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# Sandia Software Enabling Extreme-Scale Uncertainty Quantification

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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:**

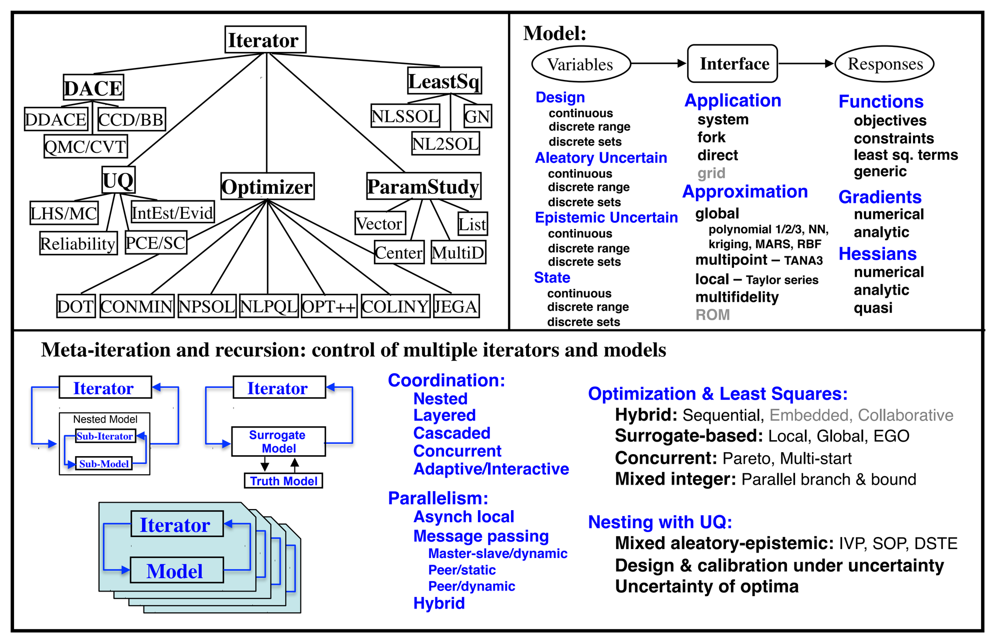
- *UQ studies:* sensitivity analysis, uncertainty propagation, statistical inference
- *Environments:* rapid prototyping in interpreted languages ⟷ production computing in compiled languages on parallel platforms
- *Intrusion:* embedded ⟷ linked ⟷ black box

**An interoperable set of tools that can be tailored:**

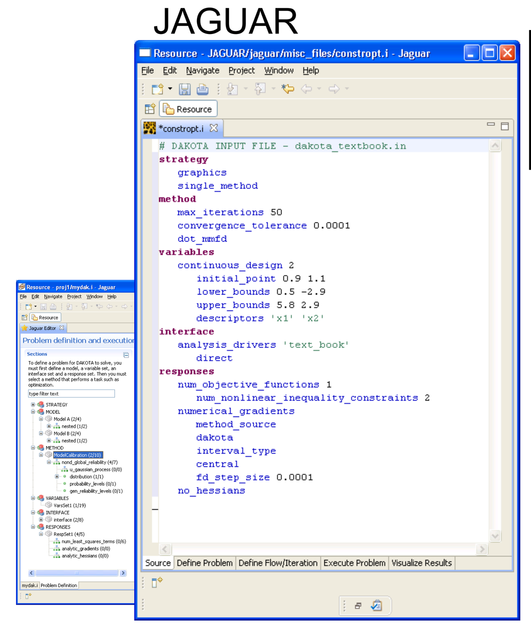
- DAKOTA + QUESO/GPMSA + PCE/SC/GP emulators
- Production deployment of stable capabilities in frameworks
- Close collaboration of SAPs with library developers for custom capabilities

