Sandia Software Enabling Extreme-Scale Uncertainty Quantification[1]

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Process of quantifying the effect of uncertainties typically includes:

- ***(Global) sensitivity analysis:*** identification of input set with greatest influence on output QoIs
- ***Uncertainty characterization:*** model or infer from observable data; parametric/non-parametric/KDE
- ***Uncertainty propagation:*** input distributions → output QoI distributions
- ***Decision making:*** model validation, prediction, design under uncertainty

SNL software tools within QUEST support a range of:

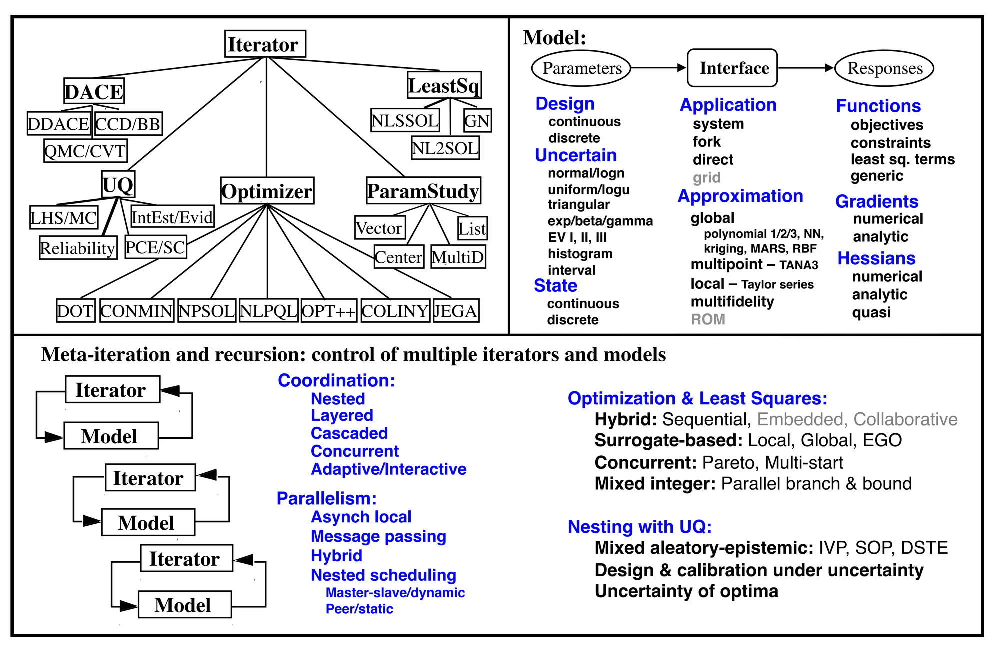
- ***UQ studies:*** sensitivity analysis, uncertainty propagation, statistical inference
- ***Environments:*** rapid prototyping in interpreted languages ⟷ production computing in compiled languages on parallel platforms
- ***Intrusion:*** embedded ⟷ linked ⟷ black box

An interoperable set of tools that can be tailored:

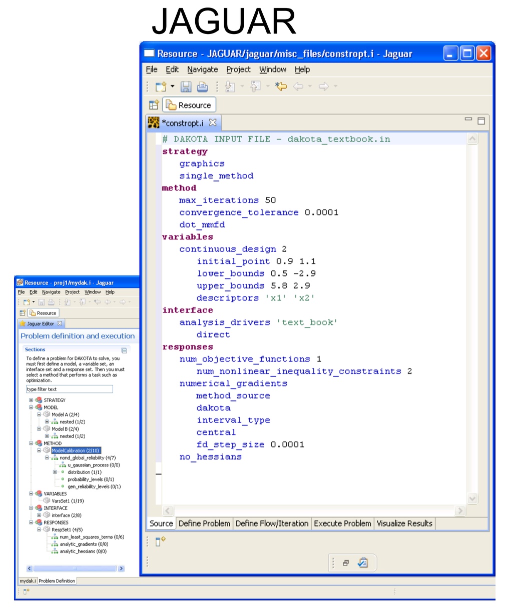
- DAKOTA + QUESO/GPMSA + PCE/SC/GP emulators
- Production deployment of stable capabilities in frameworks
- Close collaboration of SAPs with library developers for custom capabilities

DAKOTA (dakota.sandia.gov) is a C++ application that provides a variety of non-intrusive algorithms for design optimization, model calibration, uncertainty quantification, global sensitivity analysis, parameter studies, and solution verification. It can be used as either a stand-alone application or as a set of library services, and supports multiple levels of parallelism for scalability on both capability and capacity HPC resources.

