Uncertainty Quantification For A Next-Generation Global Atmosphere Model

Sandia National Laboratories
W. Spotz, J. Fike, I. Tezaur, A. Salinger, S. Bova, J. Overfelt, M. Taylor, E. Phipps

Objectives

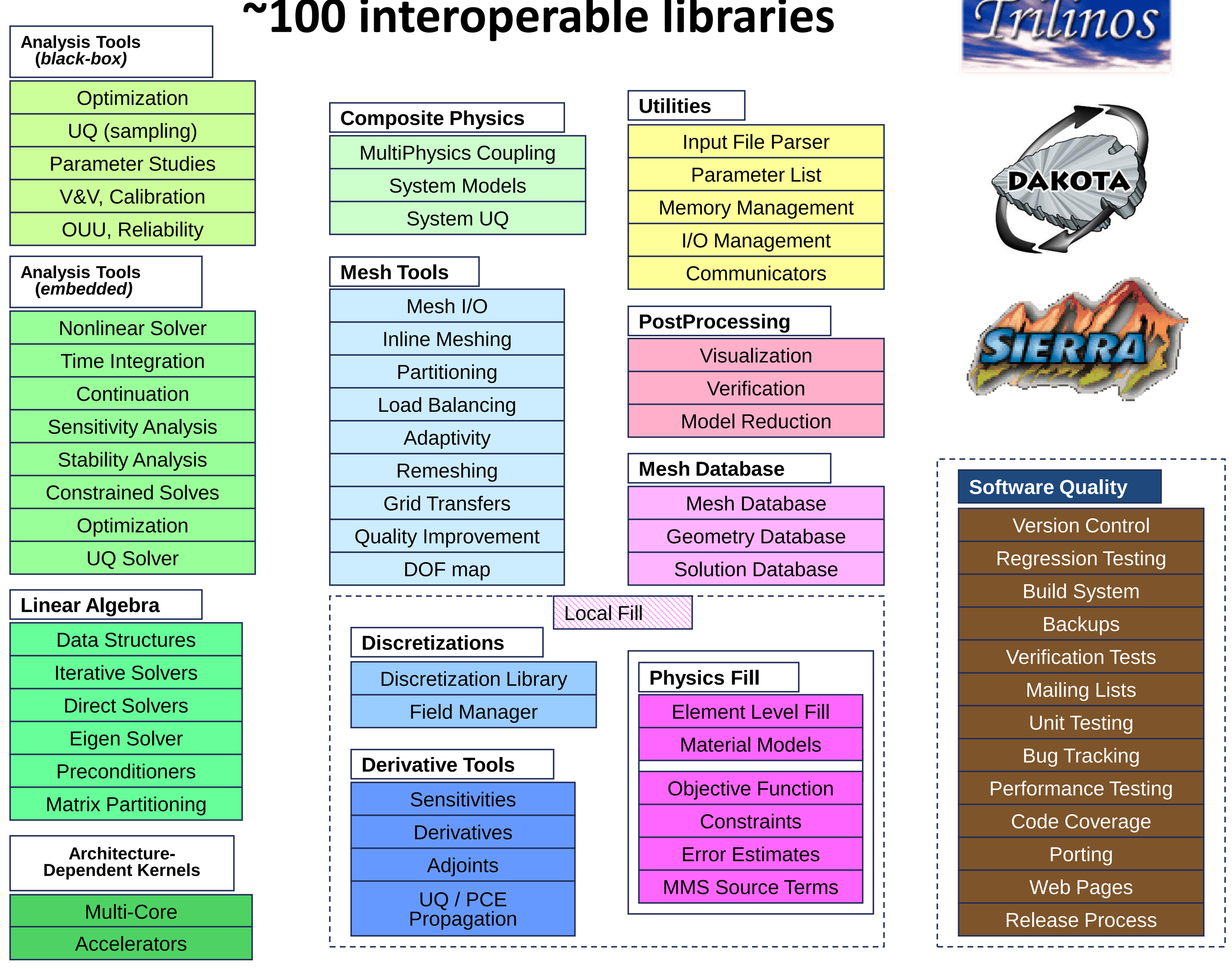
Develop a ***next-generation*** atmosphere model by leveraging Albany, a C++, parallel, implicit, unstructured-grid finite element code from Sandia National Laboratories that demonstrates ***agile components*** and enables rapid prototyping. Unique features will include embedded ***uncertainty quantification***, ***performance portability***, and a wide variety of ***discretizations***.

