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Dakota: Benefits and Challenges of Lab-developed Open Source Scientific Software

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http://dakota.sandia.gov

Scientific Software Days

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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.

Talk Goals

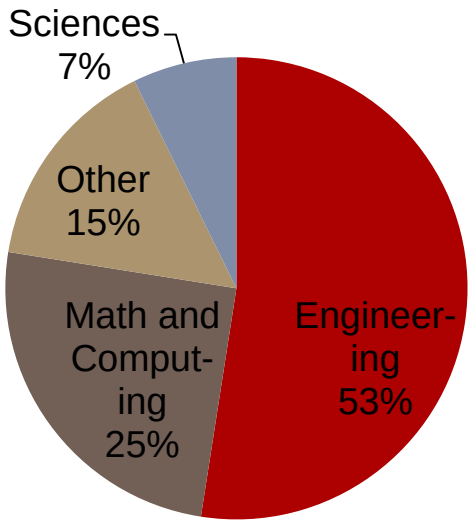
- Give perspective on national lab context for Dakota development
- Share Dakota software and project goals
- Understand drivers for (open-source) software development
- Raise challenges and get community feedback

This talk is not unique to Dakota, nor the lab environment, but I hope to seed discussion.

SNL Mission: Advanced Science and Engineering for National Security

- Nuclear Weapons
- Defense Systems and Assessments
- Energy and Climate
- International, Homeland, and Nuclear Security

- Collegial environment with 12,000 (5,000 R&D; 6,000 advanced degreed) staff in Albuquerque, NM and Livermore, CA



- Dakota Mission: *To serve Sandia's mission through state-of-the-art research and robust, usable software for optimization and uncertainty quantification.*

