UQTk

A C++/Python Toolkit for Uncertainty Quantification

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QUANTIFICATION OF UNCERTAINTY IN EXTREME SCALE COMPUTATIONS
QUEST

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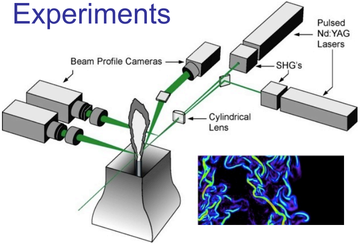
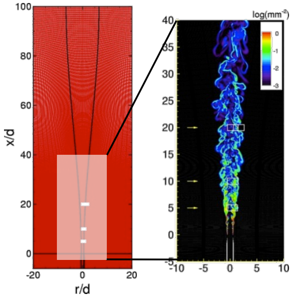
Outline

UQ is about enabling predictive simulations

Experiments



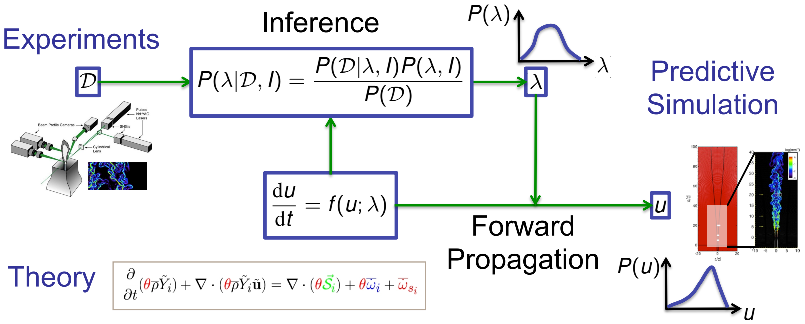
Predictive Simulation



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

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

UQTk provides tools to build a general UQ workflow

- Tools for
  - Representation of random variables and stochastic processes
  - Forward uncertainty propagation
  - Inverse problems
  - Sensitivity analysis
  - Bayesian Compressive Sensing
  - Gaussian Processes
- Tools can be used stand-alone or combined into a general workflow

We want UQTk to be straightforward to download, install and use

- Target usage:
  - Rapid prototyping of UQ workflows
  - Algorithmic research in UQ
  - Tutorials / educational
- Released under the GNU Lesser General Public License
  - `http://www.sandia.gov/UQToolkit/`
  - Current version 2.1
  - Version 3.0 coming (very) soon
- No massive third party libaries to download, install, and configure

UQTk is used in a variety of applications

- Direct collaborations
  - US DOE SciDAC QUEST UQ institute `http://www.quest-scidac.org`
  - Variety of US DOE SciDAC partnership projects
  - Part of US DOE BER ACME climate model analysis tools
  - Always welcome new applications / collaborations
- Downloads from `http://www.sandia.gov/UQToolkit`
  - $\approx$ 600 total downloads
  - $\approx$ 425 downloads of version 2.x
  - Mostly academic and laboratory research groups
- Mailing lists
  - `uqtk-announce@software.sandia.gov`
  - `uqtk-users@software.sandia.gov`
  - Join at `http://www.sandia.gov/UQToolkit`

We rely on Polynomial Chaos expansions (PCEs) to represent uncertainty

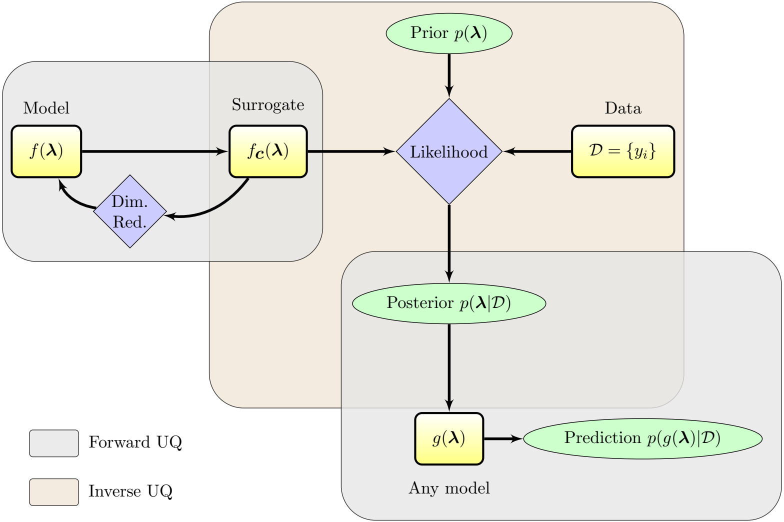
- Standard PC Basis types supported:
  - Gauss – Hermite
  - Uniform – Legendre
  - Gamma – Laguerre
  - Beta – Jacobi
- Also support for custom orthogonal polynomials
  - Defined by user-provided three-term recurrence formula
- Both intrusive and non-intrusive PC tools provided
  - Primarily Galerkin 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 based on Swig (UQTk version 3.0)
- Download as tar file and configure with `CMake`
- Examples of common workflows provided