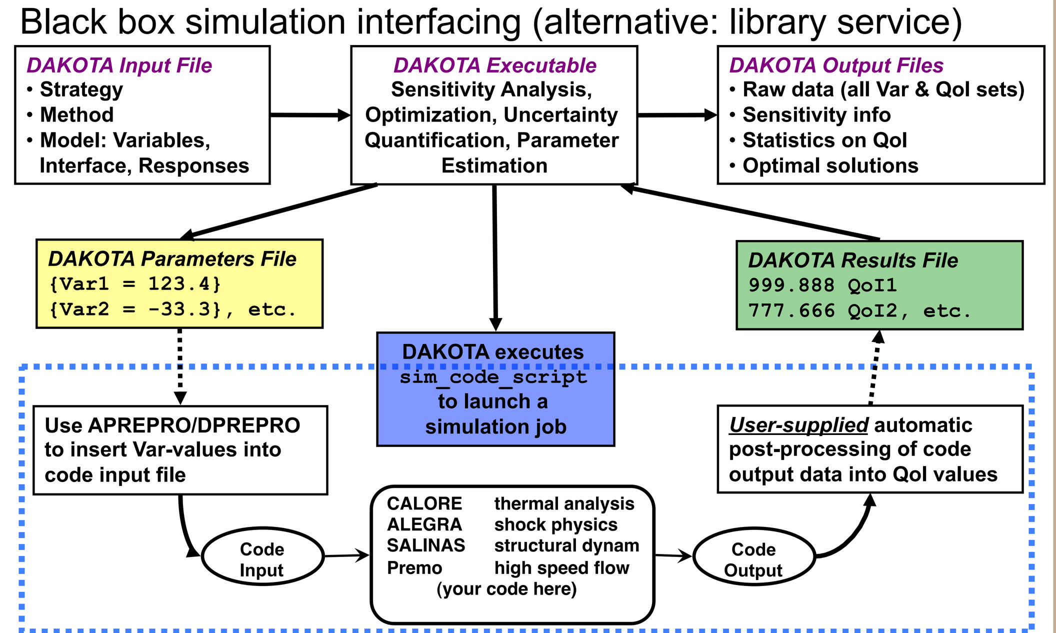
- Contact: dakota-developers@development.sandia.gov



JAGUAR



Black box simulation interfacing (alternative: library service)

