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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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Austin, TX

Exceptional service in the national interest

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

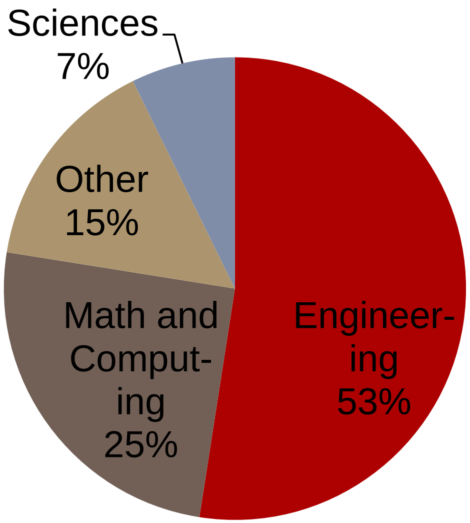
- Give perspective on national lab context for Dakota development
- Share Dakota software and project goals
- Understand drivers for (open-source) software development
- Raise challenges and get community feedback

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



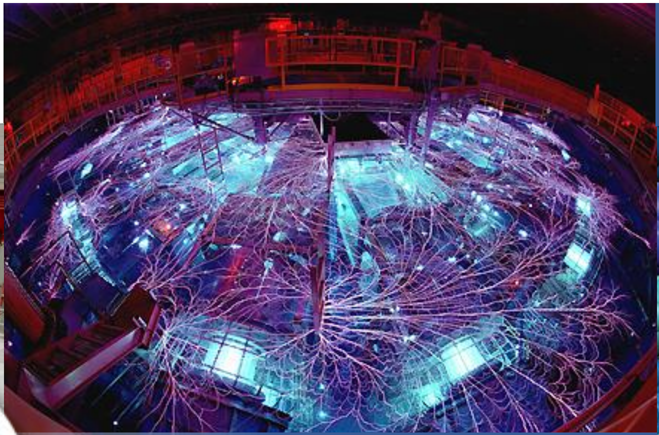
- Dakota Mission: *To serve Sandia's mission through state-of-the-art research and robust, usable software for optimization and uncertainty quantification.*