Outline

An example UQTk workflow (UQTk version 3.0)



An example UQTk workflow (UQTk version 3.0)

- Consider uncertain parameter vector $\boldsymbol{\lambda}$
- Propagate uncertainty in $\boldsymbol{\lambda}$ through model $g(\boldsymbol{\lambda})$
- First calibrate $\boldsymbol{\lambda}$ using data on function $f(\boldsymbol{\lambda})$
- Consider the following calibration functions $f(\boldsymbol{\lambda})$:
  - Gaussian: $f^G(\boldsymbol{\lambda}) = \exp\left(-\sum_{i=1}^{d} a_i^2 \lambda_i^2\right)$
  - Exponential: $f^E(\boldsymbol{\lambda}) = \exp\left(\sum_{i=1}^{d} a_i \lambda_i\right)$
  - 5 dimensional $\boldsymbol{\lambda}$: $\boldsymbol{a} = (0.4, 0.3, 0.2, 0.1, 0.05)$
- Forward models $g(\boldsymbol{\lambda})$:
  - Gaussian: $g_1(\boldsymbol{\lambda}) = f^G(\boldsymbol{\lambda})$
  - Exponential: $g_2(\boldsymbol{\lambda}) = f^E(\boldsymbol{\lambda})$
  - Summation: $g_3(\boldsymbol{\lambda}) = \sum_{i=1}^{d} \lambda_i$
- For more details, see “Handbook of Uncertainty Quantification", Springer, 2016

Surrogate models provide computationally cheap approximations for full forward model

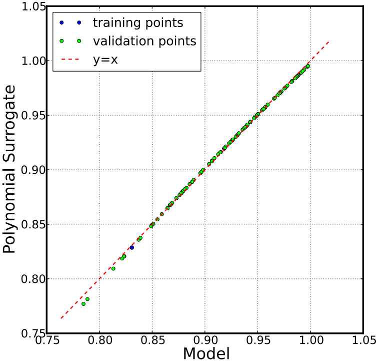
- Used instead of full forward model in computationally demanding operations such as optimization and calibration
- Use PCE surrogate model
- Same approach as forward UQ
  - Legendre-Uniform PCEs
  - Use uniform distributions over range of input parameters
  - Galerkin projection with Gauss quadrature
  - 3^{rd} order PCE using $4^5 = 1024$ quadrature points
  - 111 random validation samples to assess surrogate accuracy

Sample UQTk commands (using stand-alone apps)

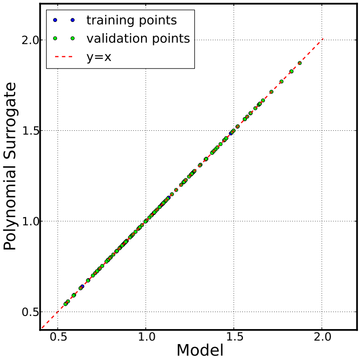
- Generate quadrature points:
  `generate_quad -d 5 -g LU -x full -p 4`
- Generate random samples for validation:
  `pce_rv -w PCvar -d 5 -n 111 -p 5 -x LU`
- Evaluate model at quadrature and validation points
- Perform Galerkin projection:
  `pce_resp -d 5 -x LEG -o 3 -e`
- Evaluate output PCE at validation points to compute error:
  `pce_eval -x PC -s LU -o 3 -f <INPC>`

Surrogate Construction

Gaussian



Exponential

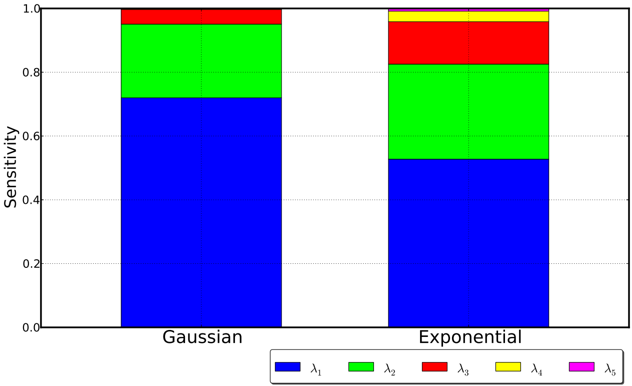


- 3^{rd} order PC surrogate accurate up to 0.1% relative error for both Gaussian and Exponential function

