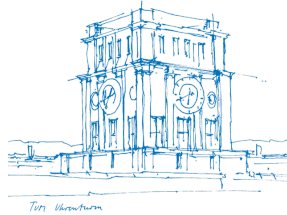


Algorithms for Uncertainty Quantification

Lecture 11: Software for UQ

ST 2018

Tobias Neckel
Scientific Computing in Computer Science
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Repetition of Previous Lecture

- random fields
 - motivation
 - application examples
 - formal definition
- stochastic processes
 - definition
 - example: Brownian motion
- approximation of random fields
 - the Karhunen-Loève expansion
 - example: approximation of the Wiener process

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Concept of Building Block:

- Time: \approx 80 minutes
- Content
 - coding from scratch vs. using existing code
 - UQ software vs. UQ packages
 - the world of UQ software: what software is available?
 - survey on selected UQ software
- Expected Learning Outcomes
 - The participants can list a variety of different software packages or libraries dealing with UQ aspects.
 - They are able to indicate advantages or target use cases for those implementations that are listed in more detail (i.e. in red in the overview).
 - For different use cases, the participants can indicate possible software and are able to give arguments for their choice.

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Coding from scratch vs. Using Packages

from scratch

- no dependency on external packages/libraries (and their changes/bugs/...)
- at least: decision, on which to rely on
- Computer Science people like it :-)
- context UQ: "Monte Carlo is so easy"

reusing existing codes

- avoid reinventing the wheel over and over again
- rely on work of others
 - faster time to solution (less debugging, testing, ...!)
 - quality of packages?
 - flexibility/portability supported?
 - maintainability of (own) code?
 - API fix or not very flexible
 - license issues?

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UQ Software vs. UQ Packages

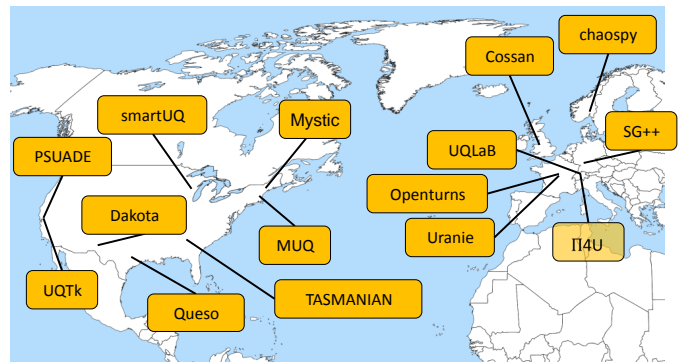
difference between software and small code packages:

- size of developing group:
single Ph.D. candidates \Leftrightarrow many life-time positions
- goal of implementations:
specific tasks \Leftrightarrow many methods/approaches, for large user base
- ease of use:
direct start with (almost) no docu \Leftrightarrow a lot of docu (to read)
- quality assurance:
manual tests (if any) \Leftrightarrow software engineering aspects, user support
- ...

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World of UQ Software



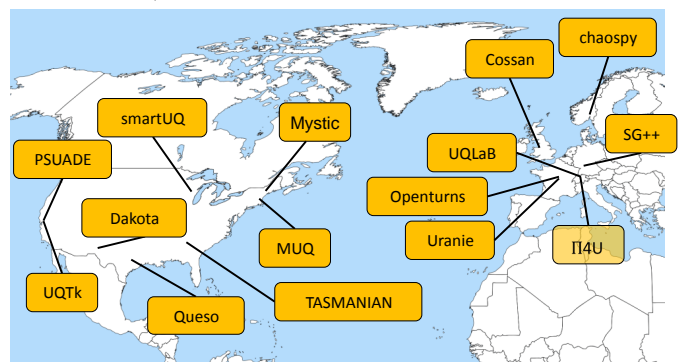
SIAM conference UQ 18, minisymposia 88, 102, 115, and 128: Software for UQ, Tobias Neckel & Dirk Pflüger
see also https://www5.in.tum.de/wiki/index.php/STAMUQ18_-_Slides_Minisym_Software4UQ

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Discussion of Evaluation!

World of UQ Software – Reloaded



SIAM conference UQ 18, minisymposia 88, 102, 115, and 128: Software for UQ, Tobias Neckel & Dirk Pflüger
see also https://www5.in.tum.de/wiki/index.php/STAMUQ18_-_Slides_Minisym_Software4UQ

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List of UQ Software

alphabetical; for sure: incomplete!

- Chaospy
- Dakota
- MUQ library
- Mystic
- NASA UQTools
- OpenCossan (matlab)
- Openturns
- Π4U
- Promethee
- Psuade
- Queso
- SG++
- SmartUQ
- TASMAMANIAN
- UQLab (matlab)
- UQ Toolkit (UQTK)
- Uranie
- ...