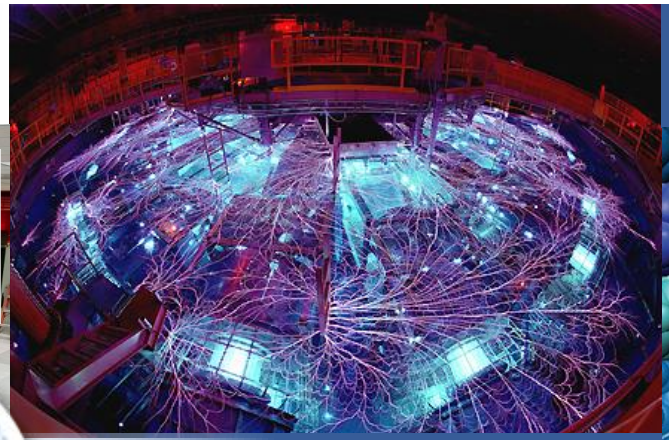
SNL's Research Framework

Strong research foundations play a differentiating role in our mission delivery

Sandia National Laboratories

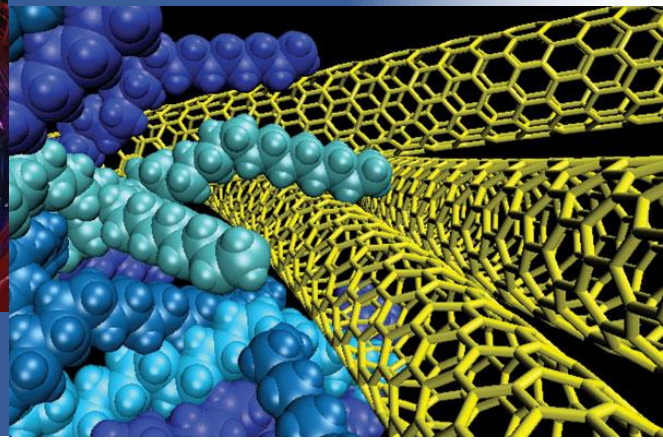
Computing & Information Sciences

Center for Computing Research
Optimization and UQ
Dakota

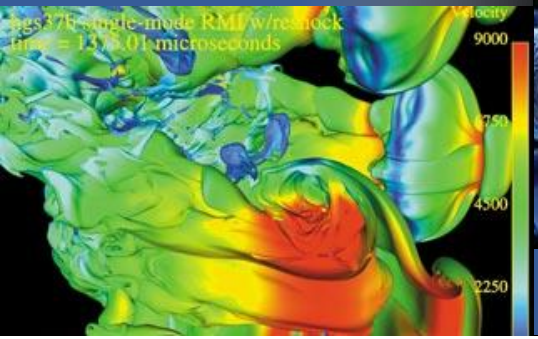


Radiation Effects & High Energy Density Science

Materials Sciences

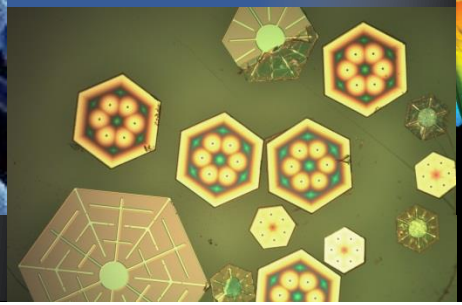


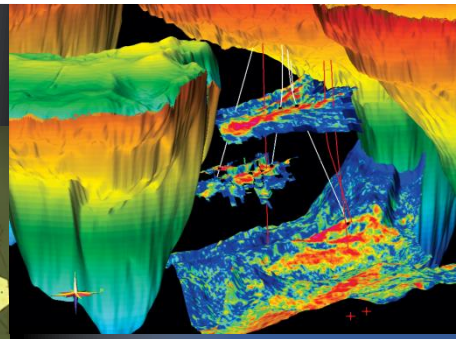
Engineering Sciences



Bioscience

Nanodevices & Microsystems

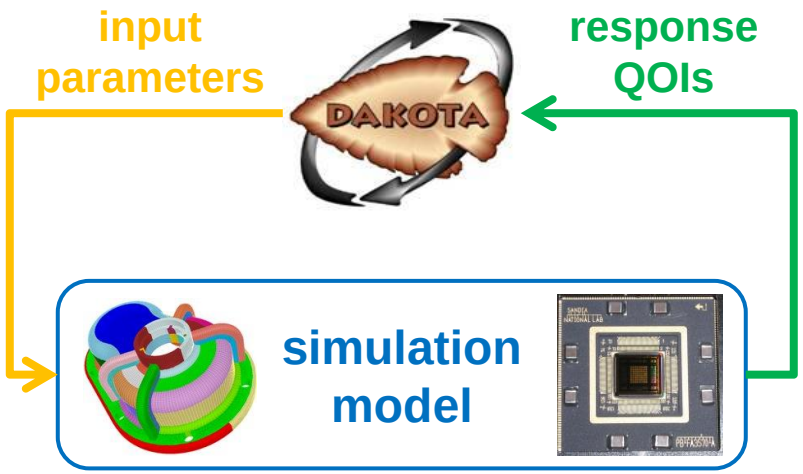




Geoscience

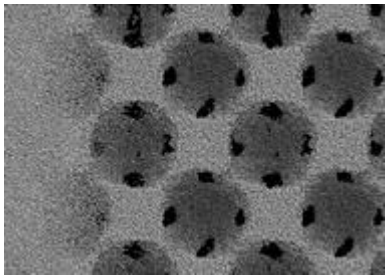
Dakota: Algorithms for Design Exploration and Simulation Credibility

- Suite of iterative mathematical and statistical methods that interface to computational models
- Makes sophisticated parametric exploration of black-box simulations practical for a computational design-analyze-test cycle:
  - Sensitivity Analysis
  - Uncertainty Quantification
  - Design Optimization
  - Model Calibration

