol{c}_{\boldsymbol{\alpha}}|\right)$$

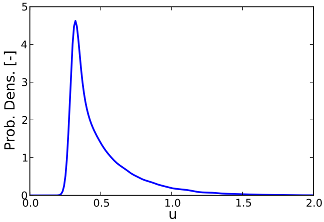
Longer Term Plans

- Coupling with other libraries
  - Better support for user specified third-party libraries, e.g. random number generators, integrators, ...
  - Coupling with DAKOTA (SNL) and MUQ (MIT) for leveraging functionality
- Mixed PC basis types
- More general multi-index specification
- Data structures amenable to parallelization and GPU acceleration
- Other developments you would like to see?
  - Let us know at `https://github.com/sandialabs/UQTk/discussions`

Polynomial Chaos Expansions represent random variables

$$u = \sum_{k=0}^{P} u_k \psi_k(\xi)$$

- u: Random Variable (RV) represented with 1D PCE
- u_k: PC coefficients (deterministic)
- ψ_k: 1D Hermite polynomial of order k
- ξ: Gaussian RV

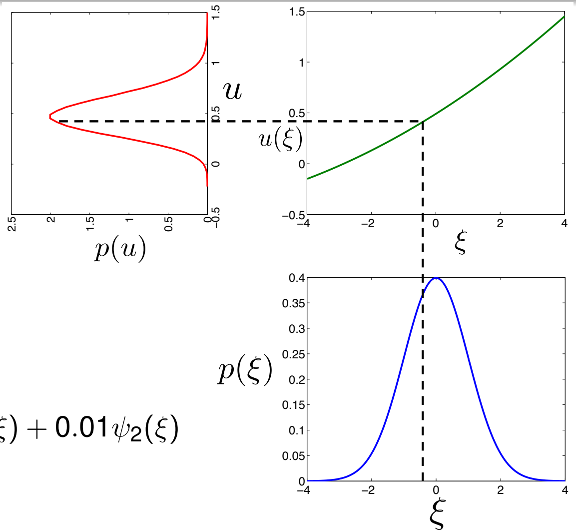


$$u = 0.5 + 0.2\psi_1(\xi) + 0.1\psi_2(\xi)$$

Expansion in terms of functions of random variables multiplied with deterministic coefficients

- Set of deterministic PC coefficients fully describes RV
- Separates randomness from deterministic dimensions

PCEs can be seen as a functional map from standard RVs to the represented RV



$$u = 0.5 + 0.2\psi_1(\xi) + 0.01\psi_2(\xi)$$

One-Dimensional Hermite Polynomials

$$\begin{aligned}\psi_0(\xi) &= 1 \\ \psi_k(\xi) &= (-1)^k e^{\xi^2/2} \frac{\mathrm{d}^k}{\mathrm{d}\xi^k} e^{-\xi^2/2}, \qquad k = 1, 2, \ldots\end{aligned}$$

$$\psi_1(\xi) = \xi, \quad \psi_2(\xi) = \xi^2 - 1, \quad \psi_3(\xi) = \xi^3 - 3\xi, \ \ldots$$

The Hermite polynomials form an orthogonal basis over $[-\infty, \infty]$ with respect to the inner product

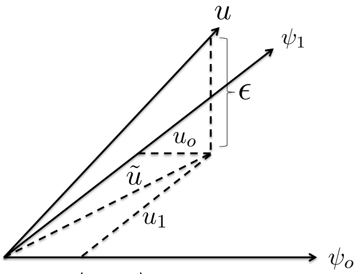
$$\langle \psi_i \psi_j \rangle \equiv \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \psi_i(\xi)\psi_j(\xi) w(\xi) d\xi = \delta_{ij} \left\langle \psi_i^2 \right\rangle$$

where $w(\xi) = e^{-\xi^2/2}$ is the weight function.