Component-Based Strategy

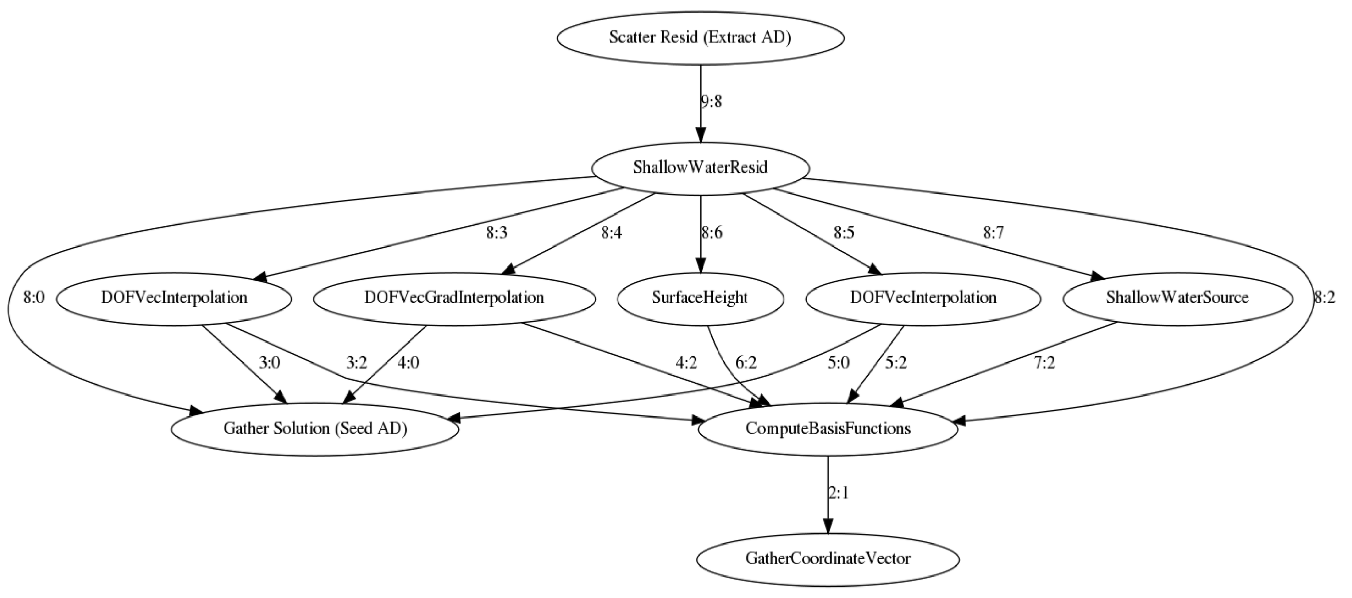
Component-based approach enables ***rapid*** development of new ***production*** codes embedded with ***transformational*** capabilities

"Components" = ☑ Libraries ☑ Software Quality Tools ☑ Interfaces ☑ Demonstration Applications

Sandia's components effort includes ~100 interoperable libraries



Verification Tools



Dependency graph of finite element assembly kernels for the Shallow Water equations. By use of operator overloading-based automatic differentiation (AD), the same code base is used for implicit and explicit calculations. Most kernels shown here are general-purpose finite element calculations that were provided by Albany.

UQ Approach for Aeras

Aeras utilizes the uncertainty quantification capabilities available in Albany through Dakota and the Trilinos package Stokhos.