SNL's Research Framework

Strong research foundations play a differentiating role in our mission delivery

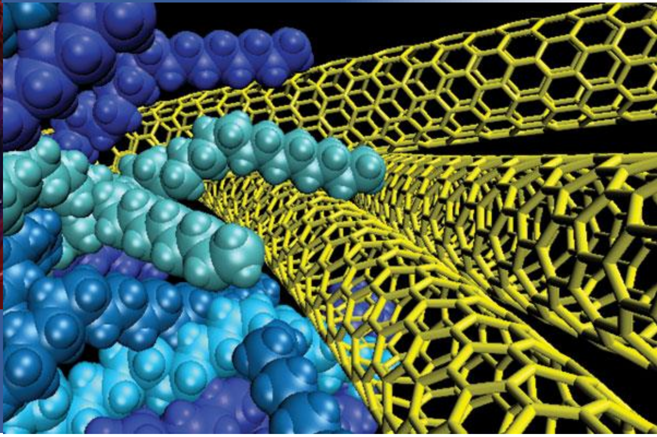
Computing & Information Sciences

Center for Computing Research
Optimization and UQ
Dakota

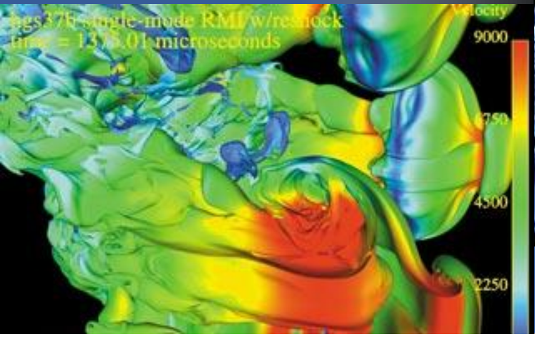


Radiation Effects & High Energy Density Science

Materials Sciences

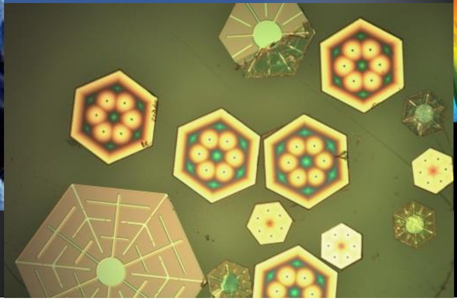


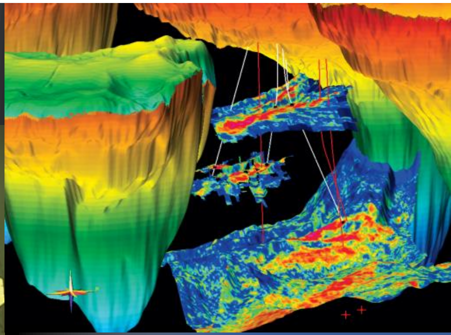
Engineering Sciences



Bioscience

Nanodevices & Microsystems

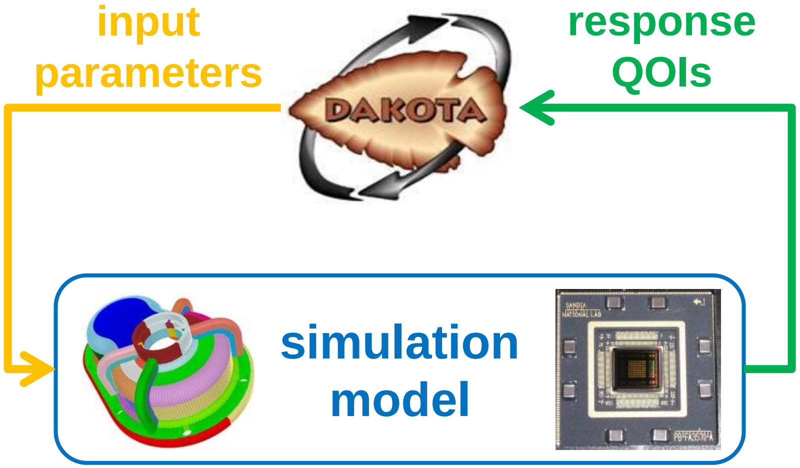




Geoscience

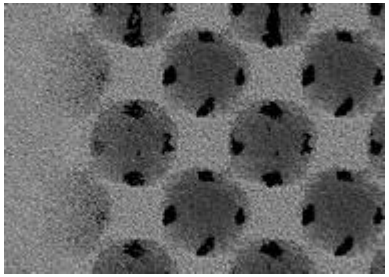
Dakota: Algorithms for Design Exploration and Simulation Credibility

- 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

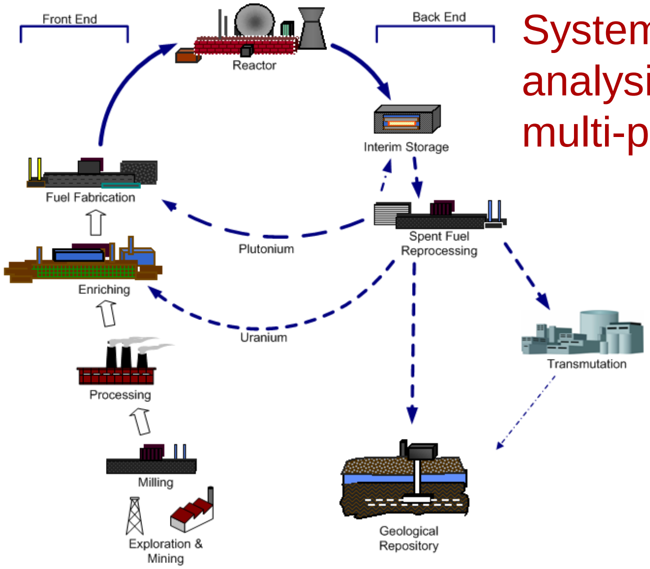


- *Goal: provide scientists and engineers (analysts, designers, decision makers) richer perspective on model predictions*