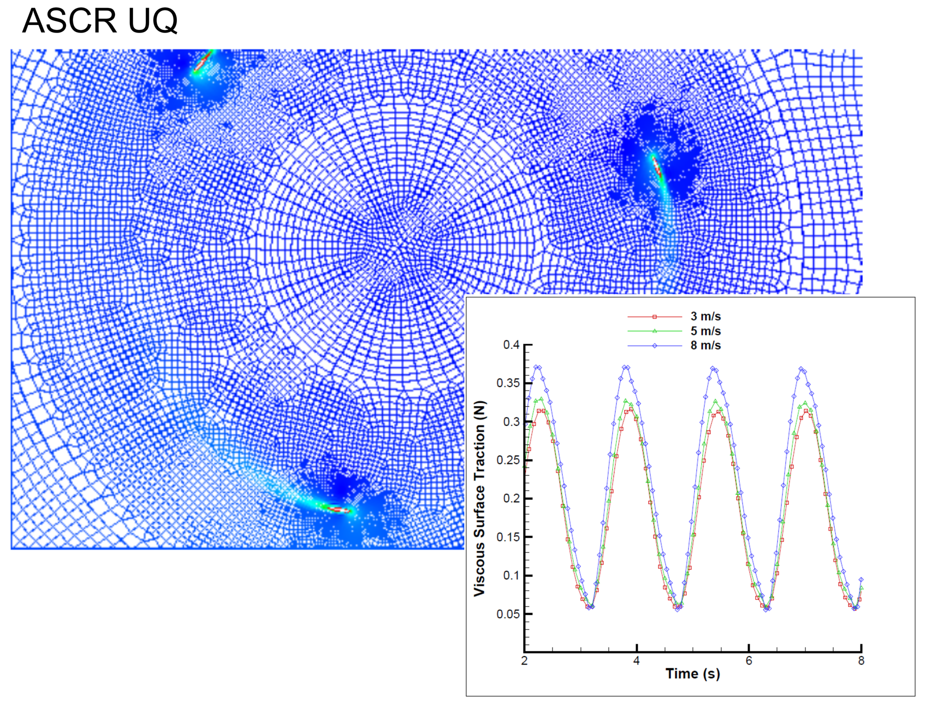


UQ Capabilities:

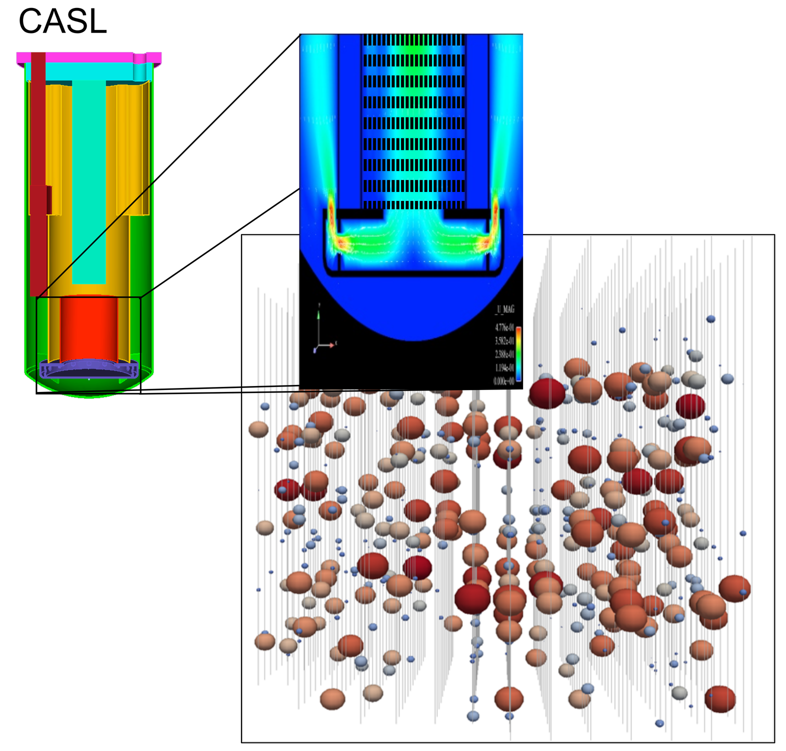
- **Sampling methods**
  - **Random: LHS, MC**
  - **Incremental random**
  - **Importance: IS, AIS, MMAIS**
  - **Adaptive: Morse-Smale et al.**
- **Reliability methods**
  - **Local: MV, AMV, AMV+, AMV[2]+, FORM, SORM**
  - **Global: EGRA, GPAIS,** POF Darts
- **Stochastic expansion methods**
  - **Polynomial chaos: projection, regression (see SNL poster)**
  - **Stochastic collocation: tensor and sparse grids**
- **Epistemic methods**
  - **Interval estimation: local, global, mixed-integer**
  - **Dempster-Shafer**
- **Bayesian methods**
  - **QUESO (see UT poster)**
  - **GPMSA (see LANL poster)**
  - **Emulator-based: PCE, SC, GP**
- **Meta-iteration and recursion**
  - **Mixed aleatory-epistemic UQ**
  - **Design / calibration under uncertainty**