**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.

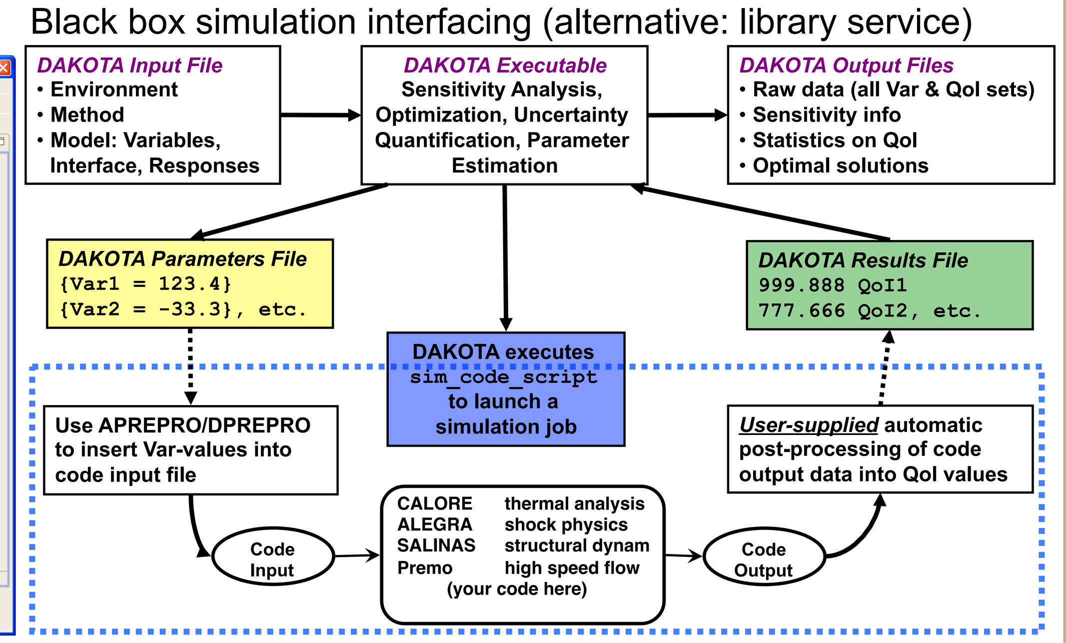
- Contact: dakota-developers@development.sandia.gov



JAGUAR



Black box simulation interfacing (alternative: library service)

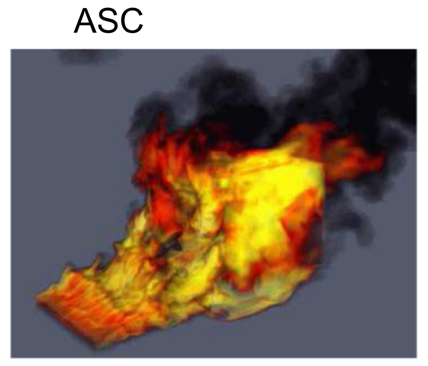



## UQ Capabilities:

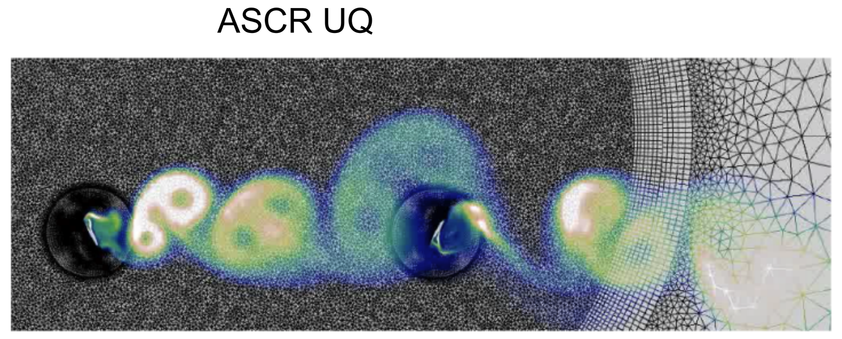
- Sampling methods
  - Random: LHS, MC, Incremental
  - Importance: IS, AIS, MMAIS
  - Adaptive: Morse-Smale et al.
- Reliability methods
  - Local: MV, AMV, AMV+, AMV$^2$+, TANA-3, FORM, SORM
  - Global: EGRA, GPAIS, POF Darts
- Stochastic expansion methods
  - Polynomial chaos: projection, regression (see Algs poster)
  - Stochastic collocation: tensor & sparse; nodal & hierarchical
- Epistemic methods
  - Interval estimation: local, global, mixed-integer
  - Dempster-Shafer
- Bayesian methods
  - QUESO, GPMSA, DREAM
  - Emulator-based MCMC: PCE, SC, GP
  - Random field inference (PISCEES at bottom)
- Meta-iteration and recursion
  - Mixed aleatory-epistemic UQ
  - Design / calibration under uncertainty

