SAND2013-9317P

High-Performance Computing Software Relevant to Wind Energy Applications

Computing Research Center and Engineering Sciences Center

Sandia National Laboratories

Albuquerque, NM

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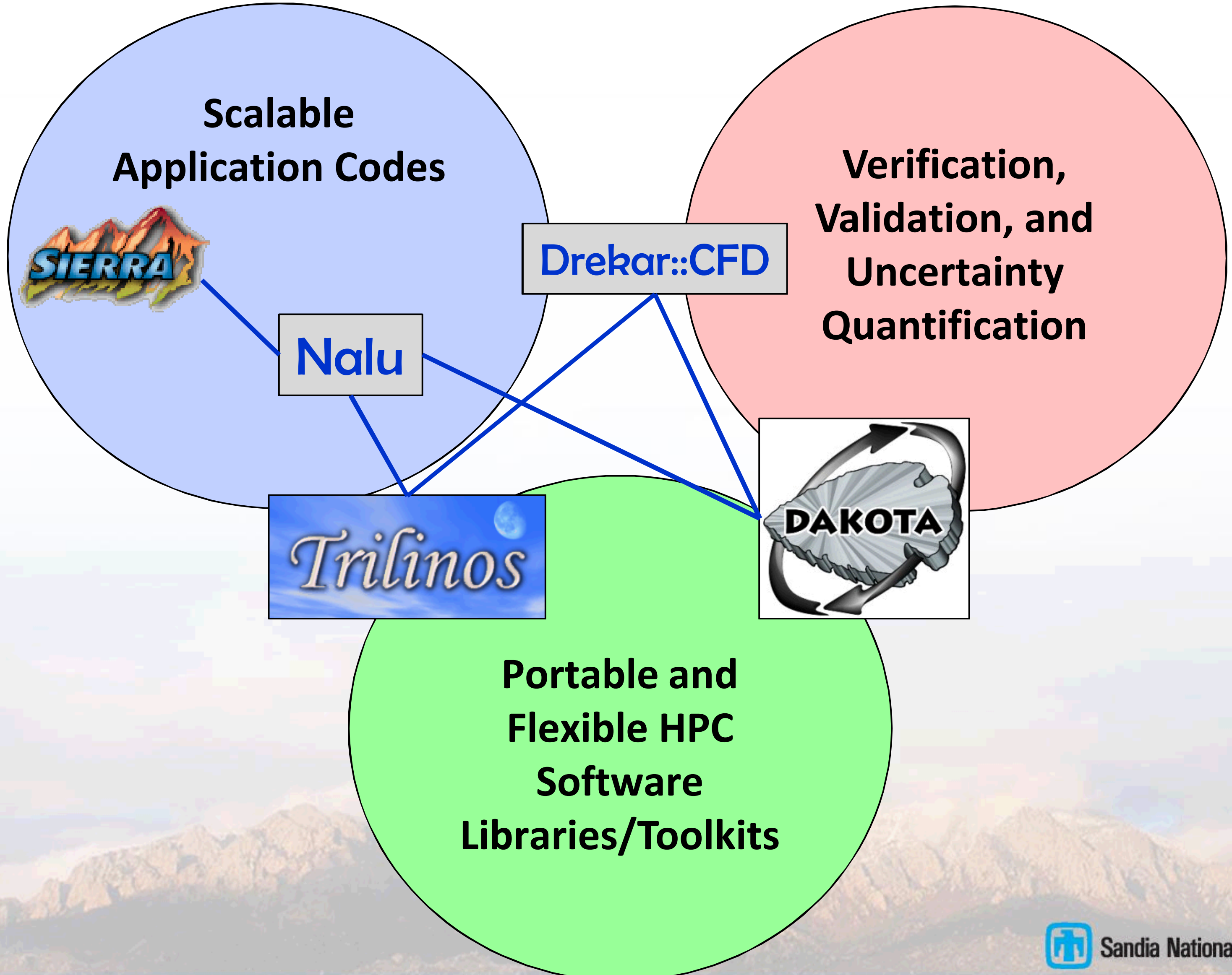
SNL HPC Software and Expertise