Office of Science Applications: wind energy, nuclear power, climate

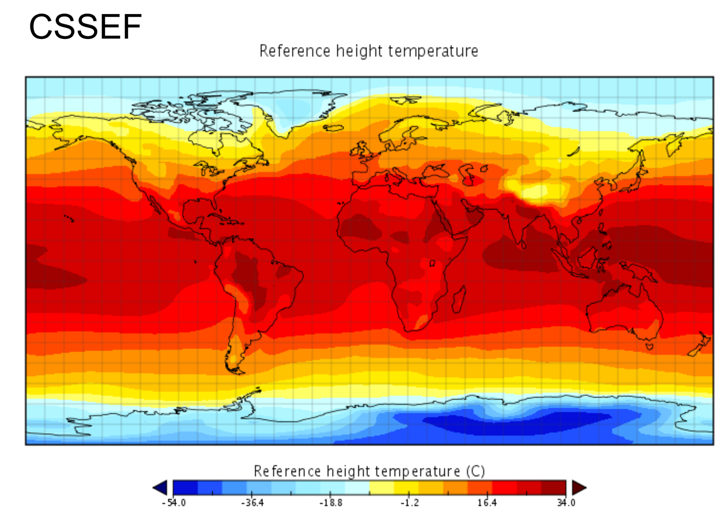
ASCR UQ



CASL

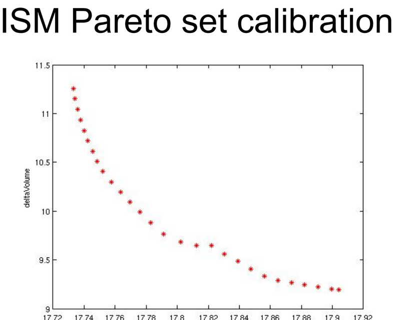


CSSEF

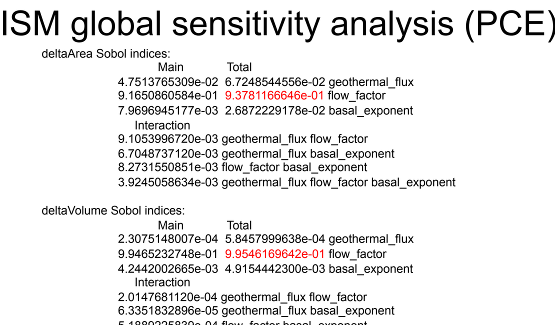


PISCEES Partnership

CISM Pareto set calibration



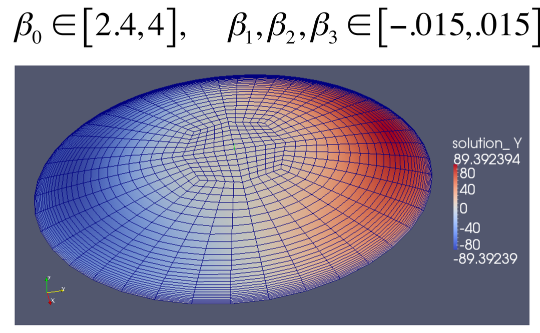
CISM global sensitivity analysis (PCE)

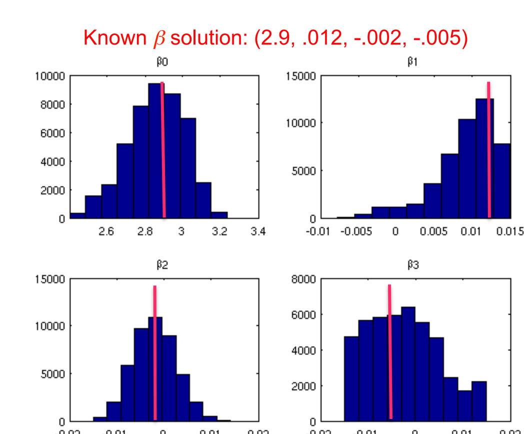


Bayesian calibration with FELIX ice dome

$$\beta(x,y)=\beta_0+\beta_1 x+\beta_2 y+\beta_3 r$$

$$\beta_0\in[2.4,4],\quad \beta_1,\beta_2,\beta_3\in[-.015,.015]$$





UQTk (www.sandia.gov/UQToolkit) is a library of C++ and Matlab functions for propagation of uncertainty through computational models.