## Defense, Science, and Energy Applications

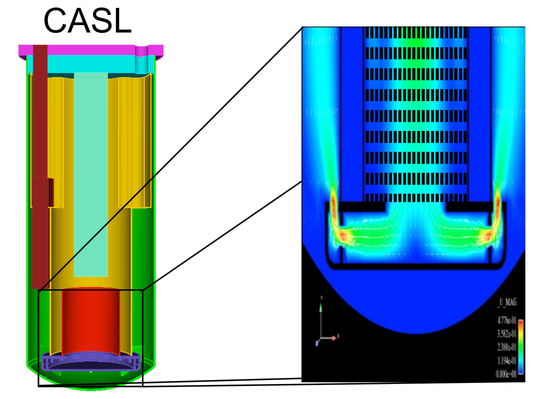
ASC



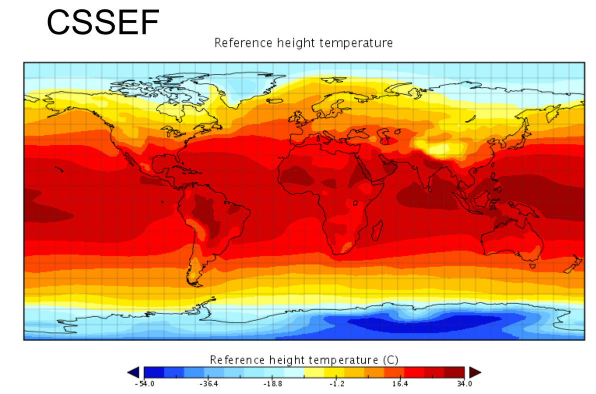
ASCR UQ



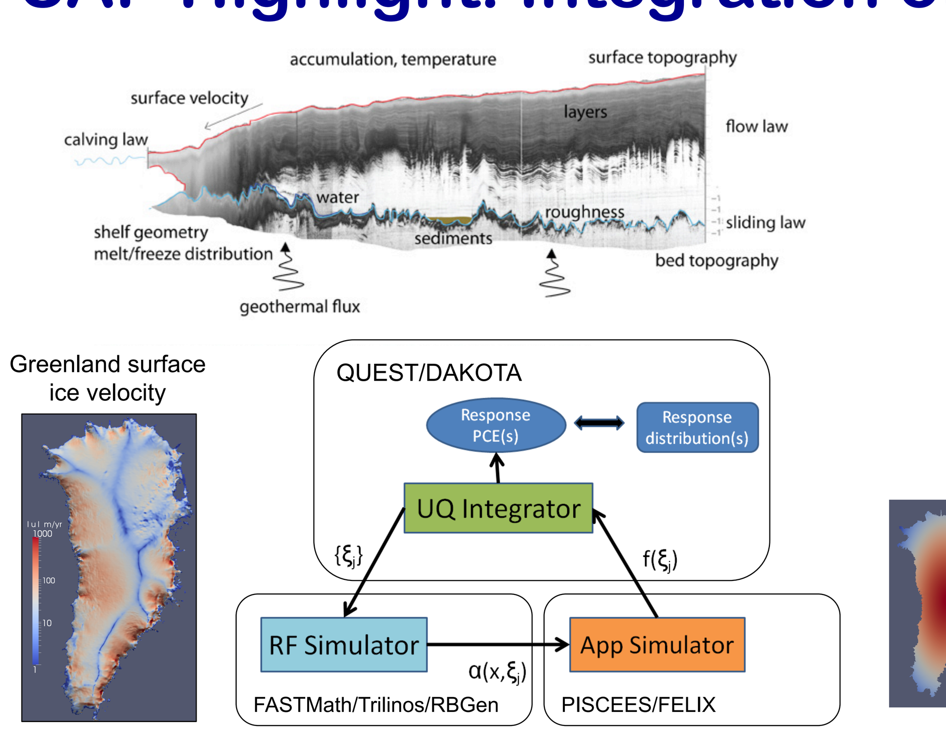
CASL



CSSEF




## SAP Highlight: Integration of Albany/Dakota/Trilinos for PISCEES



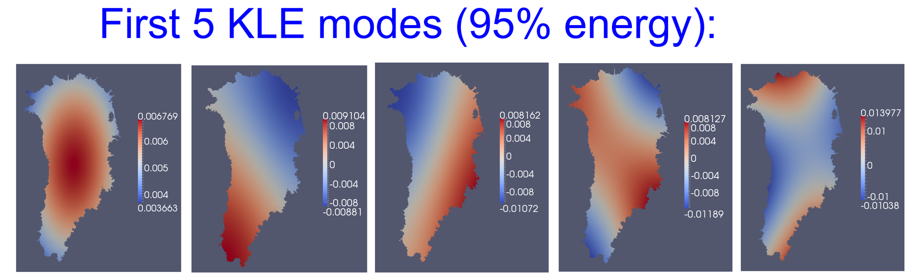
### Karhunen-Loève expansion (KLE):

Assume analytic spatial covariance kernel (squared exponential) for random field:

$$C(r_1, r_2) = e^{-(r_1 - r_2)^2 / L^2}$$

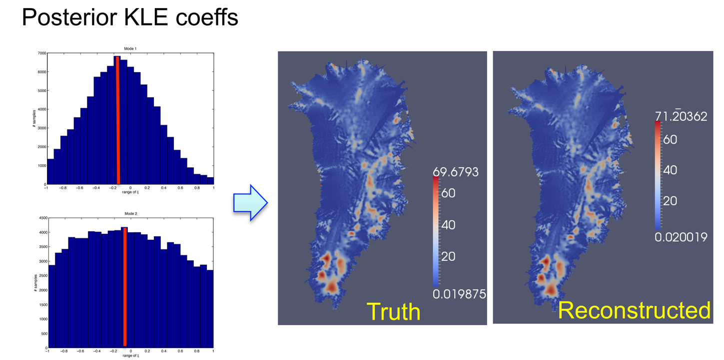