Aspects of Chaospy

| | |
|----------------------------------|---|
| URL | https://github.com/jonathf/chaospy |
| developing organisation | Jonathan Feinberg (SIMULA / private) |
| existing since | 2014? |
| main purpose | forward UQ (PCE, sampling) |
| user support | mail support, documentation, tutorials |
| type of SW | framework/library, "full" license |
| programming language | Python |
| interface language support / API | Python |
| unique selling point | high-level Python, fast prototyping, PCE pseudospectral approach |

Aspects of MUQ

| | |
|----------------------------------|---|
| URL | http://uqgroup.mit.edu/software |
| developing organisation | UQ Group (Marzouk), MIT |
| existing since | 2011 |
| main purpose | MCMC, PCE, KL, optimisation |
| user support | Q&A, example page, interactive test sessions, doxygen |
| type of SW | collection of tools, "full" license |
| programming language | C++ |
| interface language support / API | Python, C++ |
| unique selling point | advanced UQ algorithms |

Aspects of Π4U

| | |
|----------------------------------|---|
| URL | http://www.cse-lab.ethz.ch/index.php |
| developing organisation | CSE lab, ETH |
| existing since | 2014? |
| main purpose | Bayesian inversion for large-scale applications, sampling, optimisation |
| user support | tutorial |
| type of SW | framework, GPL license |
| programming language | C/C++ |
| interface language support / API | TORC library |
| unique selling point | inversion, (heterogeneous) HPC platforms |

List of UQ Software – Details

alphabetical; for sure: incomplete!

- Chaospy
- Dakota
- MUQ library
- Mystic
- NASA UQTools
- OpenCossan (matlab)
- Openturns
- Π4U
- Promethee
- Psuade
- Queso
- SG++
- SmartUQ
- TASMAMANIAN
- UQLab (matlab)
- UQ Toolkit (UQTK)
- Uranie
- ...

for some: more detailed aspects

Aspects of Dakota

| | |
|----------------------------------|---|
| URL | https://dakota.sandia.gov/ |
| developing organisation | Sandia National Laboratory |
| existing since | 1994 |
| main purpose | UQ/optimisation for HPC applications |
| user support | FAQs, maillists, trainings, manuals & tutorials |
| type of SW | toolkit, LGPL license |
| programming language | C++ |
| interface language support / API | text input files |
| unique selling point | large user base, very mature, HPC aspects |

Aspects of Openturns

| | |
|----------------------------------|---|
| URL | http://openturns.org/ |
| developing organisation | 4 companies: Airbus, EDF, IMACS, Phimeca Engineering |
| existing since | 2005 |
| main purpose | forward UQ, data analysis |
| user support | manuals, examp., mailing lists, user days |
| type of SW | library, open source LGPL license |
| programming language | C++ |
| interface language support / API | Python, symbolic |
| unique selling point | larger user base? |

Aspects of Queso

| | |
|----------------------------------|--|
| URL | http://libqueso.com/ |
| developing organisation | UT Austin |
| existing since | 2011? |
| main purpose | forward/inverse UQ for parallel applications |
| user support | maillists, doxygen |
| type of SW | collection of algorithms & functionalities, LGPL license |
| programming language | C++ |
| interface language support / API | C++ library |
| unique selling point | inversion, Software Engineering aspects; collaboration with Dakota |

Aspects of SG++

| | |
|----------------------------------|---|
| URL | http://sgpp.sparsegrids.org/ |
| developing organisation | University of Stuttgart, TUM |
| existing since | 2007? |
| main purpose | sparse grid toolbox for interpolation, quadrature, PDEs, data mining & machine learning, UQ, optimisation |
| user support | manuals, coding days, doxygen |
| type of SW | library, BSD-like license? |
| programming language | C++ |
| interface language support / API | C++, Python, Java, MATLAB |
| unique selling point | sparse grids (spatially adaptive! combination technique) |

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Aspects of UQTK

| | |
|----------------------------------|---|
| URL | http://www.sandia.gov/UQToolkit/ |
| developing organisation | Sandia National Laboratory |
| existing since | 2005+X? |
| main purpose | forward/inverse UQ |
| user support | mailing lists, doxygen, manuals |
| type of SW | collection of libraries, LGPL license |
| programming language | C++ |
| interface language support / API | C++, Python |
| unique selling point | high-level UQ, fast prototyping, many methods |

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Literature:

- References and manuals of software websites
- Overview of status at conference SIAM UQ 2018,
https://www5.in.tum.de/wiki/index.php/SIAMUQ18_-_Slides_Minisymposium_Software4UQ

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Aspects of TASMANIAN

| | |
|----------------------------------|---|
| URL | http://tasmanian.ornl.gov/ |
| developing organisation | Oak Ridge National Laboratory |
| existing since | 2013? |
| main purpose | high-dimensional integration, interpolation & parameter calibration |
| user support | manuals |
| type of SW | toolkit (libraries) |
| programming language | C++ |
| interface language support / API | C++, Python |
| unique selling point | sparse grids (combination technique) |

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Aspects of Uranie

| | |
|----------------------------------|---|
| URL | https://sourceforge.net/projects/uranie/ |
| developing organisation | CEA, France |
| existing since | 2013? |
| main purpose | data analysis, UQ, optimisation |
| user support | mail support |
| type of SW | (L)GPL |
| programming language | Python, C++, C |
| interface language support / API | CINT, Python |
| unique selling point | many use cases, support for HPC platforms |

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Summary

Software for UQ

- coding from scratch vs. using existing code
- UQ software vs. UQ packages
- the world of UQ software: what software is available?
- overview on selected UQ software
 - maturity/features
 - preparation for use case decisions

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