- Mainly relies on spectral Polynomial Chaos Expansions (PCEs) for representing random variables and stochastic processes
- Complementary to production tools, UQTk targets:
  - Rapid prototyping
  - Algorithmic research
  - Outreach: Tutorials / Educational
- Contact: Bert Debusschere: bjdebus@sandia.gov

Upcoming release (Summer 2013):

- Version 2.0 to be released under the GNU LGPL
  - Intrusive and non-intrusive (quadrature) approaches for PCE stochastic Galerkin projection
    - In C++ and Matlab
  - Markov Chain Monte Carlo library for Bayesian inference (C++)
  - Bayesian Compressive Sensing library (C++)
  - Karhunen-Loève library (C++)
  - Sparse quadrature library (C++)

Sample Applications:

- Bayesian Compressive Sensing library used in testbed for land model data processing in climate modeling
- Development of lecture material and hands-on exercises for UQ tutorials
  - SIAM UQ12, Raleigh, April 2012, Raleigh, NC
  - Summer school on UQ, Aug 2012, 2013, USC, Los Angeles, CA
  - QUEST UQ tools tutorial, Oct 2012, SNL, Livermore, CA
  - Summer School on UQ, May 2013, Katholieke Universiteit Leuven, Leuven, Belgium
    - Example problems cover operations on Polynomial Chaos expansions, intrusive and non-intrusive forward propagation of UQ, Bayesian inference

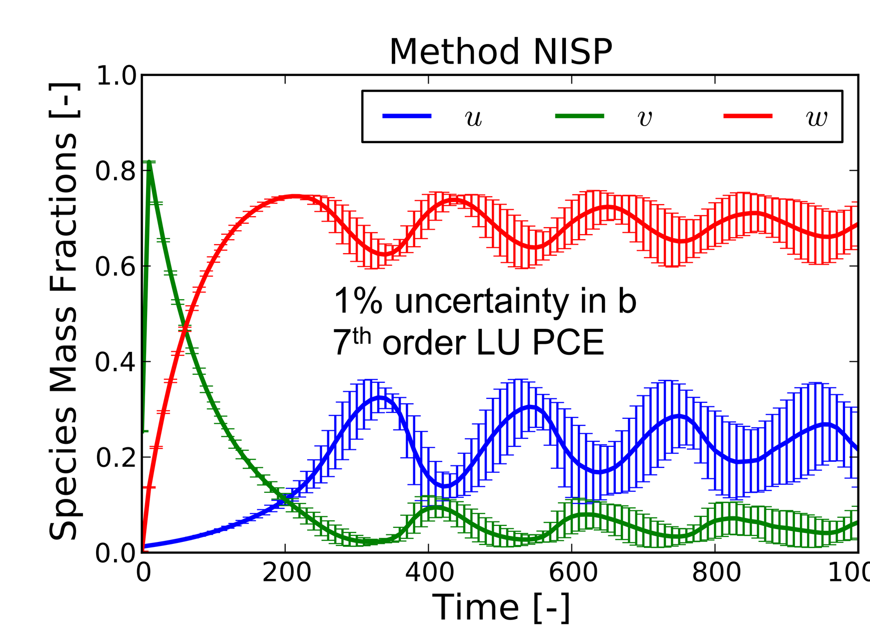
3 ODEs for a monomer (u), dimer (v), and inert species (w) adsorbing onto a surface out of gas phase.

$$\frac{du}{dt} = az - cu - 4duv$$
$$\frac{dv}{dt} = 2bz^2 - 4duv$$
$$\frac{dw}{dt} = ez - fw$$
$$z = 1 - u - v - w$$

$$u(0) = v(0) = w(0) = 0.0$$

$$a = 1.6 \quad b = 20.75 \quad c = 0.04 \quad d = 1.0 \quad e = 0.36 \quad f = 0.016$$

Method NISP



Karhunen-Loève expansion for unstructured grids:

- Enhanced capability in UQTk
- Allows representation of stochastic processes on irregular domains
- Eigenvalues and eigenmodes are computed via the Nystrom method
- 2nd order discretization of the Fredholm integral on unstructured grids