Sensitivity analysis enables dimensionality reduction

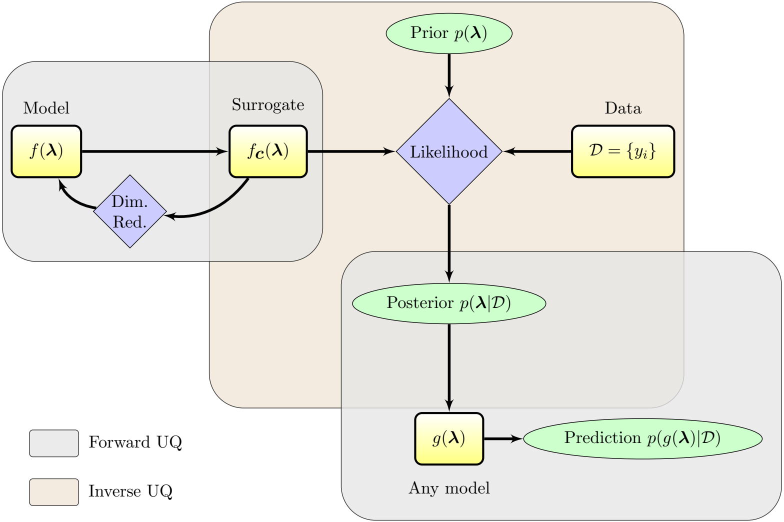
- UQTk computes main, joint, and total sensitivity coefficients
  - S_i: Fraction of variance due to λ_i only
  - S_{ij}: Fraction of variance due to both λ_i and λ_j
  - S_i^T: Fraction of variance due to λ_i by itself and in combination with any other λ_j
- Can be computed analytically from PC response surface
- `pce_sens -m mindex.dat \`
  `-f PCcoeff_quad.dat -x LU`

Components that explain most of the variance are retained



- More than 80% of variance attributed to first two components
- Include only λ_1 and λ_2 in calibration

Bayesian calibration using surrogate models



Bayesian Parameter Inference

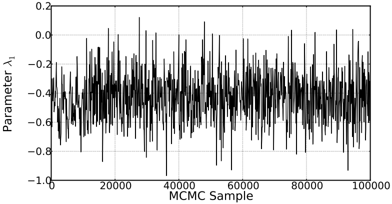
$$\overbrace{p(\boldsymbol{\lambda}|\mathcal{D})}^{\text{Posterior}} \propto \overbrace{p(\mathcal{D}|\boldsymbol{\lambda})}^{\text{Likelihood}}\,\overbrace{p(\boldsymbol{\lambda})}^{\text{Prior}}$$

$$\mathcal{L}_{\mathcal{D}}(\boldsymbol{\lambda}) = p(\mathcal{D}|\boldsymbol{\lambda}) \propto \prod_{j=1}^{R} \exp\left(-\frac{(y_j^G - f^G(\boldsymbol{\lambda}))^2}{2\sigma^2}\right) \exp\left(-\frac{(y_j^E - f^E(\boldsymbol{\lambda}))^2}{2\sigma^2}\right)$$