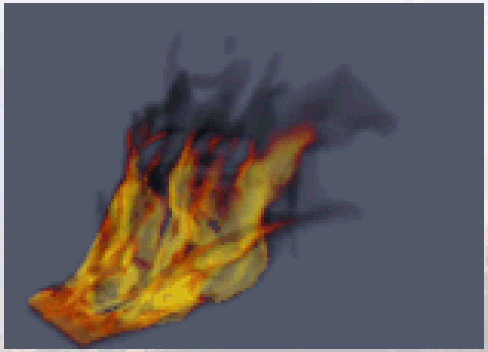


Nalu - Leveraging the NNSA CFD Code Base

http://nnsa.energy.gov/asc

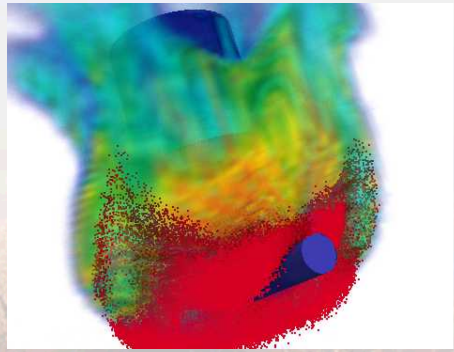
- Low-Mach fluids capability within the Sierra/Fluid Dynamics (FD) ASC IC project
  - Massively parallel computing
    - Sierra Toolkit + Trilinos => scalable solvers, support for new architectures
    - Successfully scaled to 10 billion element+ unstructured hex meshes on >130k cores
  - Low dissipation (unstructured) finite volume numerics
  - Detailed SQE plan to insure code quality
  - Nalu – CFD code for open distribution

400 million dof object in fire



Turbulent jet (17mil-10 billion DOF)

Propellant fire



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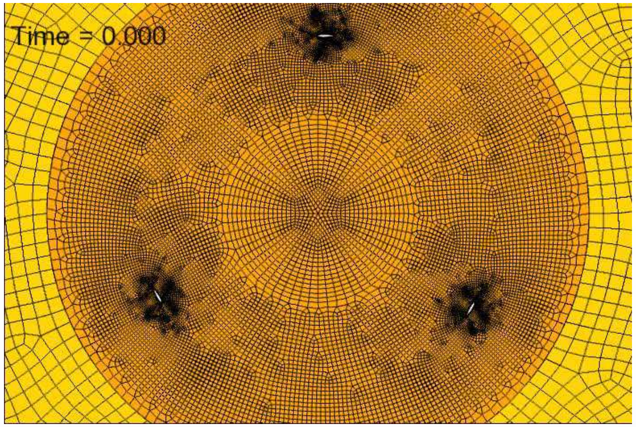
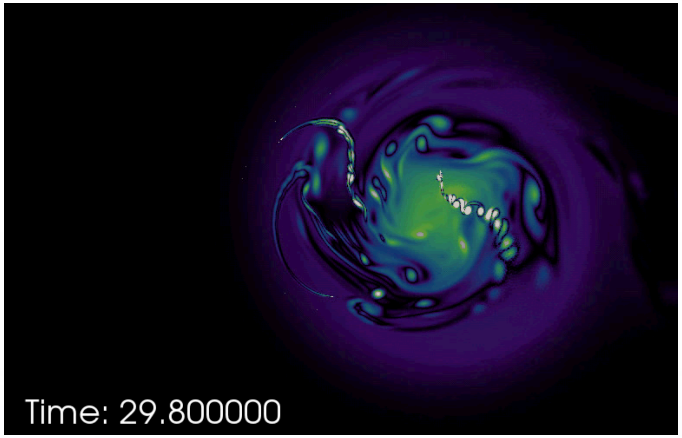
Nalu: Scalable Code for Unstructured-Mesh Large Eddy Simulation (LES)

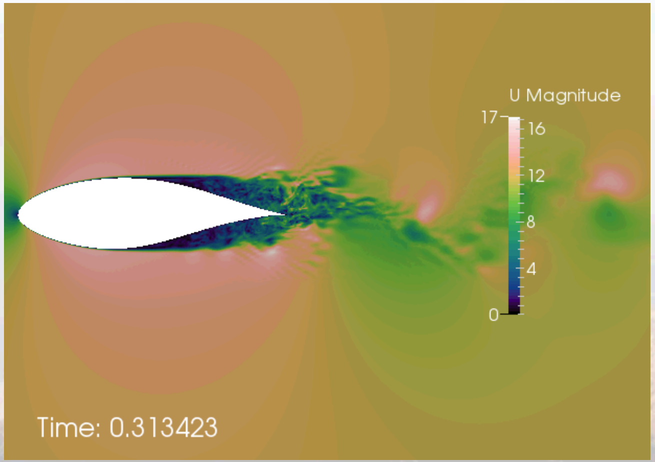
Sliding Mesh for 2D VAWT Rotor Simulation