Stokhos provides tools to enable:

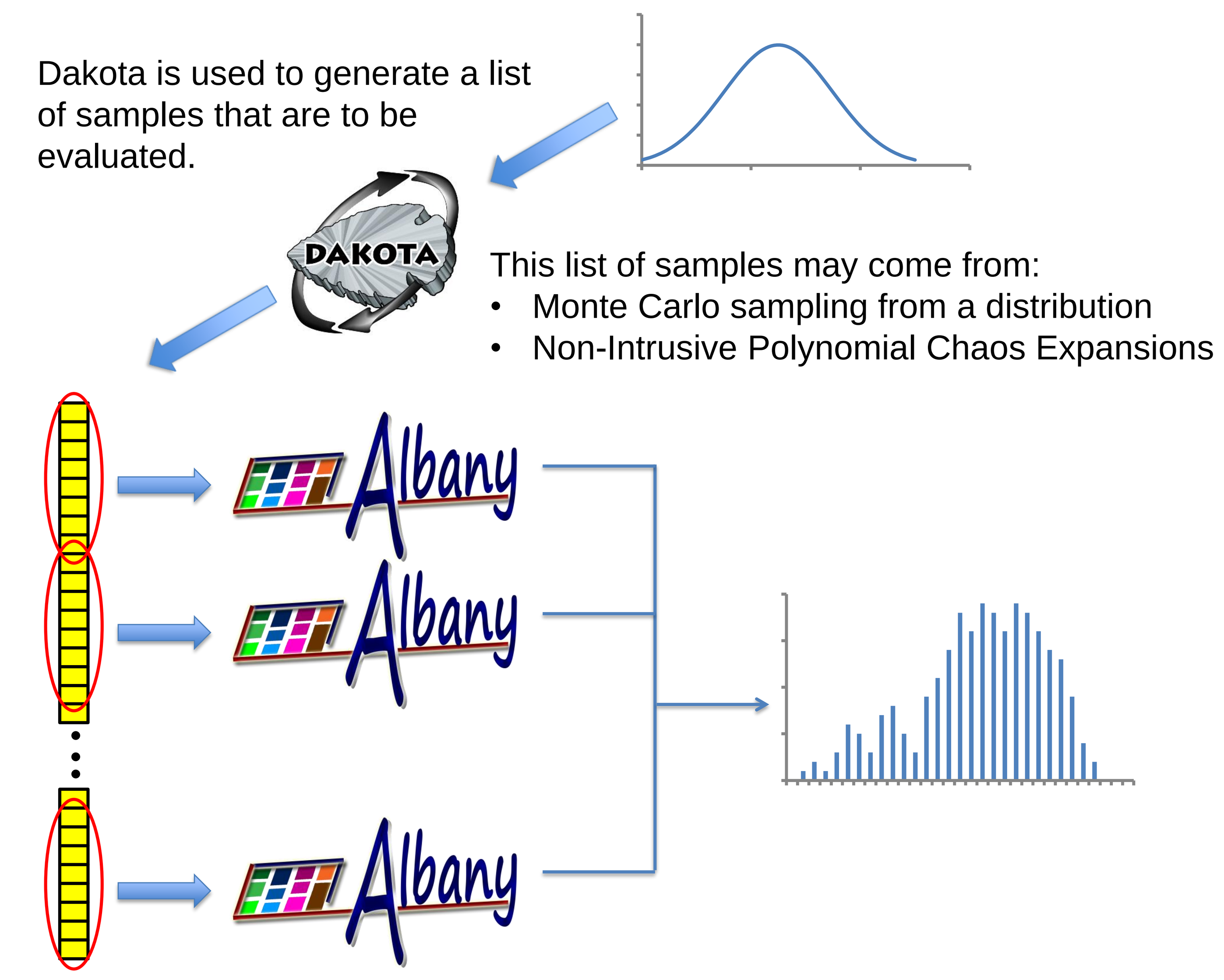
- Stochastic Galerkin Methods
- Concurrent Ensemble Sample Evaluation

Concurrent Ensemble Sample Evaluation

Aeras uses the concurrent ensemble sample evaluation capability of Stokhos to improve the computational efficiency of uncertainty quantification.

