SAND2013-8428P

Exceptional service in the national interest

Sandia National Laboratories



Scientific Computing Opportunities

Applied Mathematics, Statistics, and Computer Science

Brian M. Adams
Principal Member of Technical Staff
Optimization and Uncertainty Quantification

U.S. DEPARTMENT OF ENERGY
NNSA National Nuclear Security Administration

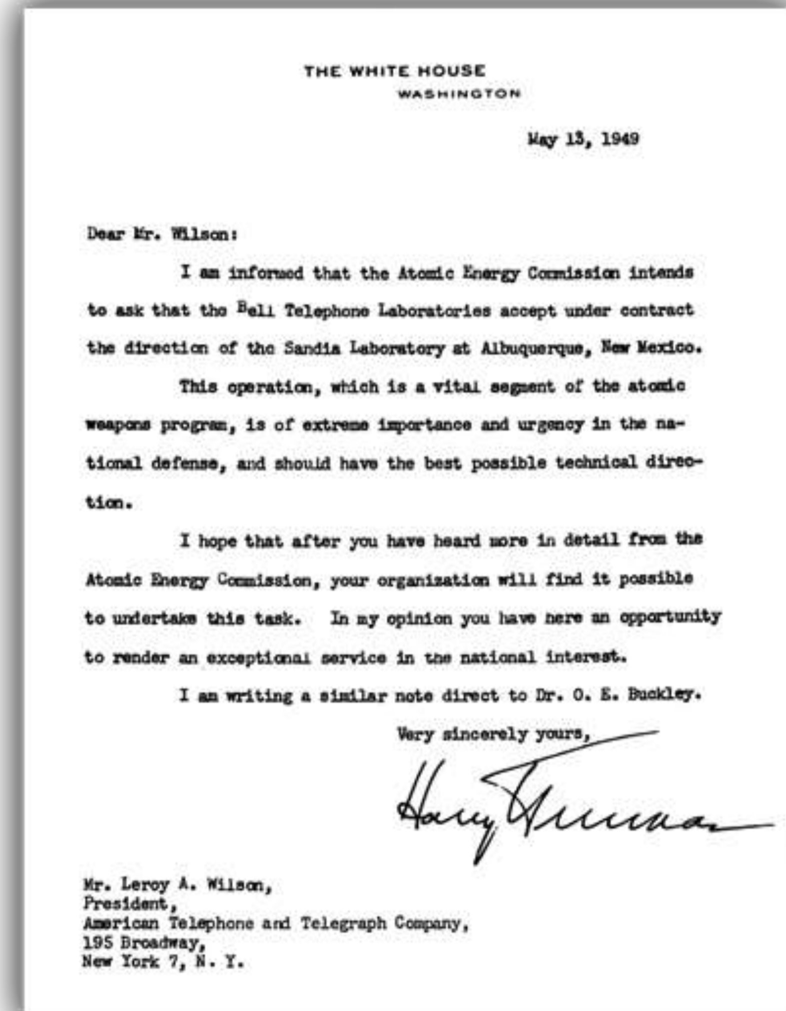
Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000. SAND No. 2013-XXXXP

- Overview of SNL
- My background and why SNL for me (benefits)
- Computing research
- Focus on my work
- Career opportunities

- SAND2012-5130P

Sandia's History

Sandia National Laboratories


THE WHITE HOUSE
WASHINGTON

May 13, 1949

Dear Mr. Wilson:

I am informed that the Atomic Energy Commission intends to ask that the Bell Telephone Laboratories accept under contract the direction of the Sandia Laboratory at Albuquerque, New Mexico.

This operation, which is a vital segment of the atomic weapons program, is of extreme importance and urgency in the national defense, and should have the best possible technical direction.

I hope that after you have heard more in detail from the Atomic Energy Commission, your organization will find it possible to undertake this task. In my opinion you have here an opportunity to render an exceptional service in the national interest.

I am writing a similar note direct to Dr. O. E. Buckley.

Very sincerely yours,

Harry Truman

Mr. Leroy A. Wilson,
President,
American Telephone and Telegraph Company,
195 Broadway,
New York 7, N. Y.

Sandia National Laboratories

Sandia's Governance Structure

Sandia Corporation

- AT&T: 1949–1993
- Martin Marietta: 1993–1995
- Lockheed Martin: 1995–present
- Existing contract expired: Sept. 30, 2012
- One-year contract extension: Sept. 30, 2013
- Two additional 3-month options: March 31, 2014

Government owned, contractor operated

Federally funded research and development center

Sandia's Sites


Albuquerque, New Mexico


Livermore, California


Kauai, Hawaii

Waste Isolation Pilot Plant, Carlsbad, New Mexico


Pantex Plant, Amarillo, Texas


Tonopah, Nevada

National Security Challenges

1950s	1960s	1970s	1980s	1990s	2000s	2010s
Nuclear weapons	Development engineering	Multiprogram laboratory	Missile defense work	Post–Cold War transition	Post 9/11	Life Extension Programs START
Production and manufacturing engineering	Vietnam conflict	Energy crisis	Cold War	Stockpile stewardship	National security	National security challenges

Nuclear Weapons

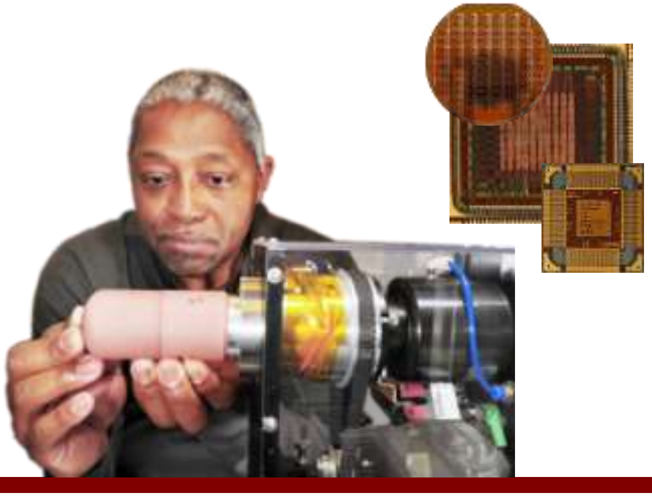
Pulsed power and radiation effects sciences

Design agency for nonnuclear components

- Neutron generators
- Arming, fuzing and firing systems
- Safety systems
- Gas transfer systems

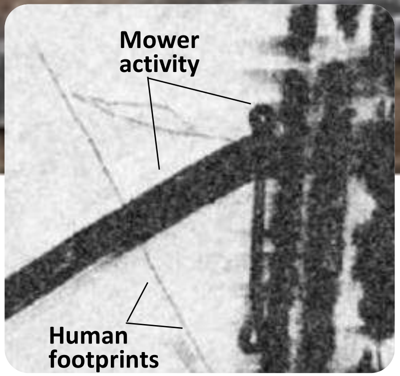
Warhead systems engineering and integration

Production agency



Defense Systems and Assessments

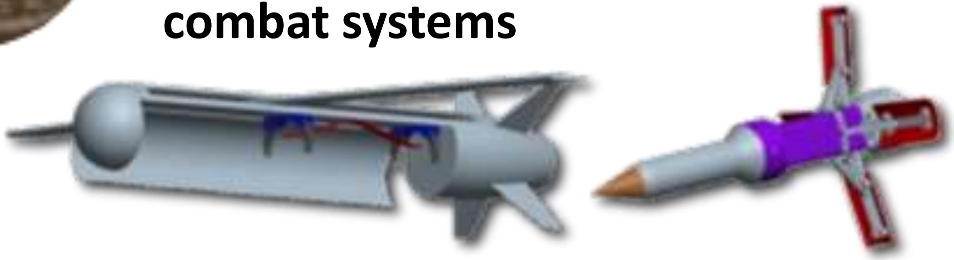
Synthetic aperture radar



Support for NASA

Support for ballistic missile defense

Ground sensors for future combat systems



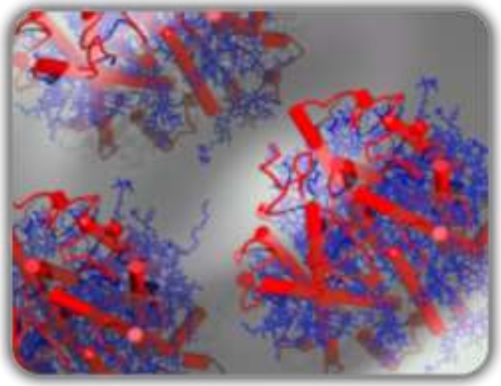
Energy, Climate, and Infrastructure Security