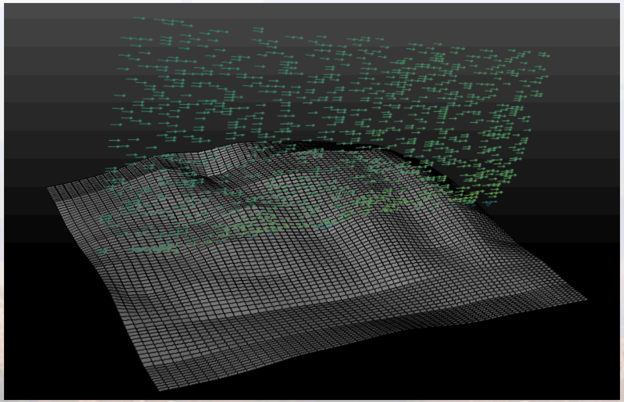
Vortical Gust Passing through VAWT rotor



LES of a Thick Wind Turbine Airfoil



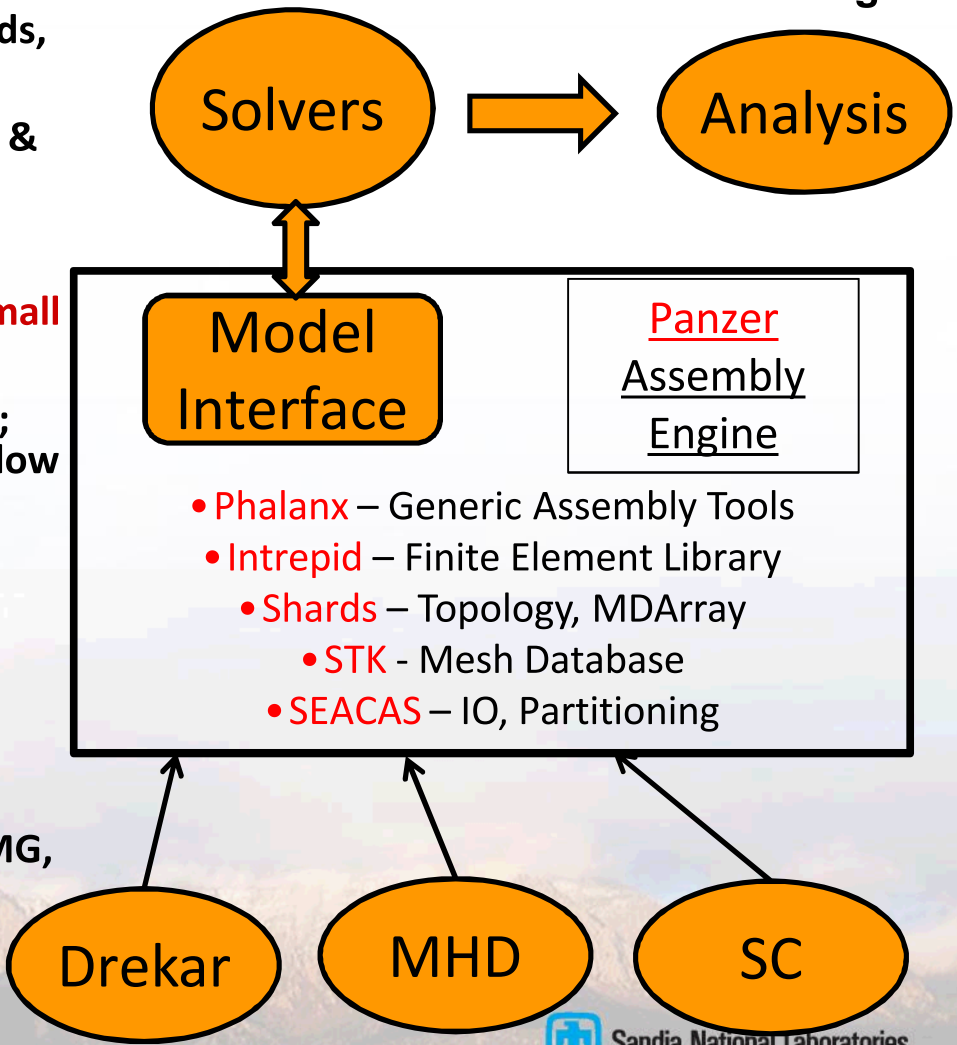
Complex Topography:
1.6 km x 1.6 km section of Angel Fire, NM