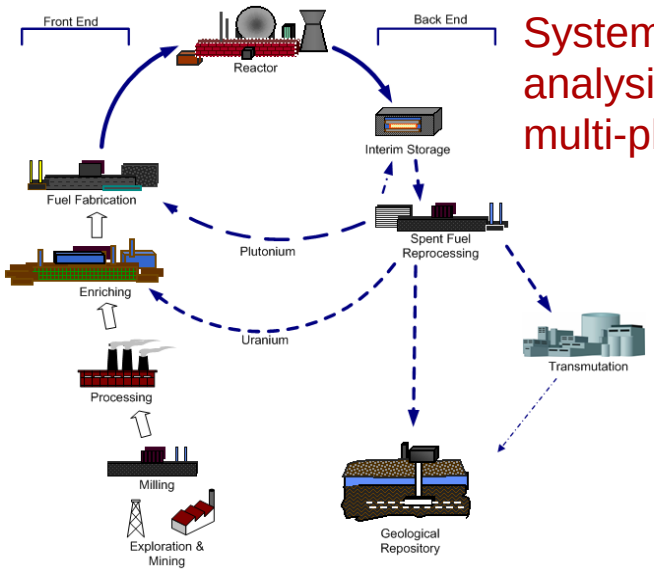


- *Goal: provide scientists and engineers (analysts, designers, decision makers) richer perspective on model predictions*

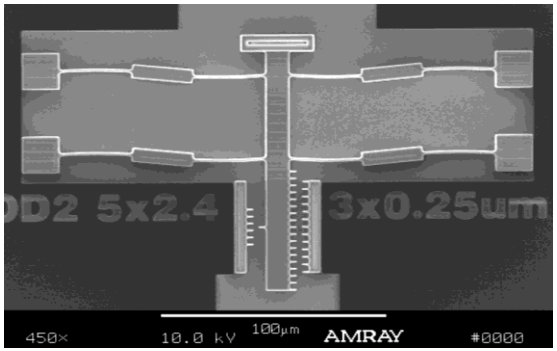
Diverse Simulations Across Scales



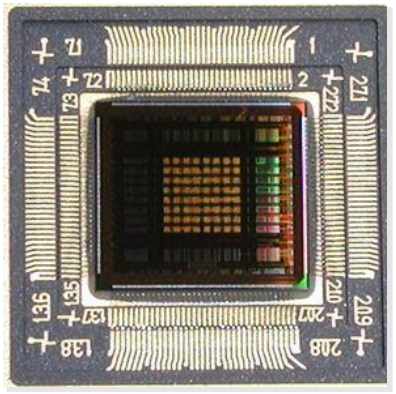
Shock loading of polymer foam: molecular dynamics



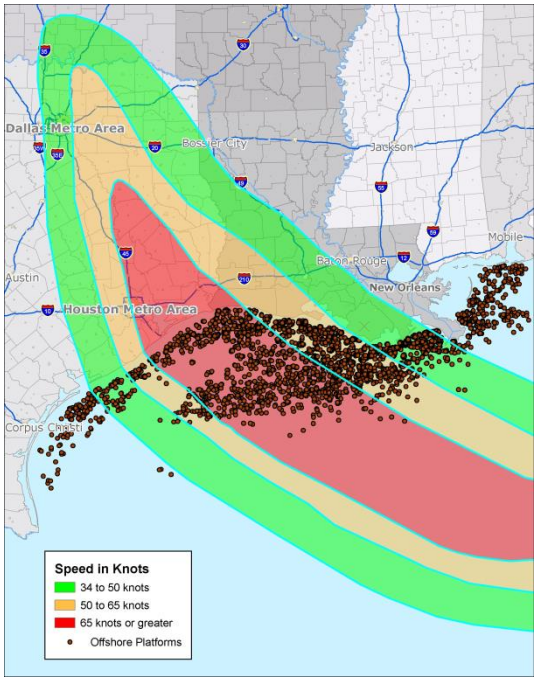
Systems of systems analysis: multi-scale, multi-phenomenon



Micro-electro-mechanical systems (MEMS): quasi-static nonlinear elasticity, process modeling



Electrical circuits: networks, PDEs, differential algebraic equations (DAEs), E&M



Emergencies: weather, logistics, economics, human behavior

Relations with Other Scientific Software

Dakota is comprised of

- Dakota and other Sandia-developed optimization, design of experiments, UQ, and surrogate model packages (only some actively developed)
- Partially DOE funded third-party libraries, e.g., FSUDace, PSUADE, QUESO
- Historical (legacy) third-party libraries (technical debt, usability challenge)
- Trilinos for numerics foundations