In this approach an ensemble of samples is propagated concurrently at the scalar level of the simulation code. This allows for:

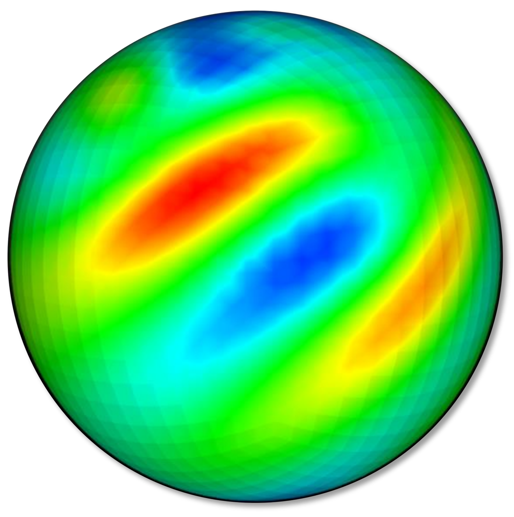
- Improved memory access patterns
- Increased vectorization of the operations
- Reduced communication overhead in MPI codes
- Increased opportunities for fine-grained parallelism



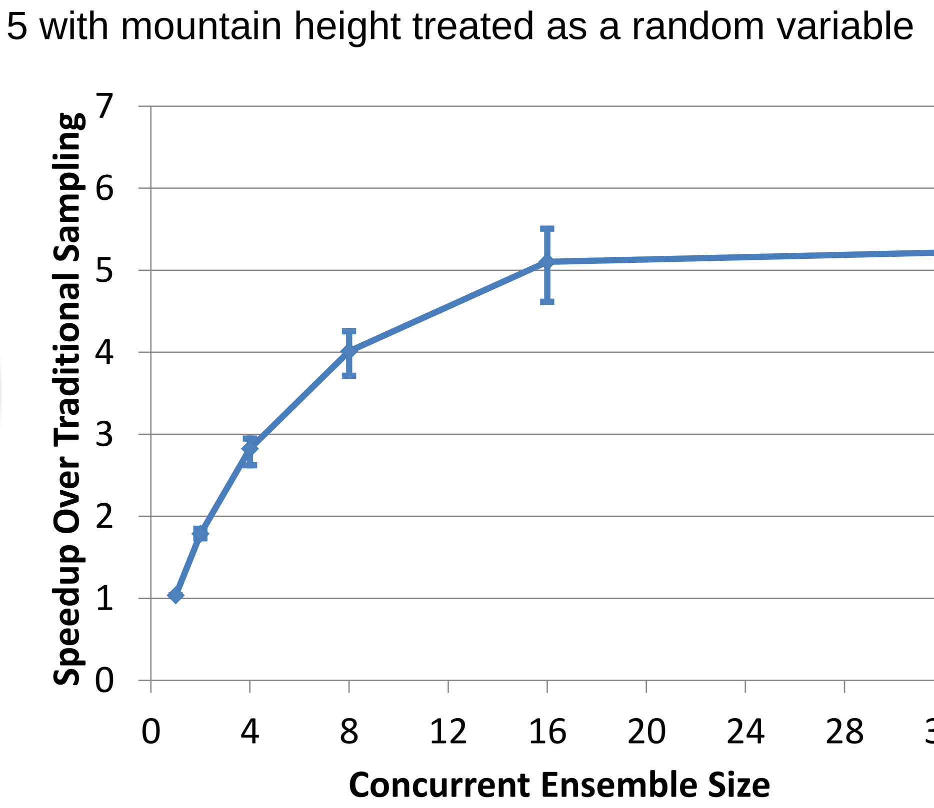
Ensembles of samples are evaluated concurrently using Albany.

Numerical Results

Shallow Water Test Case 5 with mountain height treated as a random variable



Representative Sample
Latitudinal velocity (color)
T= 6 days



Concurrent Ensemble Sample Propagation can dramatically reduce the computation time for uncertainty quantification compared to standard sampling methods in which each sample is evaluated independently.

For this test case, using a concurrent ensemble size of 32 decreases the execution time by a factor of 4 to 6 compared to standard sample evaluations.

U.S. DEPARTMENT OF ENERGY
LDRD LABORATORY DIRECTED RESEARCH & DEVELOPMENT

Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

SAND 2015-5179C

Sandia National Laboratories