Drekar::CFD

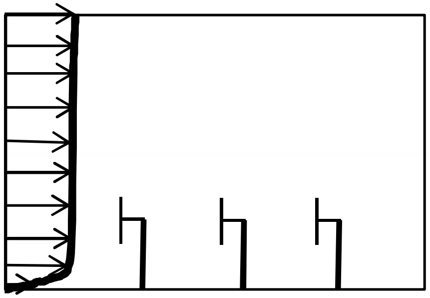
- **Massively Parallel: MPI**
- **2D & 3D Unstructured Stabilized Finite Elements**
- **Edge/face based elements, high-resolution methods, …**
- **Fully-implicit: 1st-5th variable order BDF (Rythmos) & TR**
- **Direct-to-Steady-State (NOX)**
- **Semi-implicit, IMEX, etc. under investigation for small time scale transients**
- **Eq. of State: Constant density; Bousinessq approx.; variable density: low flow Mach number approx., low flow Mach number compressible;**
- **Fully Coupled Globalized Newton-Krylov Solver**
  - **Template-based Generic Programming with Automatic Differentiation (Sacado) for NK, JFNK, Sensitivities, UQ, etc.**
  - **GMRES (AztecOO, Belos)**
- **Scalable preconditioners: Fully-coupled system AMG, physics-based (e.g. SIMPLEC)**
- **Adjoints**

trilinos.sandia.gov



Rapid Development Example
Drekar::CFD + DAKOTA

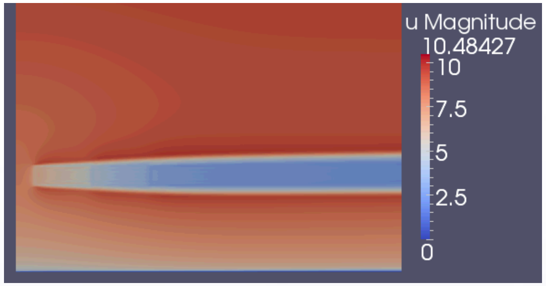
- **Drekar::CFD is an open source CFD code built from Trilinos components. It uses an unstructured finite element discretization. Problems can be solved direct-to-steady-date, pseudo-transient to steady-state and time accurate. UQ, error estimation and parameter sensitivity studies are enabled by automatic differentiation and an embedded adjoint solver. Optimization problems can be solved using Dakota driving Drekar as a black box or using adjoints. Using the ML solver library, Drekar demonstrated scalability on 5e5 cores on problems containing 1.8e8 unknowns.**



Schematic of 2D wind farm

Rapid development example: Wind farm optimization

- **Wind farm model details**
  - 2D turbulent BL with 1/7 power inflow velocity profile, Spalart-Allmaras RANS turbulence model
  - Reynolds number, ReD=10,000/m
  - Actuator Disc Rotor model: constant thrust coefficient, momentum source
- **Optimization Problem**
  - Dakota drives optimization treating Drekar as a black box
  - Nonlinear conjugate gradient method with line searching
  - Objective: maximize total power (V*T)
  - Allow the rotors to move vertically subject to practical constraints: 3 ≤ height ≤ 8
- **Outcome**
  - **Actuator Disc code development time: three days**
  - **Optimization problem development and run time: two days**
  - Initial heights: [5.0, 5.0, 5.0] - **Initial Power: 250.0 (W/m)**
  - Final heights: [8.0, 6.5, 5.2] - **Final Power: 602.3 (W/m)**