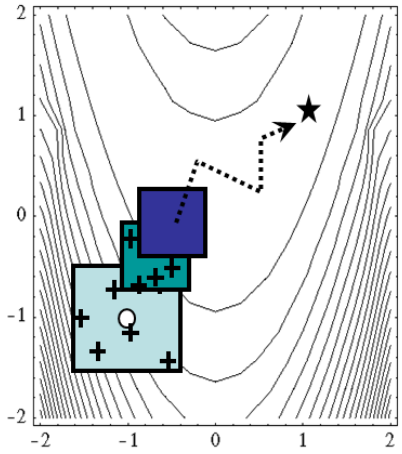
And interfaces with

- Simulation Codes (scalability is a challenge here!):
  - Sandia-developed: both loose and tight integration
  - Other open source
  - Commercial
- Visualization and post-processing tools: both for simulation output and Dakota results
- Simulation analysis environments / GUIs

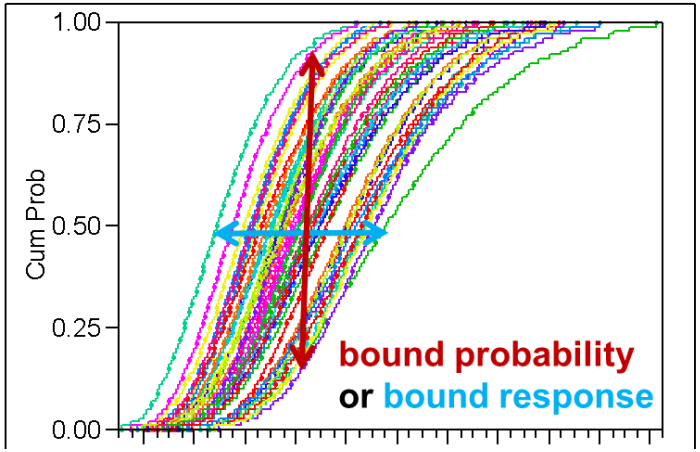
Engineering Needs Drive Dakota R&D

Develop/deploy advanced approaches to help solve practical problems:

- Characterize parameter uncertainty → Bayesian calibration
- Hybrid analysis → mix methods, surrogates, and models
- Mixed uncertainty characterizations → epistemic and mixed UQ approaches
- Costly simulations → surrogate-based optimization and UQ
- Build in safety or robustness → mixed deterministic/probabilistic methods



$$\begin{aligned} \min \quad & f(d) + W s_u(d) \\ \text{s.t.} \quad & g_l \le g(d) \le g_u \\ & h(d) = h_t \\ & d_l \le d \le d_u \\ & a_l \le A_i\, s_u(d) \le a_u \\ & A_e\, s_u(d) = a_t \end{aligned}$$



SNL Environment: Benefits/Challenges

- Rich, though challenging, problems across science/engineering domains
  "I want to do UQ with 200 parameters, but can only run two simulations."
- Healthy culture of intra- and inter-institution collaboration
- Strong Dakota name recognition and track record; hundreds of SNL users, more DOE-wide; many support requests
- Must regularly deliver and support application-ready, usable software
- Rewarded by customers/users for both time-tested and leading-edge algorithms in software as well as close consulting partnerships
- CIS research foundation and CCR expect and reward research, software, and publications, though we aren't in the commercial software business

Life of Dakota

1994

Unify engineering optimization

$: LDRD

Surrogate-based methods

Proprietary

2001

Risk-informed decision making

$: NW/ASC V&V

UQ, OUU, multi-fidelity methods

Open source v3.0 (GPL)

2006

Significant UQ investments

$: Energy, Climate

Public mailing lists

Open source v4.0 (LGPL)

2011

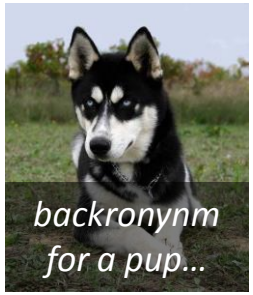
Scalable algorithms

Production support

$: Office of Science, DARPA

Agile development, v5.2

Mike Eldred
Founder



Invested developer, solving a practical problem

Why Open Source?