and integrate over domain for modes. Length scale (L) balances feature resolution vs. # KLE modes.

### First 5 KLE modes (95% energy):



### Dimension reduced inference:

- Mismatch = sum sq of surface velocity discrepancy
- PCE formed for mismatch over uniform prior distributions for isotropic sparse grid lev = 3
- MCMC on PCE with 100k samples, 1st 10k discarded




**UQTk** (www.sandia.gov/UQToolkit) is an LGPL open source library of functions for characterization and propagation of uncertainty in 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

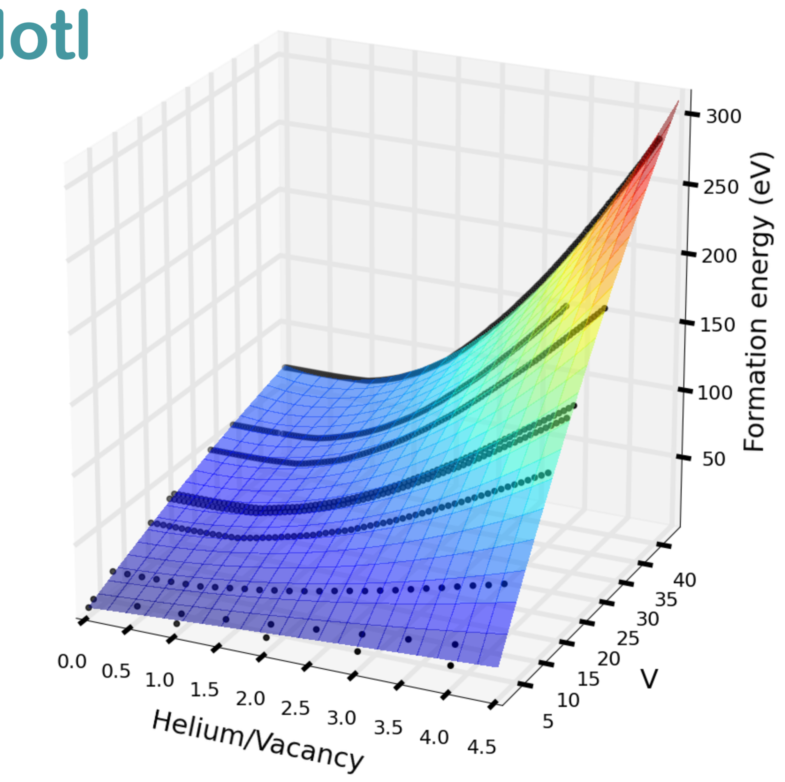
## Capabilities:

