UQTk
A C++/Python Toolkit for Uncertainty Quantification

Bert Debusschere, Khachik Sargsyan, Cosmin Safta, Kenny Chowdhary

bjdebus@sandia.gov
Sandia National Laboratories,
Livermore, CA, USA

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## Acknowledgements

<table>
<thead>
<tr>
<th>Name</th>
<th>Institution</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cosmin Safta</td>
<td>Sandia National Laboratories</td>
</tr>
<tr>
<td>Khachik Sargsyan</td>
<td>Livermore, CA, USA</td>
</tr>
<tr>
<td>Kenny Chowdhary</td>
<td></td>
</tr>
<tr>
<td>Habib Najm</td>
<td></td>
</tr>
<tr>
<td>Omar Knio</td>
<td>Duke University, Raleigh, NC, USA</td>
</tr>
<tr>
<td>Roger Ghanem</td>
<td>University of Southern California, Los Angeles, CA, USA</td>
</tr>
<tr>
<td>Olivier Le Maître</td>
<td>LIMSI-CNRS, Orsay, France</td>
</tr>
<tr>
<td>and many others</td>
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Outline

1. General Characteristics
2. An Example Workflow
3. Summary
4. References
UQ is about enabling predictive simulations

Experiments

Theory

Predictive Simulation

\[
\frac{\partial}{\partial t} (\theta \rho \tilde{Y}_i) + \nabla \cdot (\theta \rho \tilde{Y}_i \tilde{u}) = \nabla \cdot (\theta \tilde{S}_i) + \theta \tilde{\omega}_i + \tilde{\omega}_{si}
\]
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
  - Current version 2.1
  - Version 3.0 coming (very) soon
- No massive third party libraries 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
  - ≈ 600 total downloads
  - ≈ 425 downloads of version 2.x
  - Mostly academic and laboratory research groups

- Mailing lists
  - uqtk-announce@software.sandia.gov
  - uqtk-users@software.sandia.gov
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**
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1. General Characteristics
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An example UQTk workflow (UQTk version 3.0)

- **Model:** $f(\lambda)$
- **Surrogate:** $f_c(\lambda)$
- **Likelihood:**
  - Prior $p(\lambda)$
  - Data $\mathcal{D} = \{y_i\}$
- **Posterior:** $p(\lambda|\mathcal{D})$
- **Prediction:** $p(g(\lambda)|\mathcal{D})$

**Forward UQ**

**Inverse UQ**
Consider uncertain parameter vector $\lambda$  
Propagate uncertainty in $\lambda$ through model $g(\lambda)$  
First calibrate $\lambda$ using data on function $f(\lambda)$  
Consider the following calibration functions $f(\lambda)$:  
  - Gaussian: $f^G(\lambda) = \exp \left( - \sum_{i=1}^{d} a_i^2 \lambda_i^2 \right)$  
  - Exponential: $f^E(\lambda) = \exp \left( \sum_{i=1}^{d} a_i \lambda_i \right)$  
  - 5 dimensional $\lambda$: $a = (0.4, 0.3, 0.2, 0.1, 0.05)$  
Forward models $g(\lambda)$:  
  - Gaussian: $g_1(\lambda) = f^G(\lambda)$  
  - Exponential: $g_2(\lambda) = f^E(\lambda)$  
  - Summation: $g_3(\lambda) = \sum_{i=1}^{d} \lambda_i$  
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

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

Exponential
Sensitivity analysis enables dimensionality reduction

- UQTk computes main, joint, and total sensitivity coefficients
  - $S_i$: Fraction of variance due to $\lambda_i$ only
  - $S_{ij}$: Fraction of variance due to both $\lambda_i$ and $\lambda_j$
  - $S_{iT}^T$: Fraction of variance due to $\lambda_i$ by itself and in combination with any other $\lambda_j$
- Can be computed analytically from PC response surface
- `pce_sens -m minindex.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 $\lambda_1$ and $\lambda_2$ in calibration
Bayesian calibration using surrogate models

\begin{align*}
&\text{Model: } f(\lambda) \\
&\text{Surrogate: } fc(\lambda) \\
&\text{Likelihood: } p(D|\lambda) \\
&\text{Data: } D = \{y_i\} \\
&\text{Posterior: } p(\lambda|D) \\
&\text{Prediction: } p(g(\lambda)|D) \\
&\text{Forward UQ} \\
&\text{Inverse UQ}
\end{align*}
Bayesian Parameter Inference

\[ p(\lambda|D) \propto p(D|\lambda)p(\lambda) \]

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

- Generate \( R \) random noisy realizations of \( f^G(\lambda) \) and \( f^E(\lambda) \) as data \( D \)
- Assume Normally distributed priors \( N(0, 0.3) \) on \( \lambda_1 \) and \( \lambda_2 \)
- Infer \( \lambda_1 \) and \( \lambda_2 \) against data on both \( f^G(\lambda) \) and \( f^E(\lambda) \)
- `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

- The chains for both parameters show good mixing
Marginal and Joint Posterior Densities

PDF of $\lambda_1$

PDF of $\lambda_2$
Forward propagation with calibrated parameters

**Model**
- $f(\lambda)$

**Surrogate**
- $f_c(\lambda)$

**Likelihood**
- $D = \{y_i\}$

**Posterior**
- $p(\lambda|D)$

**Prior**
- $p(\lambda)$

**Prediction**
- $p(g(\lambda)|D)$

**Any model**
- $g(\lambda)$

**Forward UQ**
- Model

**Inverse UQ**
- Surrogate

**Dimension Reduction**
- Dim. Red.
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 $\lambda$
  - Galerkin projection requires map between posterior samples and $\xi$
  - Rosenblatt transformation provides this mapping
  - \texttt{pce_quad} provides this map to project samples onto PCEs
Rosenblatt mapping of quadrature points enables Galerkin projection onto Gauss-Hermite basis.

\[ \lambda_1 = \sum_{k=0}^{P} \lambda_{1k} \psi_k(\xi) \quad \lambda_{1k} \propto \int R_{\lambda_1}^{-1}(\xi) \psi_k(\xi) w(\xi) d\xi \]

\[ \lambda_2 = \sum_{k=0}^{P} \lambda_{2k} \psi_k(\xi) \quad \lambda_{2k} \propto \int R_{\lambda_2}^{-1}(\xi) \psi_k(\xi) w(\xi) d\xi \]
Forward propagation uses similar commands as surrogate construction

- Use calibrated uncertainty on $\lambda_1, \lambda_2$
- Keep prior uncertainty $N(0, 0.3)$ on $\lambda_3, \lambda_4, \lambda_5$
- Forward models $g(\lambda)$:
  - Gaussian: $g_1(\lambda) = f^G(\lambda)$
  - Exponential: $g_2(\lambda) = f^E(\lambda)$
  - Summation: $g_3(\lambda) = \sum_{i=1}^d \lambda_i$
- 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: \texttt{pce\_sens}
- For Gaussian model: more data needed to further reduce input uncertainty in $\lambda_1, \lambda_2$
- 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


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).

\[
\begin{align*}
\eta_1 &= F_1(\lambda_1) \\
\eta_2 &= F_{2|1}(\lambda_2|\lambda_1) \\
&
\vdots \\
\eta_d &= F_{d|d-1,...,1}(\lambda_d|\lambda_{d-1}, \ldots, \lambda_1)
\end{align*}
\]

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