Sandia National Laboratories

Energy

Infrastructure

Crosscuts and enablers



Climate

jbei
Joint BioEnergy Institute

International, Homeland, and Nuclear Security

Critical asset protection

Homeland defense and force protection

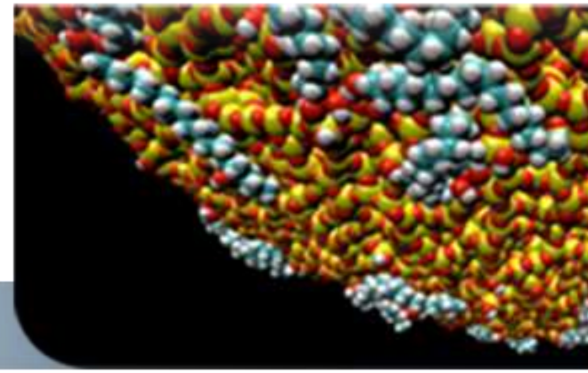
Homeland security programs

Global security

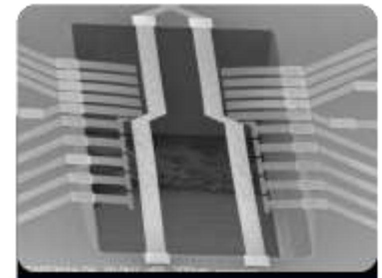
Science and Engineering Foundations

Computing and information science

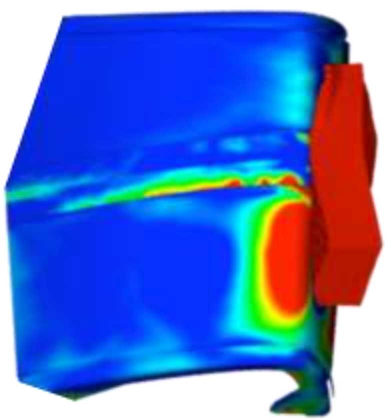
Materials science



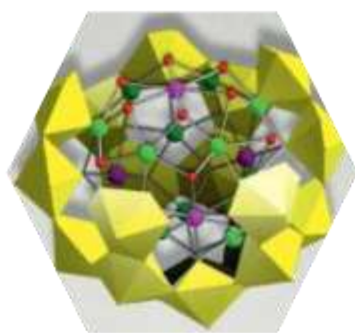
Nanodevices and microsystems



Engineering sciences

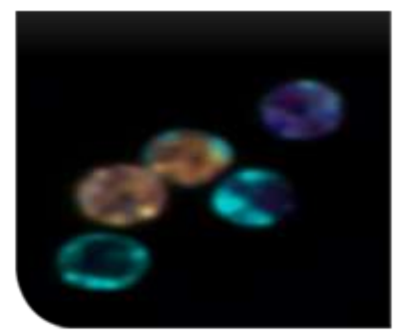


Geoscience



Radiation effects and high-energy density science

Bioscience

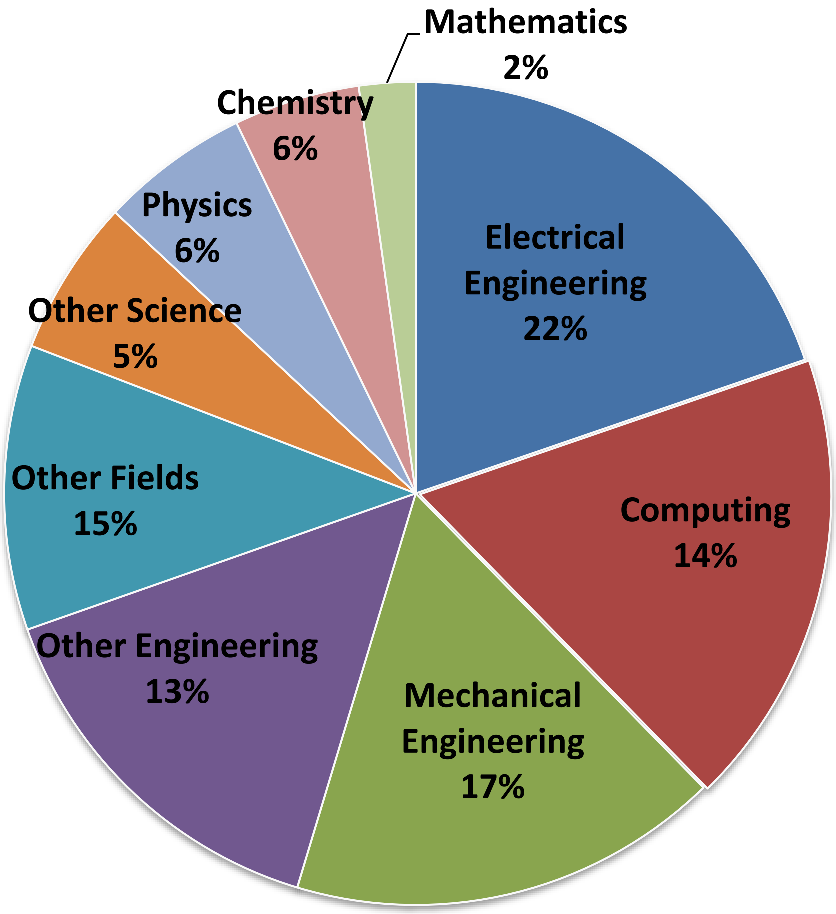


Our Workforce

- On-site workforce: 11,711
- Regular employees: 9,494
- Gross payroll: ~$1.046 billion

Data as of April 12, 2013

R&D staff (4,799) by discipline



My Path to Sandia

- St. Michael's College (VT)
  - mathematics major
  - minors: music, computer science, secondary education
  - AmeriCorps volunteer in New Orleans; IT focus

- Ph.D., Computational and Applied Mathematics, NC State
  - So, what can math be used for?
  - mathematics, statistics, computer science, immunology
  - nondeterministic model calibration (HIV)

- SNL, Albuquerque since 2005:
  - project management, algorithm development, production software
  - went for optimization focus; diversified into UQ
  - science/engineering application customers drive research and software

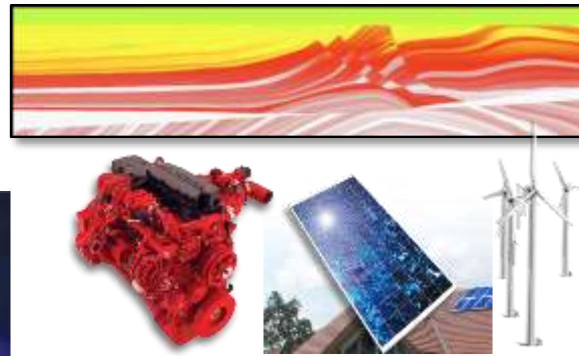
Why Sandia Suits Me

Sandia National Laboratories

- Sense of purpose: critical national security problems
- Innovation: world class, yet approachable, science and engineering staff
- Research to development to applications
- Independence and teaming
- Albuquerque: great weather, bike friendly, mid-size city
- Work/life balance

- *Mathematics, statistics, and computer science are critical partners to engineering and disciplinary science in executing Sandia National Laboratories' mission*

Computing Research Supports Mission Decisions



Sandia Strategic Thrusts

- Nuclear Security
- Energy Security
- Cyber Security

Computer Science Application Themes

- Nuclear Weapons Engineering
- Energy/Climate Security
- Cyber Assurance
- Decision Support

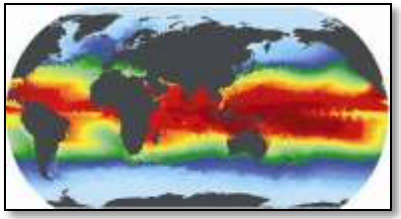
Computer Science Technology Themes

- Predictive Simulation
- Scalable Computing
- Scalable Informatics
- Cognitive Science
- Enabling Technologies

Why Computational Modeling or Simulation?

Researchers and designers at SNL need to understand complex engineering and science phenomena, but physical experimentation might not be feasible, due to, e.g.,:

- Safety: dangerous to test a mechanical component or new type of chemical reaction in the regime of interest
- Laws/ethics: may prohibit nuclear weapons testing; human subjects or genetics experiments
- Practicality: can't readily experiment with climate, economics, or the universe, except at reduced scale
- Cost/availability: building prototypes, destructive testing on legacy systems or in extreme environments often prohibitively expensive



In these cases, we pair limited experimentation and data with computational models intended to represent reality.