Initial rotor placement, velocity magnitude

Final rotor placement, velocity magnitude

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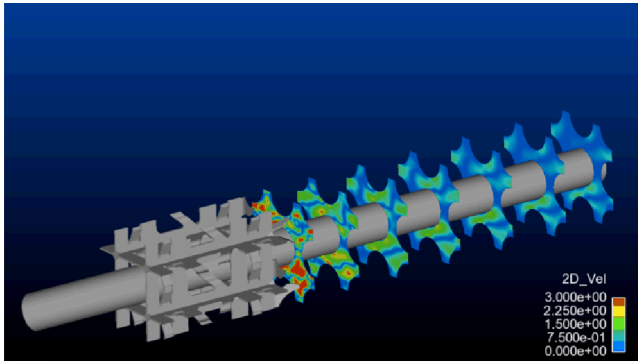
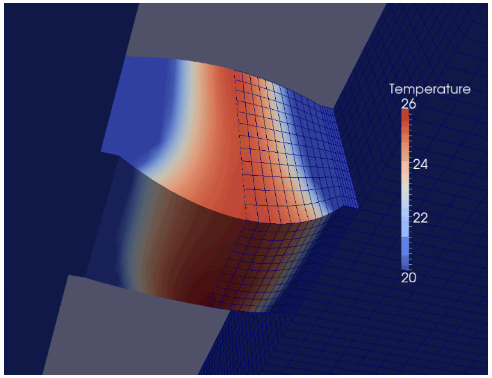
Component-Based Code Design Maximizes the Leveraging of Foundational Technologies

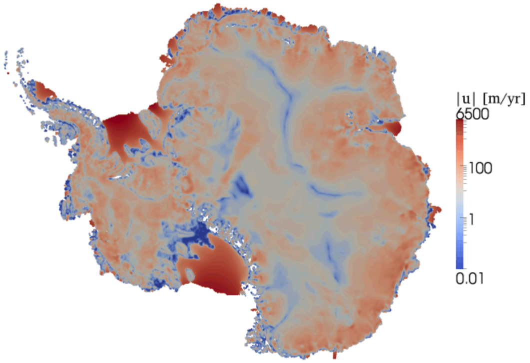
-- Codes are Born with Sophisticated Design Capabilities



LES calculation to Analyze Vibrations of Fuel Rods



Shape Optimization of Contactor



Calibration of Antarctic Ice Sheet Flow Model

Trilinos **(Open Source Components)**

Parallelization Tools
Data Structures
Partitioning
Load Balancing
Architecture-Dependent Kernels

Linear Solvers
Iterative Solvers
Direct Solvers
Eigen Solver
Preconditioners
Multi-Level Algs

Analysis Tools
Nonlinear Solver
Time Integration
Stability Analysis
Optimization
UQ Algorithms
Reduced Order Models

Software Quality
Version Control
Regression Testing
Build System
Verification Tests
Bug Tracking
Web Documentation

Codes are written quickly with robust and scalable solvers, embedded analysis capabilities, and modern software tools. →Continued leveraging of ongoing projects (e.g. port to GPUs).

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DAKOTA: Research, development, & deployment of advanced iterative algorithms for simulation-based assessment and design

DAKOTA
Optimization
Uncertainty Quant.
Parameter Est.
Sensitivity Analysis

Model Parameters

Black box:
Sandia simulation codes
Commercial simulation codes
Library mode (semi-intrusive):
ALEGRA (shock physics),
Xyce (circuits), Sage (CFD),
Albany/TriKota (Trilinos-based),
MATLAB, Python, ModelCenter,
SIERRA (multiphysics)

Design Metrics

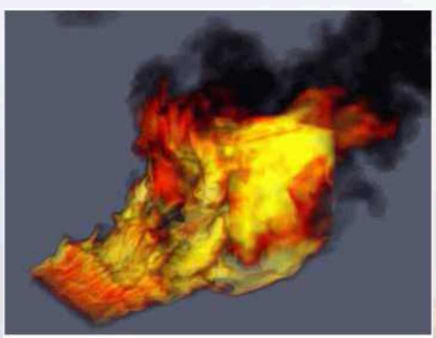
Iterative systems analysis

Multilevel parallel computing

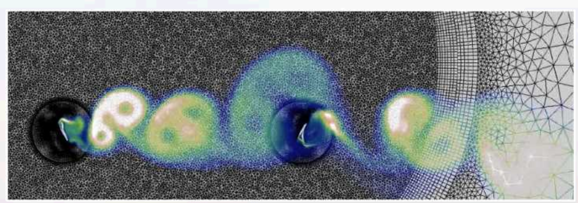
Simulation management

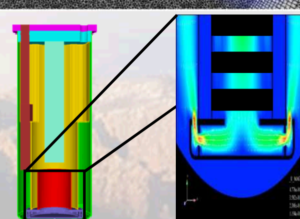
Impact across a variety of DOE mission areas