Note that $\frac{e^{-\xi^2/2}}{\sqrt{2\pi}}$ is the density of a standard normal random variable

Propagation of Uncertain Inputs Represented with PCEs

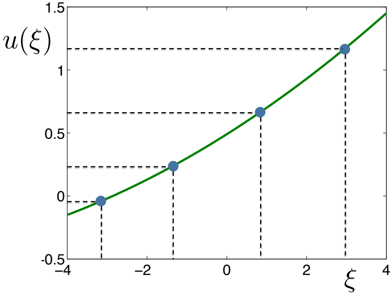
Galerkin Projection



$$u_k = \frac{\langle u\Psi_k\rangle}{\langle \Psi_k^2\rangle}, \quad k = 0, \ldots, P$$

Residual orthogonal to space covered by basis functions

Collocation



Match PCE to random variable at chosen sample points: interpolation or regression

Galerkin projection methods are either intrusive or non-intrusive

- Use same projection but in different ways

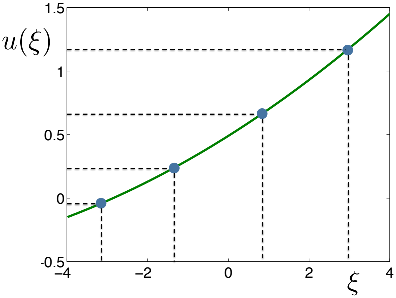
$$u_k = \frac{\langle u\Psi_k \rangle}{\langle \Psi_k^2 \rangle}, \quad k = 0, \dots, P$$

- Intrusive methods apply Galerkin projection to governing equations
  - Results in set of equations for the PC coefficients
  - Requires redesign of computer code
  - PCEs for all uncertain variables in system
- Non-intrusive approaches apply Galerkin projection to outputs of interest
  - Sampling to evaluate projection operator
  - Can use existing code as black box
  - Only computes PCEs for quantities of interest

Collocation approaches are non-intrusive and minimize errors at sample points

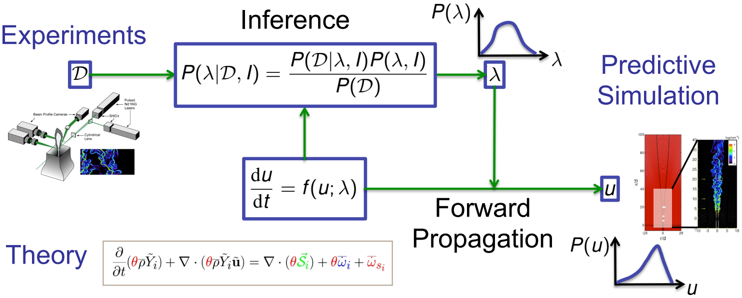
$$\sum_{k=0}^{P} u_k \Psi_k(\xi_i) = u(\xi_i)$$

$$i = 1, \ldots, N_c$$



- Use functional representation point of view
- Can use interpolation, e.g. Lagrange interpolants
- Or use regression approaches: $P + 1$ degrees of freedom to fit N_c points
- Can position points where most accuracy desired

Bayesian inference offers a probabilistic approach for inverse problems



- Bayesian inference can handle various sources of data
- Probabilistic formulation readily accommodates various sources of uncertainty

Bayes' rule updates prior belief with information extracted from data

- Bayes' rule

$$\overbrace{P(\boldsymbol{\lambda}|\mathcal{D})}^{\text{Posterior}} = \frac{\overbrace{P(\mathcal{D}|\boldsymbol{\lambda})}^{\text{Likelihood}}\,\overbrace{P(\boldsymbol{\lambda})}^{\text{Prior}}}{\underbrace{P(\mathcal{D})}_{\text{Evidence}}} \propto P(\mathcal{D}|\boldsymbol{\lambda})P(\boldsymbol{\lambda})$$

- Update prior distribution/knowledge about parameter $\boldsymbol{\lambda}$ to posterior distribution given data $\mathcal{D}$, using likelihood function $\mathcal{L}(\boldsymbol{\lambda}) \equiv P(\mathcal{D}|\boldsymbol{\lambda})$
- Data $\mathcal{D} = \{d_i\}_{i=1}^N$ - measurements of *some* quantities of interest (QoIs)
- Evidence $P(\mathcal{D})$ can be seen as a normalizing term

The prior distribution represents prior information about the inferred quantities

- Based on prior data, literature, or expert opinion
- Prior distribution helps to keep inference well defined, *e.g.* if quantity needs to remain positive
- If not much data available, posterior will be strongly influenced by the prior
- When a lot of data available, data will have predominant influence on posterior
- Prior is both powerful and dangerous
- If no prior information is available, non-informative priors can be used
  - *E.g.* uniform from $-\infty$ to $+\infty$