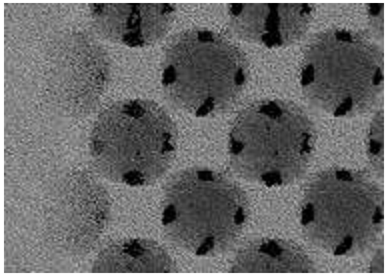
Benefits of Computational Models

- Quickly test theories/hypotheses
- Explore engineering designs with fewer prototypes
- Make predictions in regimes where testing impractical
- Gain new insights about reality
- Advise limited data collection (design of experiments)

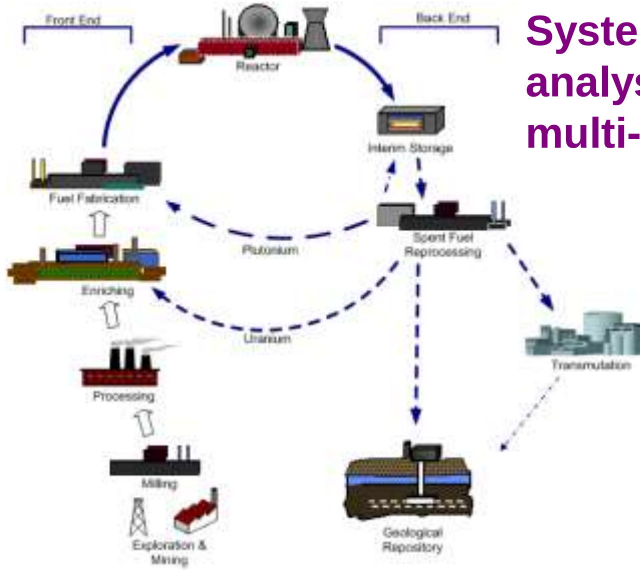
But!

- Each modeling stage makes assumptions and approximations; conclusions must be qualified and relevance vetted
- Solving equations numerically introduces approximation errors, which must be quantified
- And that's all assuming the computer code is correct!

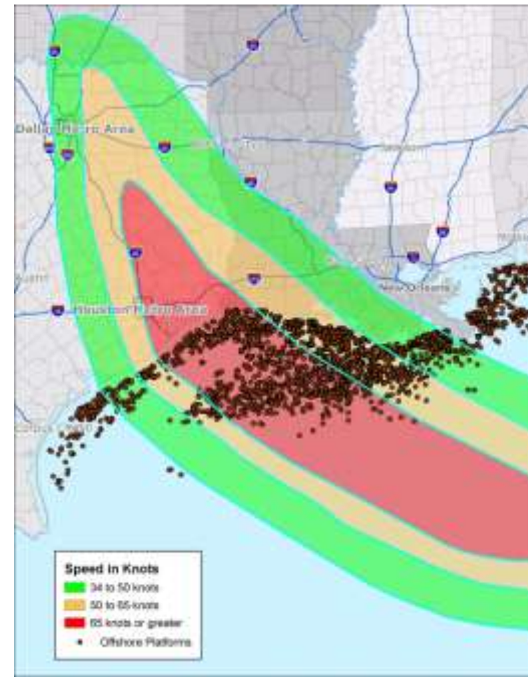
Diverse simulations across scales



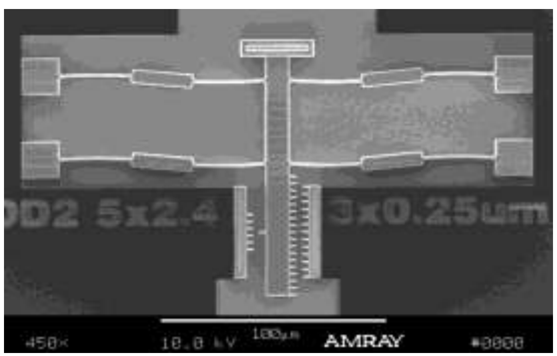
Shock loading of polymer foam: molecular dynamics



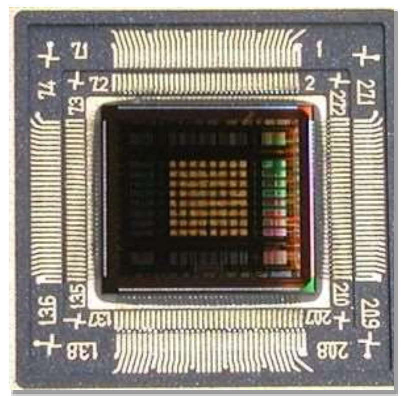
Systems of systems analysis: multi-scale, multi-phenomenon



Emergencies: weather, logistics, economics, human behavior



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

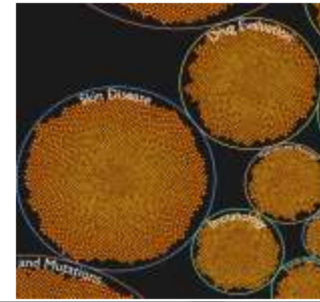


Electrical circuits: networks, PDEs, differential algebraic equations (DAEs), E&M

Why Data Analytics, Informatics, and Visualization?

- Actionable understanding from complex data
  - Voluminous, possibly distributed
  - Transient, streaming data, real-time
  - Cyber, social, water, power networks
- Demands:
  - Collecting, managing, and processing large unstructured data
  - Data intensive/centric methods and computing
  - Relationship-based analytic methods
  - Domain-specific visualization

PubMed clustering



Air traffic networks

Ensemble analysis

Computing Research at Sandia: Enabling Simulation and Analytics

- Routine engineering or decision making with models often cannot be done on a desktop computer…
  - simulate digital circuits with millions of transistors
  - solve PDEs with billions of degrees of freedom
  - simulate disaster response with millions of actors
  - process high bandwidth streaming data in real time
- Scientific discovery, such as for climate or fusion energy, might require ground-breaking fidelity and computational power to resolve a range of scales
- Supercomputers grow and architectures change rapidly

- *Multidisciplinary hardware, algorithms, software research make large-scale simulation and analysis practical*

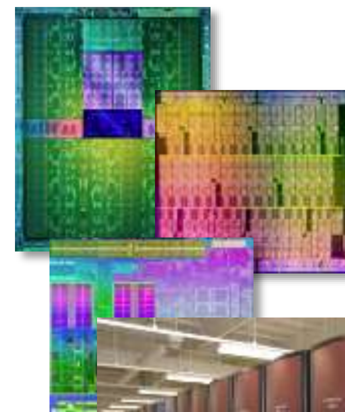
Extreme Scale Computing
Advanced Architectures and Operating Systems

- HPC Platforms
  - Cielo, Sequoia (SNL)
  - Titan (ORNL),
  - Intrepid (ANL)
  - Edison (NERSC)

Cielo
142272 cores
6^{th} on TOP500

- Many-core, FPGA, GPU, PIM, NIC, active storage/NVRAM, …
  - There will be processing capabilities everywhere that are ideal for analysis & viz