Stockpile (NNSA ASC)
Abnormal environments

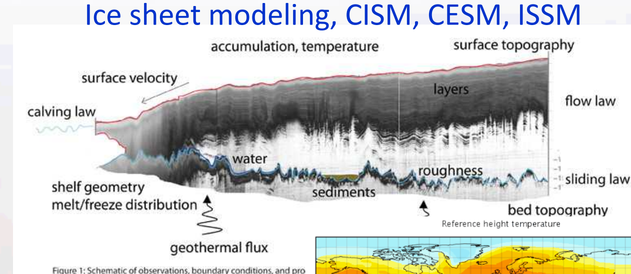


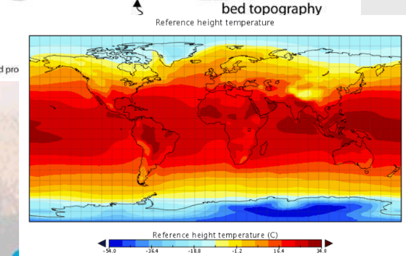
Energy (ASCR, EERE, NE)
Wind turbines, nuclear reactors





Climate (SciDAC, CSSEF)
Ice sheet modeling, CISM, CESM, ISSM





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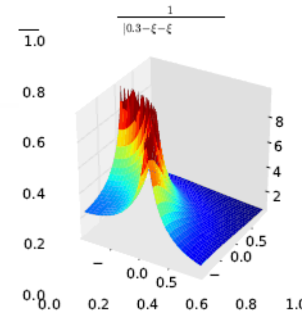
DAKOTA: Emphasis on Scalable Methods for High-fidelity UQ on HPC

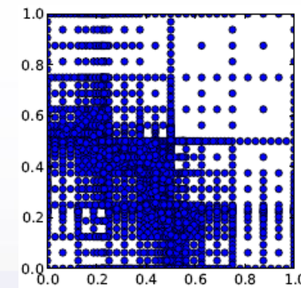
Key Challenges:

- **Severe simulation budget constraints** (e.g., a handful of high-fidelity runs)
- **Moderate to high-dimensional** in random variables: O(10) to O(100)
- **Compounding effects**:
  - Mixed aleatory-epistemic uncertainties (→ nested iteration)
  - Requirement to evaluate probability of rare events (e.g., safety criteria)
  - Nonsmooth responses (→ difficulty with fast converging spectral UQ methods)



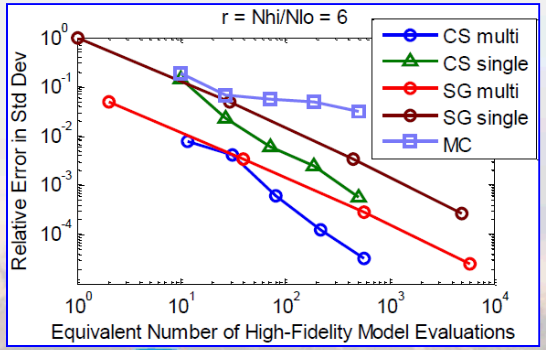
Core UQ Capabilities:

- **Sampling methods**: LHS, MC, QMC, incremental
- **Reliability methods**: local (MV, AMV+, FORM), global (EGRA, GPAIS, POFDarts)
- **Stochastic expansion methods**: polynomial chaos, stochastic collocation
- **Epistemic methods**: interval estimation, Dempster-Shafer evidence



Research Thrusts:

- **Compute dominant uncertainty effects** despite key challenges above
- **Scalable UQ foundation**
  - Adaptive refinement, Adjoint enhancement, Sparsity detection
- Leverage this foundation within **component-based meta-iteration**
  - Mixed UQ, Model form UQ, Multifidelity UQ, Bayesian methods



Overview of Hardware Available to SNL Users

Tri-Lab Capability Computers

Cielo

- 1.3 Pflops*
- 142,000 cores
- LANL/SNL/LLNL resource (NNSA)

Sequoia

- 20 Pflops
- 1.5 million cores
- LANL/SNL/LLNL resource (NNSA)

New Trinity and Tri-Lab Cluster in the works

- Trinity ~ 30 Pflops

SNL Institutional Clusters

Red Sky/Red Mesa

- 444 Tflops*
- 37,888 cores
- Red Mesa allocated to SNL energy work FY14

Unity/Glory/Whitney

- 114 Tflops
- 13,056 cores
- Available for non-NW work Q4 FY2013

New HP Cluster 4Q FY2013

- 150 Tflops

Next Generation Institutional Computers based on Trinity and Tri-Lab architectures

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*1 Petaflop = 1,000 Teraflop