The likelihood function measures goodness-of-fit

- The key component that connects the model inputs to measured QoIs
- The *noise model* accounts for disagreement between model and data
  - Common case is i.i.d. Gaussian measurement noise in each data point

$$\mathcal{L}(\boldsymbol{\lambda}) = P(\mathcal{D}|\boldsymbol{\lambda}) = \frac{1}{(2\pi)^{N/2}\sigma^N} \exp\left(-\sum_{i=1}^{N} \frac{(d_i - f_i(\boldsymbol{\lambda}))^2}{2\sigma^2} \right)$$

  - If the model itself is uncertain, then the noise model needs to reflect that
- Generally the log-likelihood is used to avoid underflow

$$\ln \mathcal{L}(\boldsymbol{\lambda}) = \ln P(\mathcal{D}|\boldsymbol{\lambda}) = -\frac{N}{2}\ln(2\pi) - N\ln(\sigma) - \sum_{i=1}^{N} \frac{(d_i - f_i(\boldsymbol{\lambda}))^2}{2\sigma^2}$$

The posterior contains updated knowledge about inferred parameters

- Gives the inferred values of the parameters as well as their uncertainty based on all sources of uncertainty
- The maximum value is referred to as the *Maximum A Posteriori* (MAP) value
- Posterior distribution generally not analytically tractable
- Commonly people resort to MCMC sampling approaches to draw samples from this distribution
  - Samples can then be used to construct a PCE expansion for the inferred parameters
  - Can be fed into other models for forward propagation

Bayes' rule derives from elementary probability theory

Conditional probability:

$$P(A, B) = P(A|B)P(B) = P(B|A)P(A)$$

$$P(A|B) = \frac{P(B|A)P(A)}{P(B)}$$

Outline

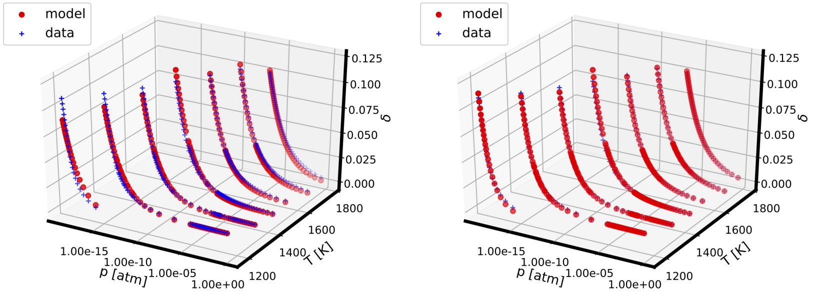
Bayesian Inference and Model Comparison

- Model for thermodynamic properties of RedOx active materials
- Used in design of materials for solar thermochemical hydrogen production
- General model form $\delta = f(p_{O_2}, T)$
  - Model A: 4 parameters
  - Model B: 8 parameters
- Bayesian parameter inference and model comparison
- Joint work with Dr. Ellen Stechel at Arizona State University and Tony McDaniel at Sandia
- Funded by the DOE Office of Energy Efficiency and Renewable Energy (EERE)

Bayesian Inference and Model Comparison

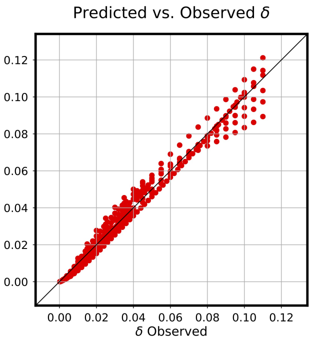
- Employed UQTk Python Bayesian Inference tools to infer parameters and compare the two models
- Model properties and numerical settings specified via flexible xml input file
- Python postprocessing and model evidence computation
- Workflow is an example included in the UQTk release

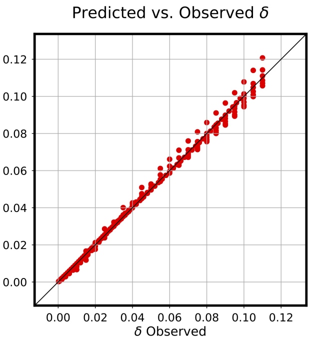
Both models agree well with data



- Model A (left) and Model B (right)