NVIDIA+x86
Intel MIC
AMD Fusion

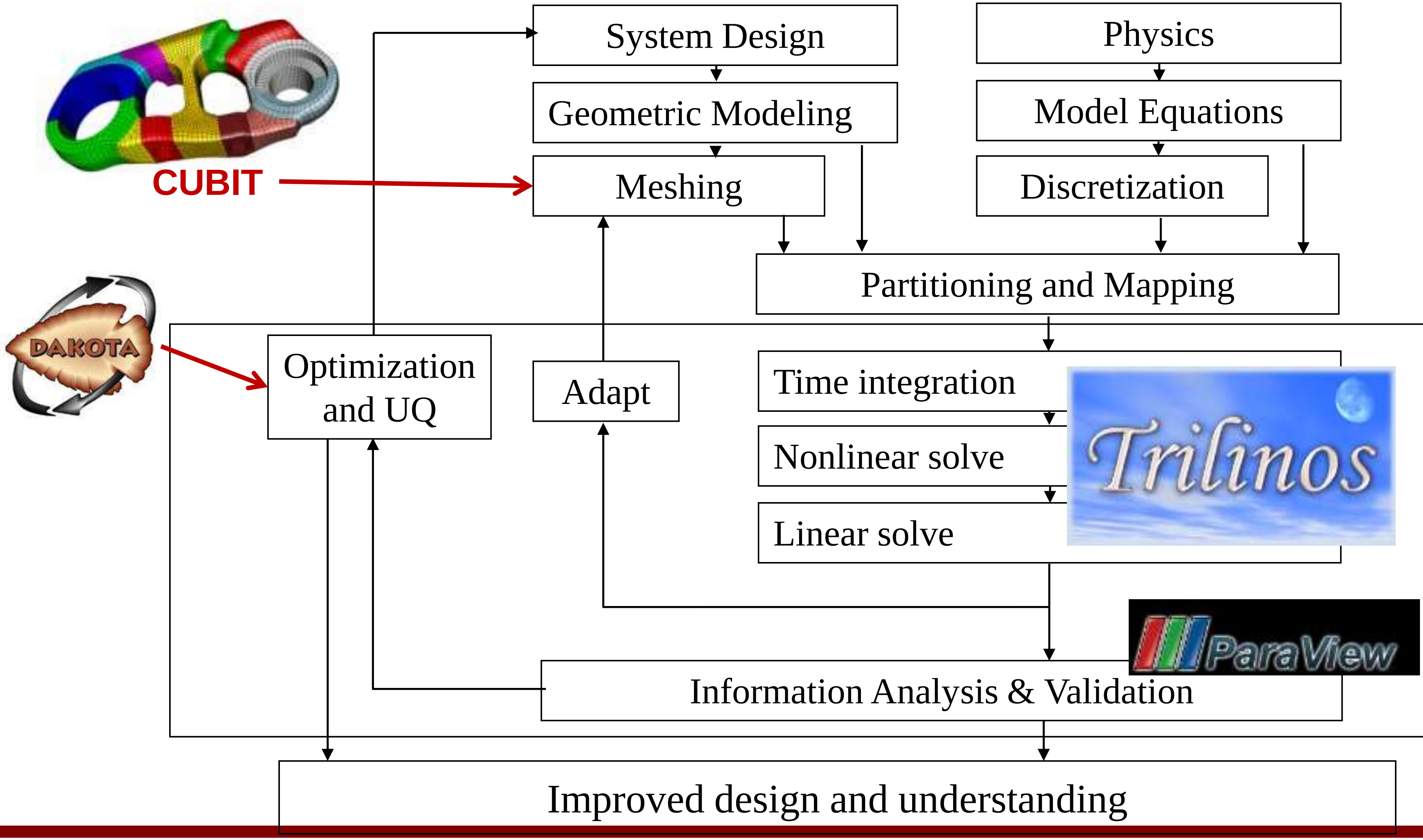


- Special architectures for "big data" analytics
  - New Urika – Graph-based analytics
  - Netezza – Large-scale SQL-based analytics
- Quantum computing

YarcData

IBM Netezza

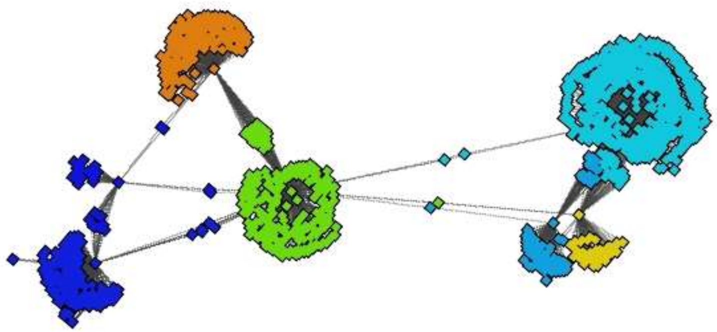
Algorithm R&D Transforms Computational Modeling & Simulation

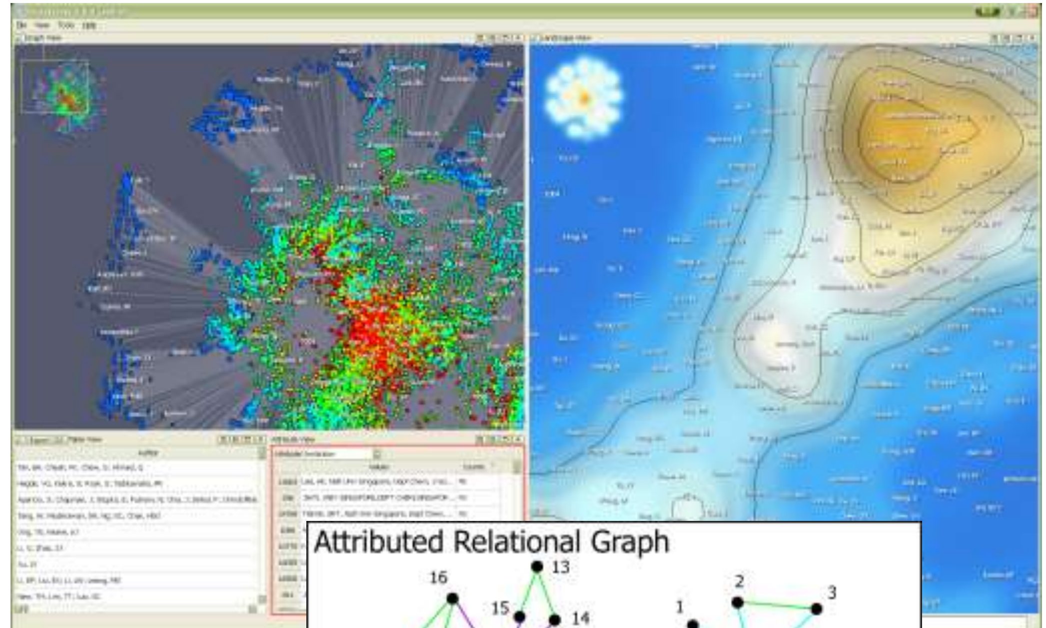


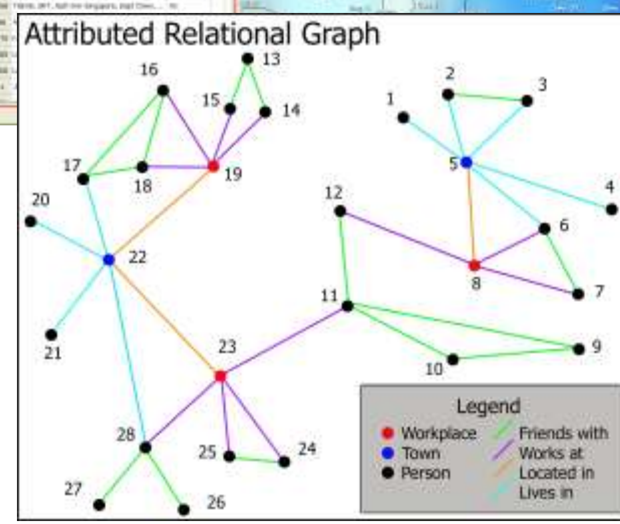
Scalable Informatics and Visualization

Sandia National Laboratories

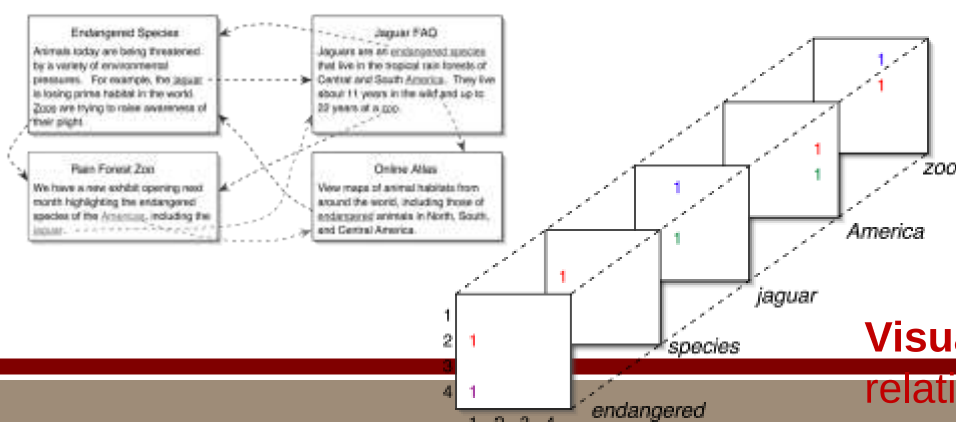
Advanced Graph Analysis: Community Clustering focuses on a smaller subset of interest.