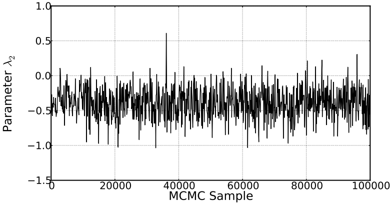
- Generate R random noisy realizations of $f^G(\boldsymbol{\lambda})$ and $f^E(\boldsymbol{\lambda})$ as data $\mathcal{D}$
- Assume Normally distributed priors $N(0, 0.3)$ on λ_1 and λ_2
- Infer λ_1 and λ_2 against data on both $f^G(\boldsymbol{\lambda})$ and $f^E(\boldsymbol{\lambda})$
- ```
  model_inf -x xfile.dat -y yfile.dat -f pc \
    -l classical -m 100000 -e 0.01 -i normal
  ```
  ```

Markov Chain Monte Carlo generates a set of posterior samples

λ_1

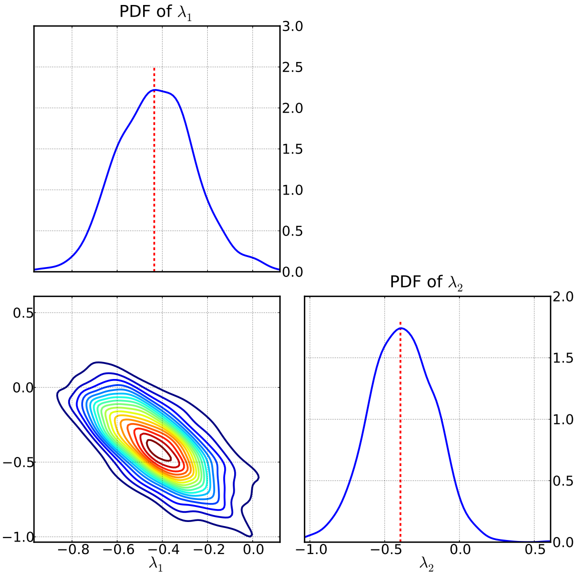


λ_2

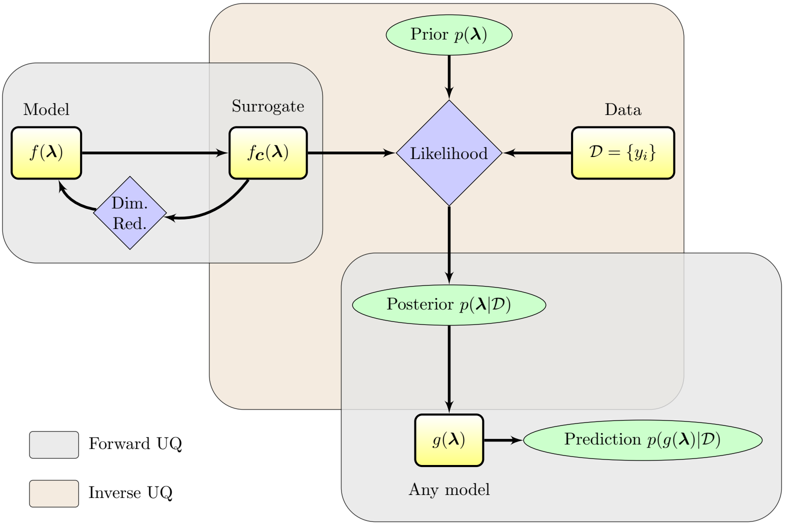


- The chains for both parameters show good mixing

Marginal and Joint Posterior Densities



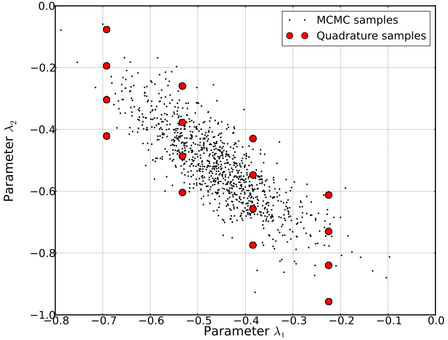
Forward propagation with calibrated parameters



The Rosenblatt transformation maps the posterior samples to standard Gaussian random variables

- Posterior distributions represent the parameter uncertainties
- Set of MCMC samples characterizes these posteriors
- Need to project these posteriors onto Gauss-Hermite PC basis to get PCE for $\boldsymbol{\lambda}$
  - Galerkin projection requires map between posterior samples and $\boldsymbol{\xi}$
  - Rosenblatt transformation provides this mapping
  - `pce_quad` provides this map to project samples onto PCEs

Rosenblatt mapping of quadrature points enables Galerkin projection onto Gauss-Hermite basis



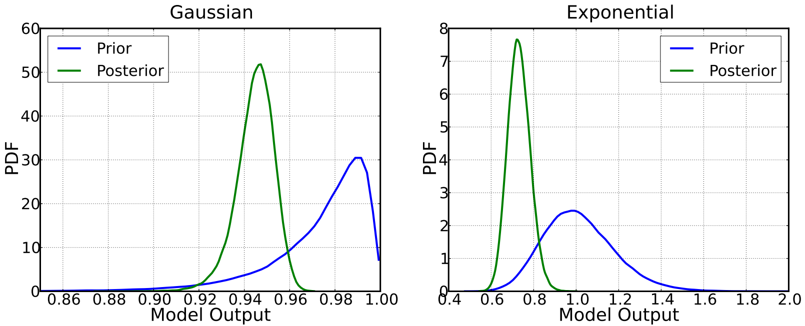
$$\lambda_1 = \sum_{k=0}^{P} \lambda_{1k} \Psi_k(\xi) \qquad \lambda_{1k} \propto \int \underbrace{R_{\lambda_1}^{-1}(\xi)}_{\lambda_1} \Psi_k(\xi) w(\xi) d\xi$$

$$\lambda_2 = \sum_{k=0}^{P} \lambda_{2k} \Psi_k(\xi) \qquad \lambda_{2k} \propto \int \underbrace{R_{\lambda_2}^{-1}(\xi)}_{\lambda_2} \Psi_k(\xi) w(\xi) d\xi$$

Forward propagation uses similar commands as surrogate construction

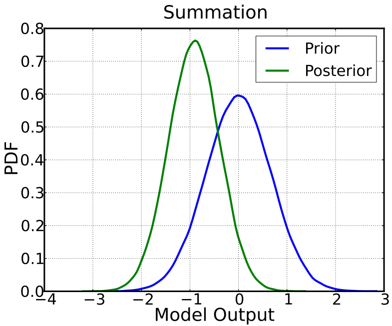
- Use calibrated uncertainty on λ_1, λ_2
- Keep prior uncertainty $N(0, 0.3)$ on $\lambda_3, \lambda_4, \lambda_5$
- Forward models $g(\boldsymbol{\lambda})$:
  - Gaussian: $g_1(\boldsymbol{\lambda}) = f^G(\boldsymbol{\lambda})$