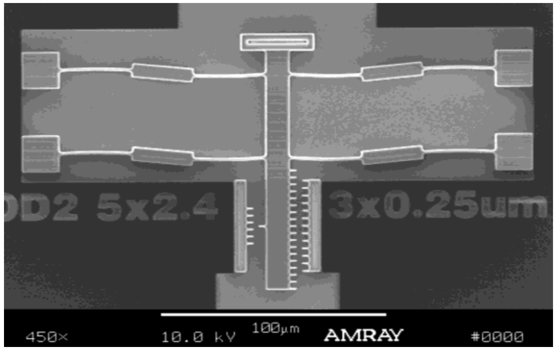
Diverse Simulations Across Scales



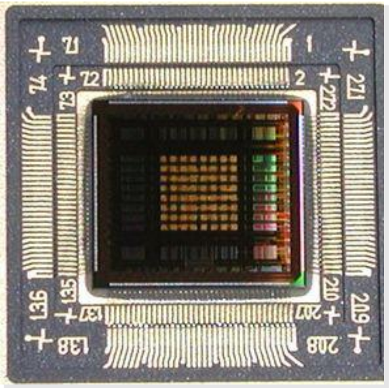
Shock loading of polymer foam: molecular dynamics



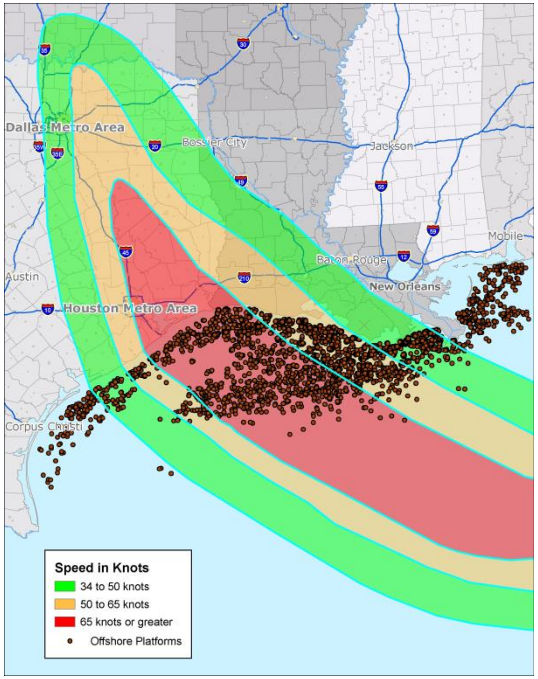
Systems of systems analysis: multi-scale, multi-phenomenon



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

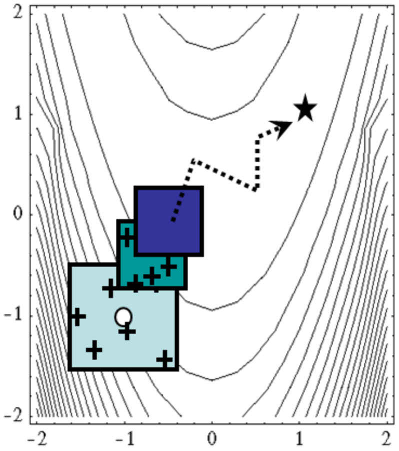
And interfaces with

- 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

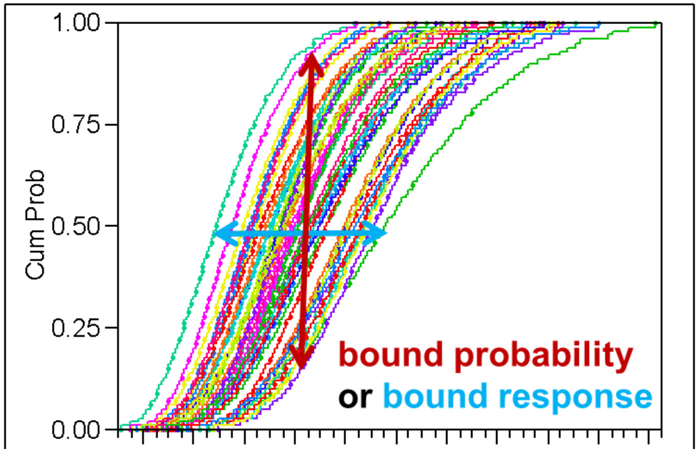
Engineering Needs Drive Dakota R&D

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



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



bound probability
or bound response

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

2009: v5.0 (LGPL)