- Lab default is (typically) government use, then commercial license
- Open source (2001) for easier collaboration on algorithm development, primarily with faculty and students (before, during, after internships)
  - Vanderbilt: reliability methods for UQ
  - MIT: surrogate-based and multi-fidelity optimization
  - Stanford: UQ and active subspace methods; PSAAP applications
  - UT Austin: Bayesian inference
- Also attract integrators across sectors, e.g.,
  - NREL/NASA integration into OpenMDAO
  - Lockheed Martin integration with ModelCenter
  - Use with OpenFOAM; integration with CAESES commercial CFD
- Better scale with user base: create an engaged user community
- *Over 20,000 package downloads since 2010 across all sectors (impact?)*
- *Whether we are genuinely, all-in open source hasn't been tested…*

Dakota Project as a Competency

- Dakota is more than software: an enthusiastic team (of fractional persons) with balanced strengths in algorithm research, software design and development, and application deployment and support
  - Mathematicians, statisticians, computer scientists, computational engineers
  - Expertise in sensitivity analysis, optimization, calibration, UQ, surrogate modelling
  - Software engineering with C++, Python, Java
  - User support to deep consulting
- But core team entirely at SNL!
- *How do we grow the team / contributors as the user community grows?*
- *Or more critically, how do we realize benefits of open source to help scale?*

Funding Picture

- Dakota strives to maintain a balanced funding portfolio; across
  - Research to production spectrum
  - Sponsor type and sizes: both core stewardship and smaller exploratory
  - Application domains
- Dakota often central to proposals, e.g., CASL, DARPA
- Example balanced portfolio:
  LDRD, ASCR, SciDAC, DARPA, CASL, NW/ASC Software, NEAMS, Industry

- Discussion points *(how do audience members manage?)*:
  - Individually funded PIs may bring their capability to Dakota
  - How to steward Dakota capability base and manage technical debt; may not be valued by some sponsors
  - How to pool / manage small funded requests, whether development or training/support?
  - What drives much needed usability efforts?

Dakota Community

- Extensive website: documentation, training materials, downloads
- Active public mailing list, *though not browsable;* moving to online forums
- Publicly readable Subversion repository

- High usage in and outside labs
- Solicited for both research and commercial engagements, mostly small scale
- Receive a few patches and bug reports monthly (many languish; perhaps due to misalignment)
- Team cannot respond to all user (or developer) requests nor reach all analysis domains
- Some users help each other, including a few superstars

Toward a Self-Sustaining Community

- We would like to build a more engaged community that
  - Helps itself (basic usage, advanced support)
  - Improves portability and interfaces by deploying to new platforms and application codes
  - Contributes to software development

- What should our team put priority on to attract and build trust with a user/developer community?
  - Incentivize use case contributions?
  - Explicitly prioritize engagements with certain super-users?
  - Better web resources (can be challenging in the lab environment)? Clear public interfaces for bugs, patches, discussion?
  - User / developer group meetings?
  - External partnerships for deployment and user support?

Technical Growth to Promote Engagement

Potential development priorities to increase contribution

- Improved modularity so users can extend, contribute, components, e.g.,
  - Surrogate model module with Python bindings
  - More usable simulation interfacing that encourages best practices
- Community repository of contributed code, examples, scripts
- Clear development practices, e.g., principles, code standards, easier build/test on new platforms
- Remain on cutting edge of algorithms to encourage it as a research vehicle. Representative current directions:
  - Bayesian calibration and model discrepancy
  - Multi-fidelity UQ and inference
  - Portability to extreme scale computers, growth into hybrid parallel
  - SA and UQ scalability with active subspaces; generalize to random fields
  - Expanding mixed-integer optimization

Questions

Thanks for your attention!

To seed discussion:

- What approaches and resources have you found most helpful in creating a vibrant user community?
- What investments or behaviors have yielded the most effective developer contributions?
- How do you set, communicate, and manage expectations and priorities?

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