  - Exponential: $g_2(\boldsymbol{\lambda}) = f^E(\boldsymbol{\lambda})$
  - Summation: $g_3(\boldsymbol{\lambda}) = \sum_{i=1}^{d} \lambda_i$
- Quadrature Galerkin projection
  - `generate_quad -d 5 -g HG -x full -p 4`
  - Evaluate model at quadrature points
  - `pce_resp -d 5 -x HG -o 3`

Input calibration reduces output uncertainty



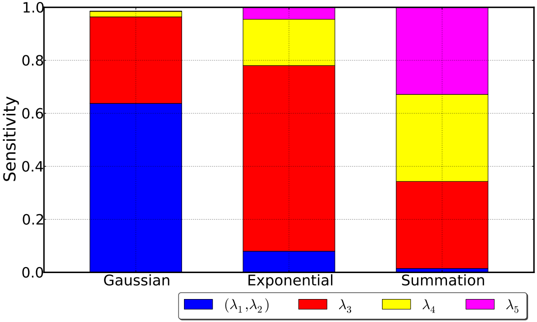
- After calibration: output distributions narrow and shift

Input calibration reduces output uncertainty



- After calibration: output distributions narrow and shift

Attribution relates output uncertainties to specific inputs



- Attribution uses sensitivity analysis tools: `pce_sens`
- For Gaussian model: more data needed to further reduce input uncertainty in λ_1, λ_2
- For other two models, need to calibrate other inputs

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 based on Swig (UQTk version 3.0)
- Version 3.0 soon at
  `http://www.sandia.gov/UQToolkit`
- Do not hesitate to contact us
  `uqtk-users@software.sandia.gov`

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.
- K. Sargsyan, *et al.*, “Dimensionality reduction for complex models via bayesian compressive sensing", *Int. J. of Uncertainty Quantification*, 4, 1:63-93, 2014.
- “Handbook of Uncertainty Quantification", R. Ghanem, D. Higdon, H. Owhadi (Eds.), Springer, 2016, `http://www.springer.com/us/book/9783319123844`
- UQ Tutorials: `http://www.quest-scidac.org/outreach/tutorials/`

Rosenblatt Transformation for Multi-D RVs

- Assume samples of multi-D RVs are (*e.g.* from MCMC sampling of posterior parameter distribution)
- Rosenblatt transformation maps any (not necessarily independent) set of random variables $(\lambda_1, \ldots, \lambda_d)$ to uniform i.i.d.'s $\{\eta_i\}_{i=1}^d$ (Rosenblatt, 1952).

$$
\begin{aligned}
\eta_1 &= F_1(\lambda_1) \\
\eta_2 &= F_{2|1}(\lambda_2|\lambda_1) \\
&\vdots \\
\eta_d &= F_{d|d-1,\ldots,1}(\lambda_d|\lambda_{d-1}, \ldots, \lambda_1)
\end{aligned}
$$

- Rosenblatt transformation is a multi-D generalization of 1D CDF mapping.
- Conditional CDFs are harder to evaluate in high dimensions