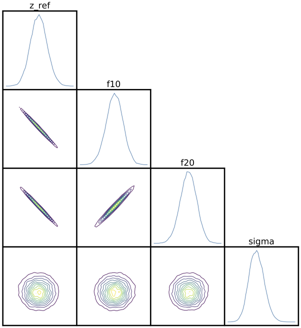
Both models agree well with data

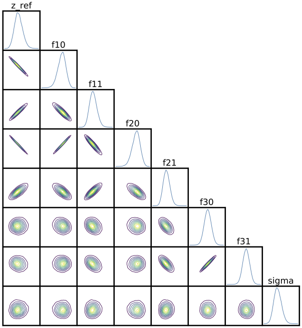




- Model B (right) has smaller residuals

Posterior distributions were sampled with adaptive MCMC





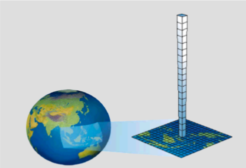
- Well-defined unimodal distributions
- Model B has more dependencies between its parameters

Model evidence favors model B

- Model evidence computed from posterior samples, using a Gaussian approximation
  - Model A: Ln(evidence) = 1580
  - Model B: Ln(evidence) = 1939
- Despite its higher complexity, model B is clearly favored.
- For situations with more measurement noise, or fewer data points, a simpler model may be preferred

Outline

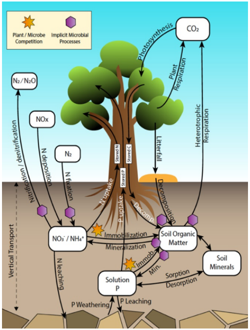
SciDAC BER Partnership Application

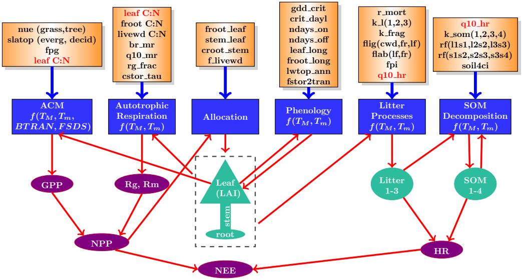


- Optimization of Sensor Networks for Improving Climate Model Predictions
- PI: Daniel Ricciuto at ORNL
- Joint work with MIT FASTMath team (Youssef Marzouk)
- Two applications of UQTk
    - Surrogate models for Global Sensitivity Analysis (GSA) – Cosmin Safta (SNL)
    - Bayesian calibration with model error – Khachik Sargsyan (SNL)

E3SM Land Model (ELM)

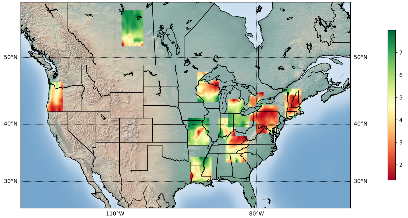
- US Department of Energy (DOE) sponsored Earth system model
- Land, atmosphere, ocean, ice, human system components
- High-resolution, employ DOE leadership-class computing facilities
- Some of the results shown here are with ELM-LF: a lower-fidelity, python version



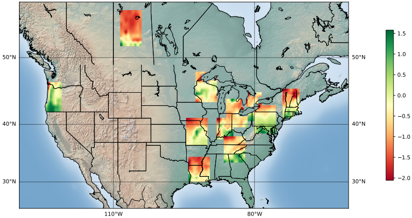


GSA is needed for multiple Quantities of Interest.

Gross Primary Production (GPP, July 2004)



Net Ecosystem Exchange (NEE, July 2004)

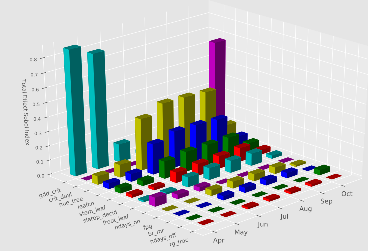


Quantities of Interest

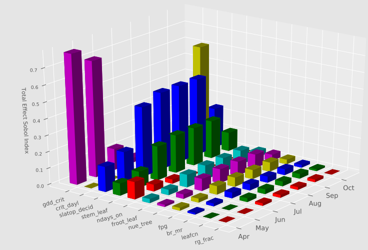
- Gross Primary Production (GPP)
- Total Leaf Area Index (LAI)
- Net Ecosystem Exchange (NEE)
- . . .