Advanced linear algebra and multi-way tensors to infer missing links and help recognize patterns



Visual Informatics: understand complex relationships; detect anomalies

Example TEVA-SPOT for Optimization of Water Sensor Networks

Goal: design a sensor network with optimal sensor locations

Motivating Applications:

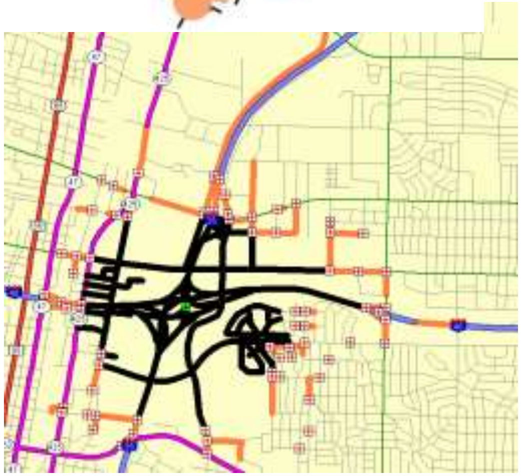
- Detect contaminants in water networks
- Protect air networks in sensitive buildings
- Detect intruders in road networks
- Physical site security protection

Discrete Mathematics:

- Is used to solve large problems quickly
- Can determine optimality of the final solution
- Reduce problem size to solve on commodity computers

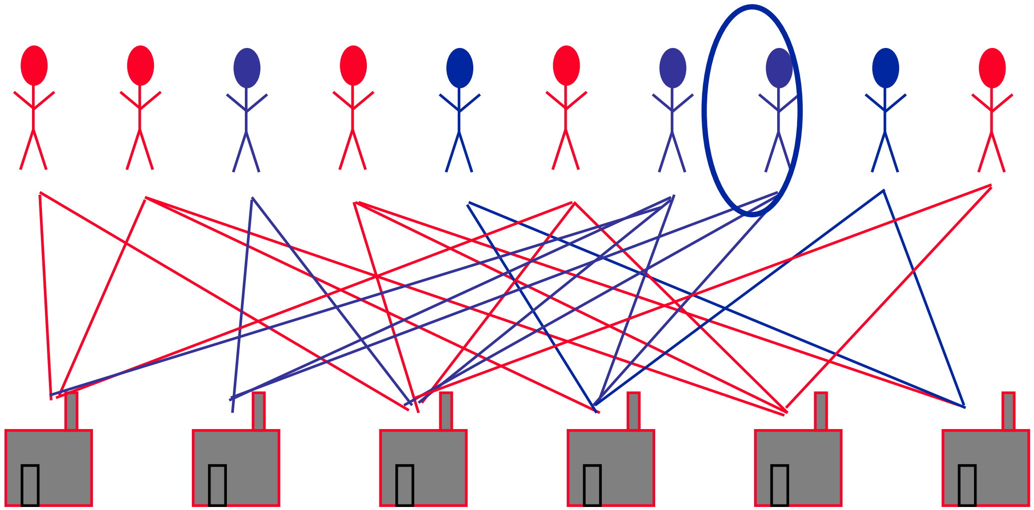
Impact:

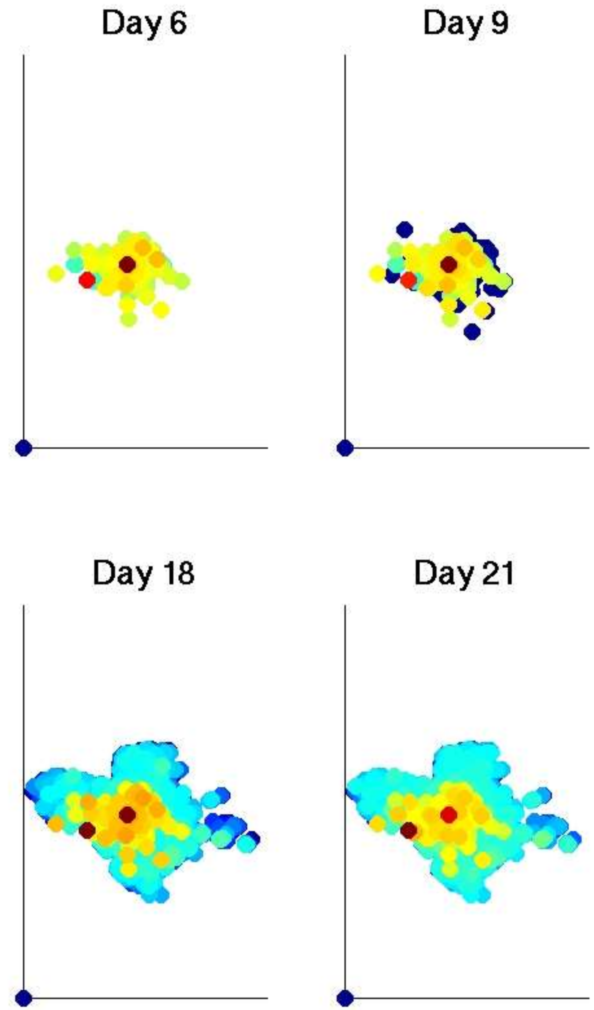
- Sensor placements designed for 8 large U.S. cities
- Sensors installed at 4 U.S. cities based on these designs
- Estimated fatalities from high consequence attacks on drinking water are decreased by a median of 48%
- The estimated value of lives lost due to high consequence attacks is reduced by a median of $19 billion dollars



Example: Agent/network-based Disease Model to Identify Outbreaks

Determine source and magnitude of natural or terrorist disease outbreak, given patients presenting for treatment

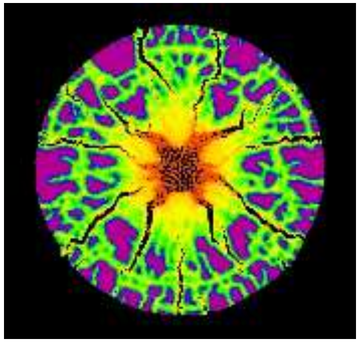




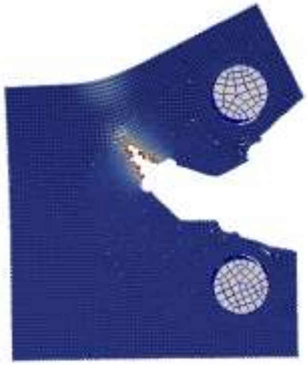
- Bayesian source inversion
- Graph theory for parallel partitioning and r analysis on bipartite graph)
- Math biology for in-host disease models (p transmission (epidemiology); discrete DEs
- Scalable parallelism via MPI for efficient simulations

Example: Peridynamics

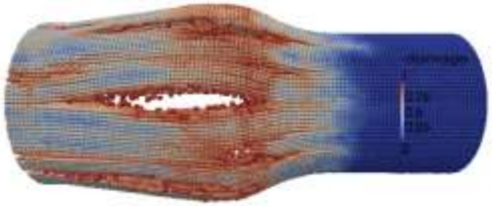
- What it is: a mathematical theory that unifies the mechanics of continuous media, cracks, and discrete particles.
- Current efforts:
  - Theory:
    - Coarse-graining & multiscale (NASA)
    - Nonlocal advection-diffusion (ASCR)
    - Material modeling (CSRF)
  - Code & algorithm development:
    - Peridigm (CSRF)
    - Sierra Mechanics (ASC)
  - Applications:
    - Composite material fracture (Boeing)
    - Ductile failure X-prize (ASC)
    - Rock blasting and drilling (ExxonMobil, Orica)
    - Fragmenting munitions (ARL)
    - Structural vulnerability (NRC)