2011

Scalable algorithms

Production support

$: Office of Science, DARPA

Agile development, v5.2

Mike Eldred Founder

backronynm for a pup…

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

2013 Employee Recognition Award-Winning Team

- 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?*

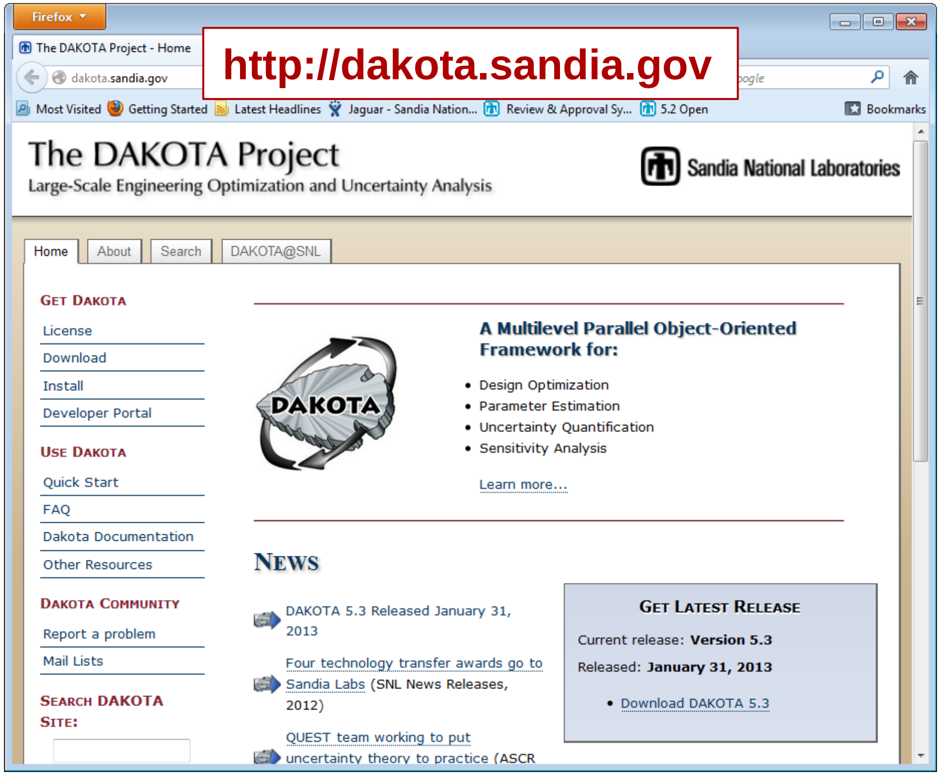
Funding Picture

- 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



http://dakota.sandia.gov

The DAKOTA Project

Large-Scale Engineering Optimization and Uncertainty Analysis

Sandia National Laboratories

GET DAKOTA

- License
- Download
- Install
- Developer Portal

USE DAKOTA

- Quick Start
- FAQ
- Dakota Documentation
- Other Resources

DAKOTA COMMUNITY

- Report a problem
- Mail Lists

SEARCH DAKOTA SITE:

A Multilevel Parallel Object-Oriented Framework for:

- Design Optimization
- Parameter Estimation
- Uncertainty Quantification
- Sensitivity Analysis

Learn more...

NEWS

DAKOTA 5.3 Released January 31, 2013

Four technology transfer awards go to Sandia Labs (SNL News Releases, 2012)

QUEST team working to put uncertainty theory to practice (ASCR

GET LATEST RELEASE

Current release: **Version 5.3**

Released: **January 31, 2013**

- Download DAKOTA 5.3

- 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

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?

- Regrets I can’t stay long today…
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  http://dakota.sandia.gov

Thanks for your attention!