- Intrusive and non-intrusive (quadrature) approaches for PCE stochastic Galerkin projection
  - Full and sparse quadrature approaches
- Markov Chain Monte Carlo library for Bayesian inference
- Bayesian Compressive Sensing
- Karhunen-Loève expansions
- Sensitivity analysis
- Core libraries in C++
- Examples and postprocessing tools in Python
- Fully functional Python interface planned for Fall 2014 release

## Applications:

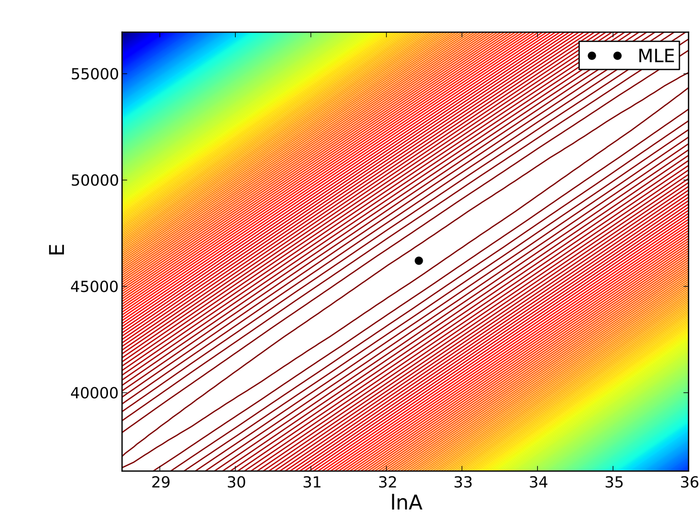
- UQTk components can be combined as needed into an end-to-end UQ workflow:
  - Surrogate construction ➔ sensitivity analysis ➔ parameter inference ➔ PCE construction ➔ forward propagation
  - Bayesian compressive sensing used in climate modeling for surrogate construction and dimensionality reduction of land, atmosphere and cloud models (CSSEF, ACME, Multiscale Earth Models, ACES4GCM)
  - UQ workflows set up in multiple SciDAC partnership projects: e.g. UQ in Xolotl (PSI)
- Development of lecture material and hands-on exercises for UQ tutorials
  - Nationally and Internationally

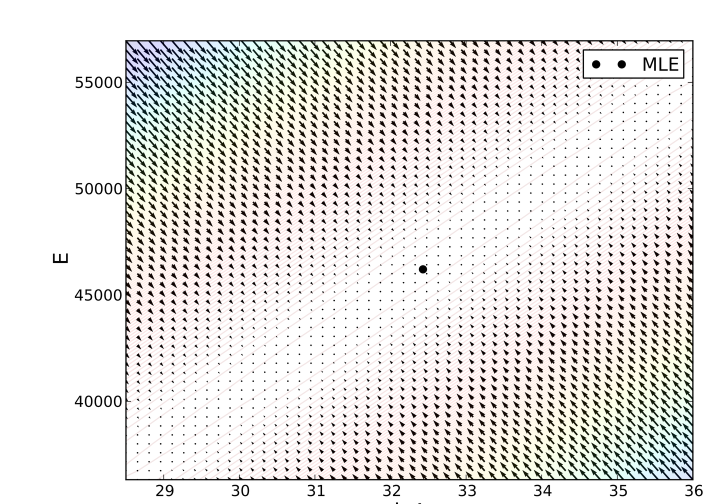
### Uncertainty Quantification in Xolotl



- 2nd order Legendre-Uniform PC surrogate obtained with Bayesian regression from formation energies computed with MD
- Input to Xolotl, which computes cluster dissociation rates in plasma-surface interactions

### Inference of Combustion Model Parameters





- 5th order Legendre-Uniform PC surrogate for an ignition time model, as a function of activation energy and pre-exponential (top left)
- Derivative of the surrogate (bottom left)
- Both the surrogate and its derivative obtained with UQTk
- Used in optimization to get better initial guess for MCMC
- Used to accelerate likelihood computation in MCMC