Rock fragmentation



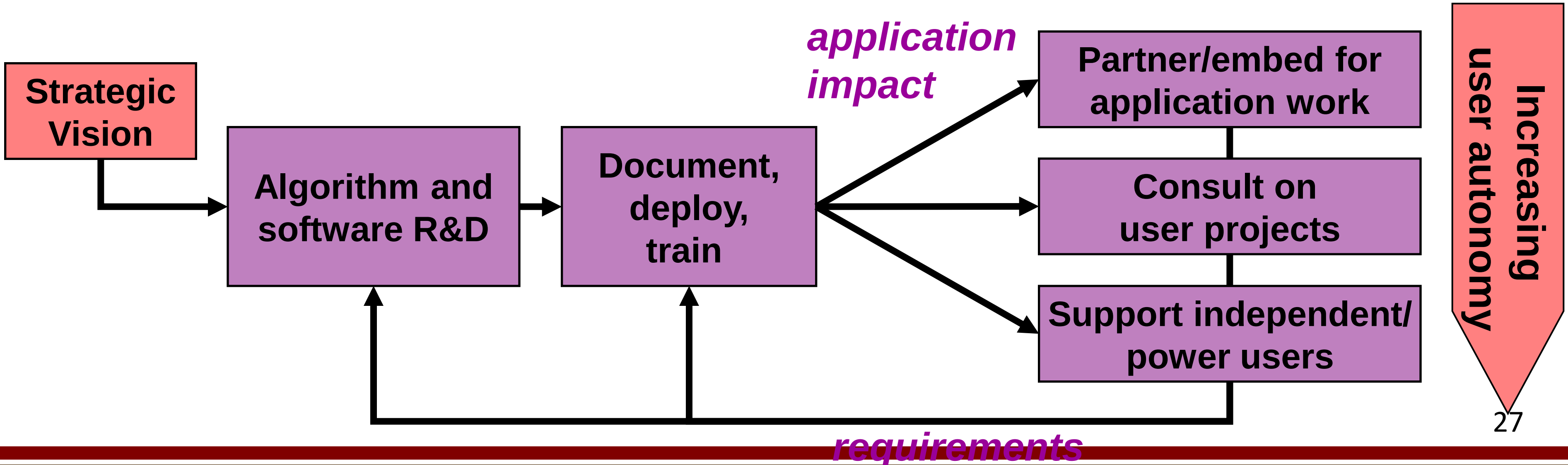
Ductile failure



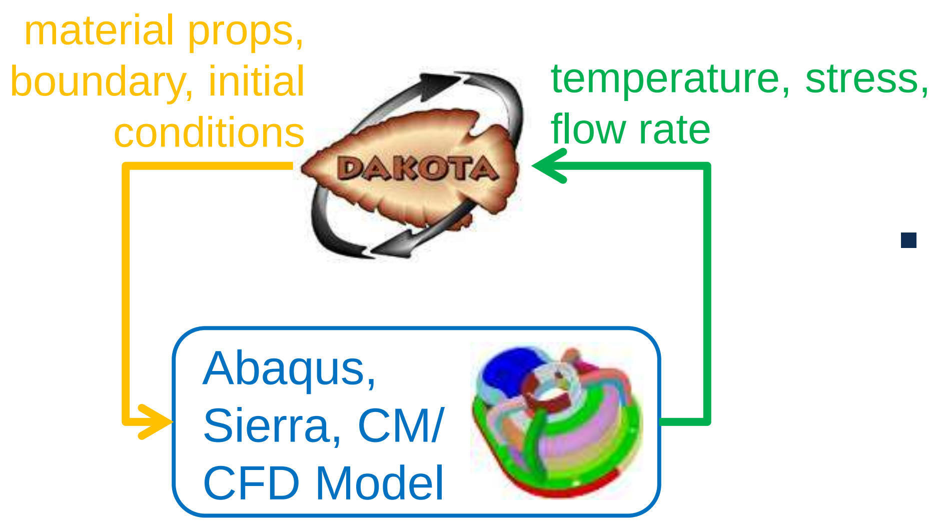
Shock loading of a metal cylinder

My Work Life
Largely Centers on DAKOTA

- Algorithm and software development
  - Implement new algorithms and infrastructure in C++
  - Collaborate with labs and universities; publish important results
- Software project management
  - Manage priorities in team development environment
  - Deliver usable algorithms to customers; enable team do research
- Application to nuclear energy and beyond
  - Solve nuclear energy and other national security problems
  - Help people understand and use our software



Dakota Supports Engineering Transformation



Automate typical "parameter variation" studies with various advanced methods and a generic interface to your simulation.

- Simulation-based engineering design: optimize computational prototypes
- Risk analysis and quantification of margins and uncertainty (QMU): assess the effect of parametric uncertainty on the probability of achieving desired system performance
- Verification and validation: automate mesh convergence or solver tolerance studies, generate ensembles of simulations and statistics to compare to experimental data

DAKOTA in a Nutshell

DAKOTA supports engineering transformation through advanced modeling & simulation. Adds value by answering science and engineering questions via iterative analysis of computational models:

- Sensitivity: what are the crucial factors/parameters and how do they affect key metrics?
  - Which of *m, c*, or *k*, is system performance most sensitive to?
- How safe, reliable, robust, or variable is my system? *(quantification of margins and uncertainty: QMU, UQ)*
  - If the damping *c* is known inexactly or it varies in manufacturing, how much variability will there be in the performance?
- What is the best performing design or control? *(optimization)*
  - What spring and damper will stabilize the car quickly without over-stressing it?
- What models and parameters best match experimental data? *(calibration)*
  - Given experimental data, calibrate *m, c*, and *k* in the math model to the real world. Does it then predict unseen scenarios (validation)?

Simulation Challenges DAKOTA Addresses

Sandia National Laboratories

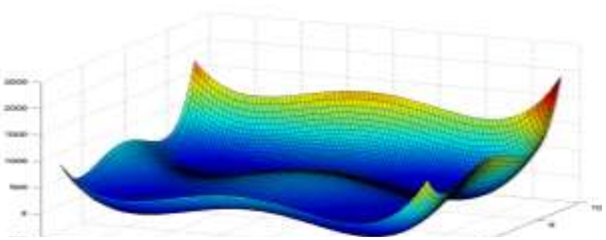
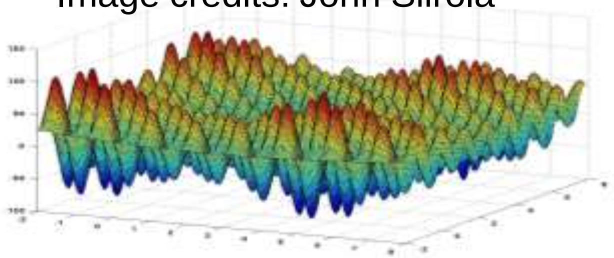
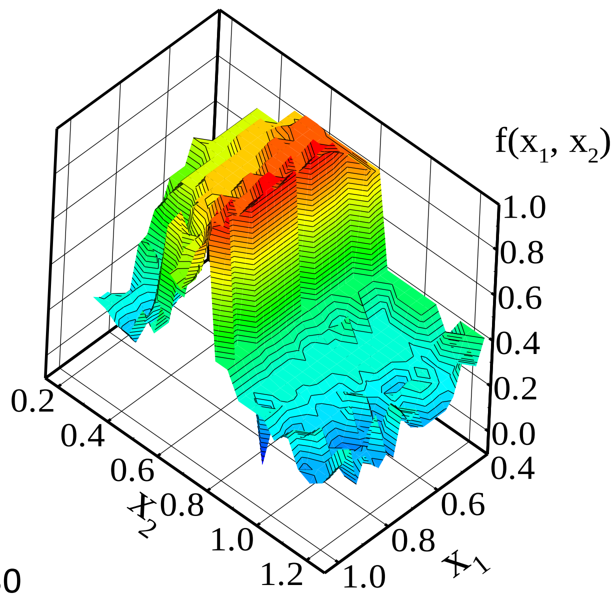


Image credits: John Siirola



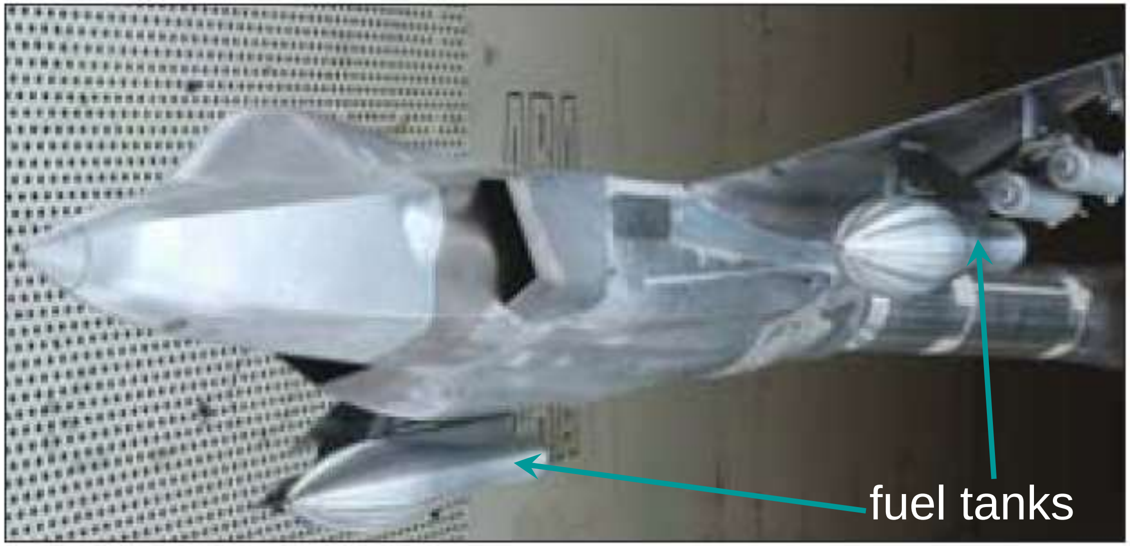


In science and engineering problems of interest, we typically have:

- no explicit function for $f(x_1,x_2)$
  - can't leverage algebraic structure
- limited number of evaluations/samples
  - expensive to evaluate $f(x_1,x_2)$ (long runtime even on many processors)
  - simulation may fail (hidden constraints)
- noisy / non-smooth
  - can't reliably estimate derivatives
- local extrema, non-convex
  - globally optimal solutions challenging

Considerable research has been done to mitigate these issues.

Optimization for Lockheed-Martin F-35 External Fuel Tank Design



This wind tunnel model of F-35 features an optimized external fuel tank.