Total Effect Sobol' Indices for Model Parameters Relevant at US-Ha1 ($42.5^\circ N$, $72.2^\circ W$)

GPP



LAI

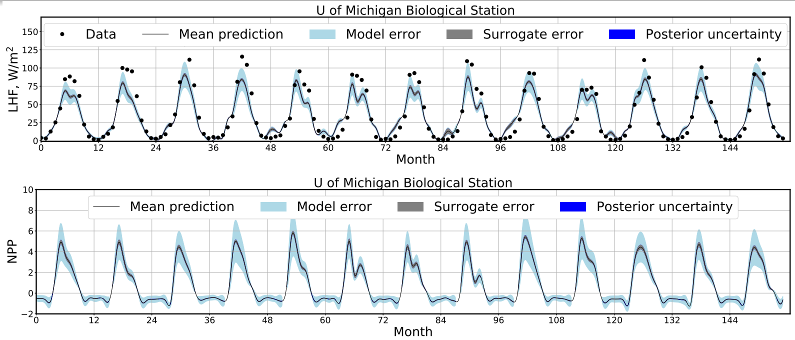


- Sparse regression model accuracy around 10%
- Identified a set of 8-12 parameters (out of 47) that control model outputs of interest.
- Expected time dependencies recovered via sparse regression techniques.

Calibration with *embedded* model error

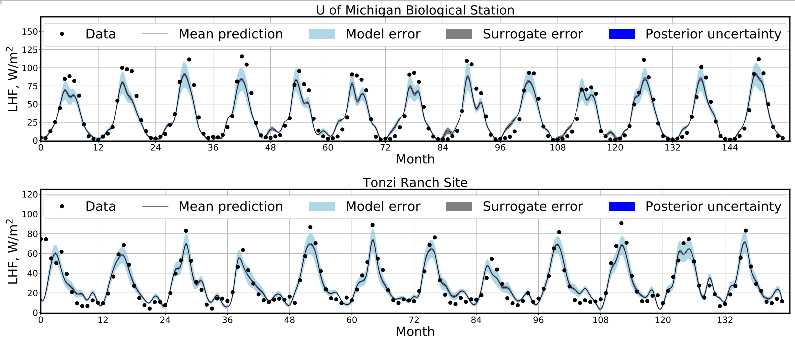
- Model structural error embedding approach [Sargsyan, et al. 2015, 2019]
  - $g(x) = f(x; \lambda + \delta(x)) + \epsilon$
  - Physics-driven model correction
  - Meaningful extrapolation to full set of QoI predictions
  - Disambiguation between model error and data noise
- Simultaneous Bayesian inference of physical parameters and embedded model correction parameters
- Likelihood computation requires uncertainty propagation of embedded stochastic terms
- UQTk provides machinery for both Bayesian inference (adaptive MCMC) and uncertainty propagation via Polynomial Chaos (non-intrusive spectral projection)

ELM calibration with FLUXNET observations



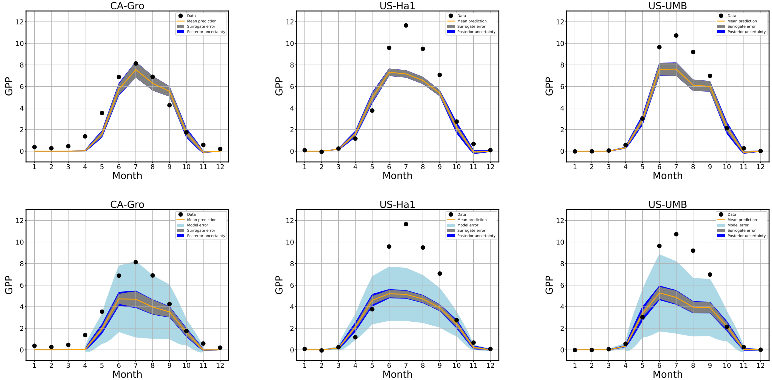
- Predictive variance decomposition with model-error component
- Allows meaningful prediction of other QoIs (e.g. no data/observable)
- Allows (a more dangerous) extrapolation to other sites

ELM calibration with FLUXNET observations



- Predictive variance decomposition with model-error component
- Allows meaningful prediction of other QoIs (e.g. no data/observable)
- Allows (a more dangerous) extrapolation to other sites

ELM-LF calibration with FLUXNET observations



- Embedding removes biases and avoids overfitting
- Model error is the dominant uncertainty component