Appeared in Aerospace America

F-35: stealth and supersonic cruise
~ $20 billion cost
~ 2600 aircraft (USN, USAF, USMC, UK & other foreign buyers)

LM CFD code
- *Expensive*: 8 hrs/job on 16 processors
- Fluid flow around tank *highly sensitive* to shape changes

Optimization Problem
- Goal: Minimize DRAG and YAW over possible values of shape parameters
- Shape parameters must be bounded to fit within prescribed area
- Design must be sufficiently safe and strong

Objective Function: quantity for which we are trying to find the extreme value over parameter ranges

Parameters: quantities to be varied

Constraints: conditions that cannot be violated

Problem Formulation: Objectives and Constraints

Information with which to configure the solver:

Minimize: $f(x_1, ..., x_N)$ ***Objective function(s)****

Subject to: $g_{LB} \le g(x) \le g_{UB}$ ***Nonlinear inequality constraints***

$h(x) = h_E$ ***Nonlinear equality constraints***

(Metrics above are typically implicit: computed by/extracted from a simulation code)

(Algebraic metrics below are typically specified directly to an optimization solver)

$A_I x \le b_I$ ***Linear inequality constraints***

$A_E x = b_E$ ***Linear equality constraints***

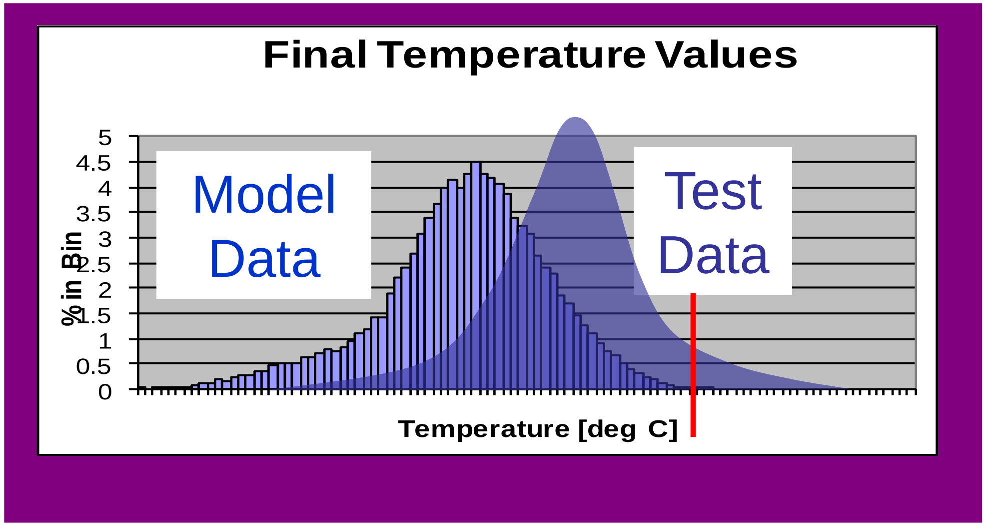
$x_{LB} \le x \le x_{UB}$ ***Bound constraints***

**** In practice, multiple f-values can comprise the objective function ("multi-objective optimization"), and there can be multiple constraints of each type.***

Uncertainty:
"But I wrote down and solved the equations!"

A *few* uncertainties affecting computational model output/results:

- physics/science parameters
- statistical variation, inherent randomness
- model form / accuracy
- material properties
- manufacturing quality
- operating environment, interference
- initial, boundary conditions; forcing
- geometry / structure / connectivity
- experimental error (measurement error, measurement bias)
- numerical accuracy (mesh, solvers); approximation error
- human reliability, subjective judgment, linguistic imprecision



The effect of these on model outputs should be integral to an analyst's deliverable: *best estimate PLUS uncertainty!*

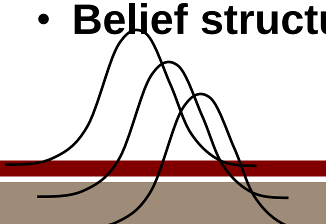
Mechanics of (Parametric) Uncertainty Quantification

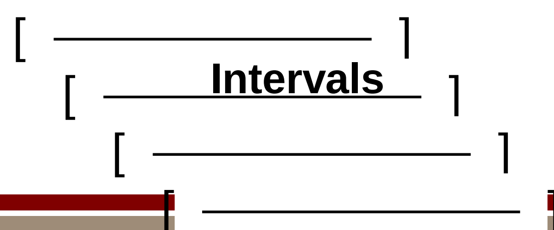
- **Identify and characterize uncertain variables (may not be normal, uniform)**
- ***Forward propagate: quantify the effect that (potentially correlated) uncertain (nondeterministic) input variables have on model output:***

Input Variables *u* **(physics parameters, geometry, initial and boundary conditions)** → **Computational Model** → **Variable Performance Measures *f(u)***

Uncertainties on inputs

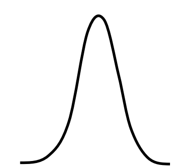
- **Parameterized distributions: normal, uniform, gumbel, etc.**
- **Means, standard deviations**
- **PDF, CDF from data**
- **Intervals**
- **Belief structures**





Uncertainties on outputs

- Means, standard deviations
- Probabilities
- Reliabilities
- PDF, CDF
- Intervals
- Belief, plausibility

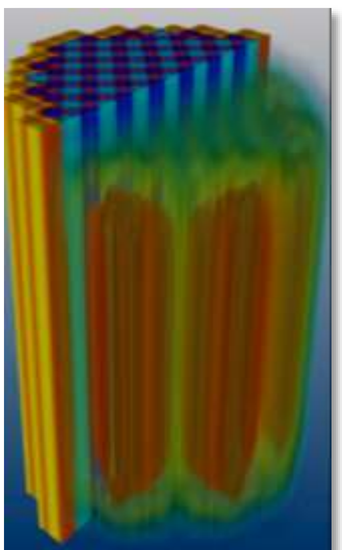


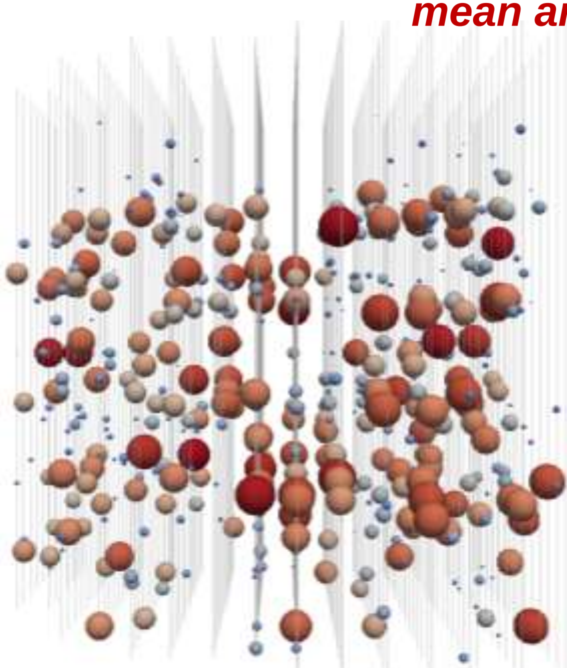
Uncertainty in Boiling Rate for Nuclear Reactor Quarter Core

DAKOTA UQ coupled to VIPRE-W thermal-hydraulics code that predicts boiling

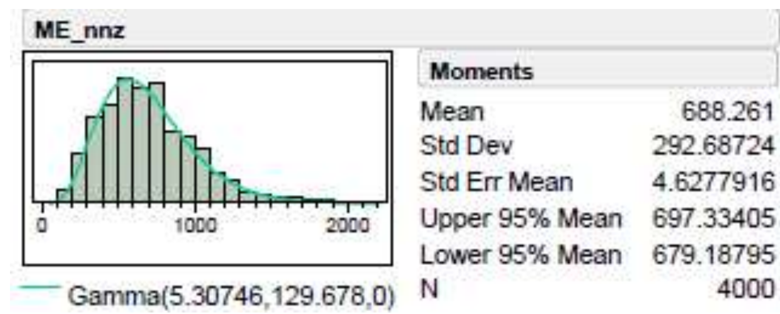
Method	ME_nnz		ME_meannz		ME_max	
	Mean	Std Dev	Mean	Std Dev	Mean	Std Dev
LHS (40)	651.225	297.039	127.836	27.723	361.204	55.862
LHS (400)	647.33	286.146	127.796	25.779	361.581	51.874
LHS (4000)	688.261	292.687	129.175	25.450	364.317	50.884
PCE (Θ(2))	687.875	288.140	129.151	25.7015	364.366	50.315
PCE (Θ (3))	688.083	292.974	129.231	25.3989	364.310	50.869
PCE (Θ (4))	688.099	292.808	129.213	25.4491	364.313	50.872

mean and standard deviation of key metrics



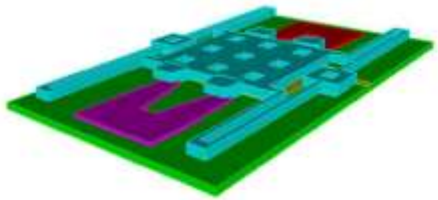


anisotropic uncertainty distribution in boiling rate throughout quarter core model

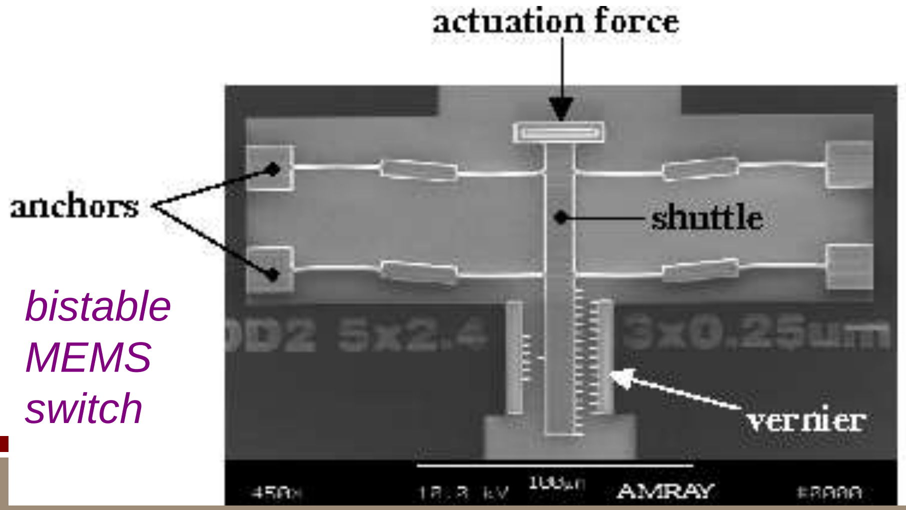


normally distributed inputs need not give rise to normal outputs…

Shape Optimization of Compliant MEMS



- Micro-electromechanical system (MEMS): typically made from silicon, polymers, or metals; used as micro-scale sensors, actuators, switches, and machines
- MEMS designs are subject to substantial variability and lack historical knowledge base. Materials and micromachining, photo lithography, etching processes all yield uncertainty.
- Resulting part yields can be low or have poor cycle durability
- Goal: shape optimize finite element mechanics model of bistable switch
  - Achieve prescribed reliability in actuation force
  - Minimize sensitivity to uncertainties (robustness)

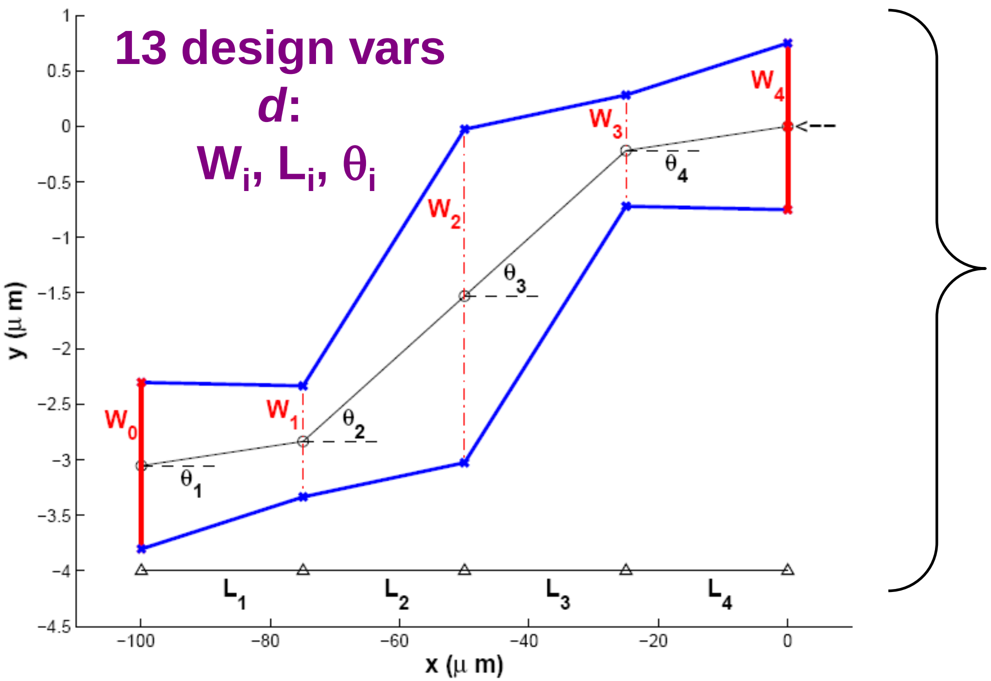


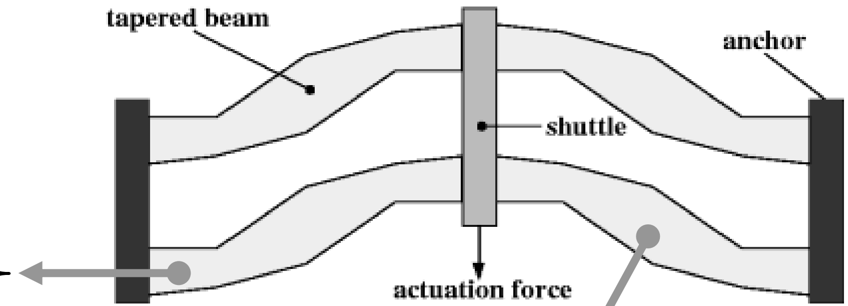
bistable MEMS switch

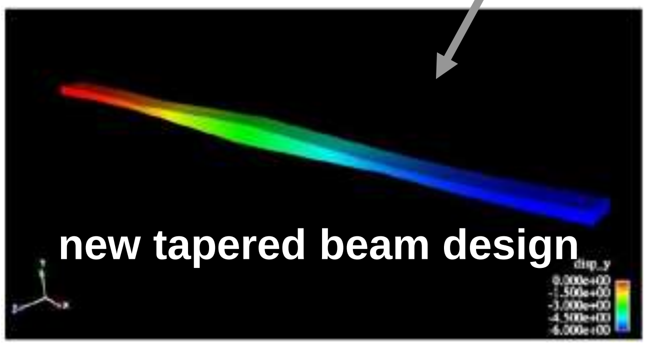
uncertainties to be considered (edge bias and residual stress)

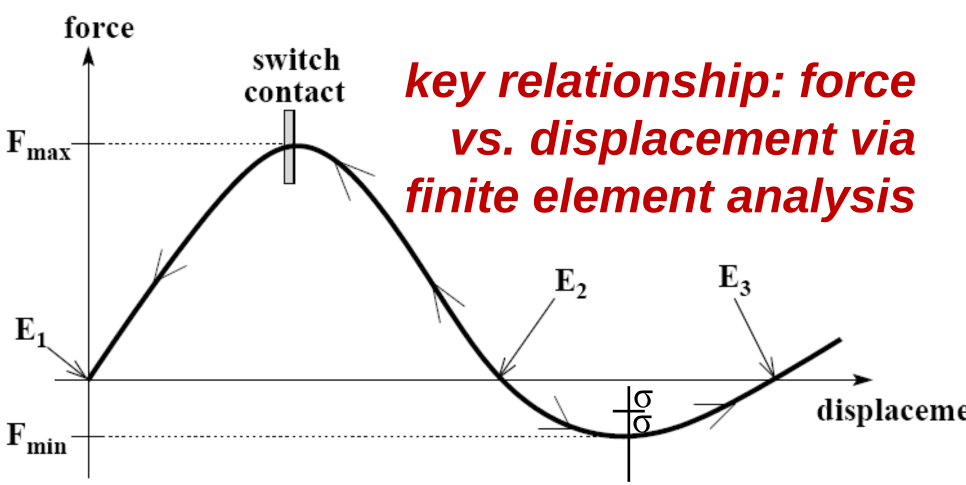
variable	mean	std. dev.	distribution
Δw	-0.2 μm	0.08	normal
S_r	-11 Mpa	4.13	normal

MEMS Switch Design: Geometry Optimization









key relationship: force vs. displacement via finite element analysis

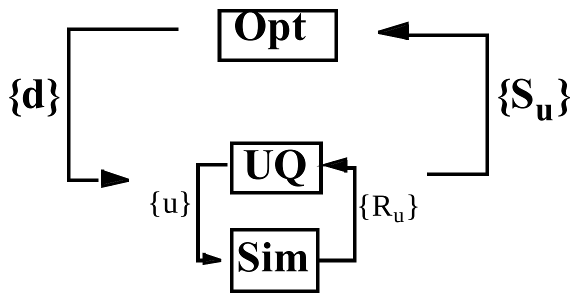
Typical design specifications:

- **actuation force F_{min} reliably 5 μN**
- **bistable ($F_{max} > 0$, $F_{min} < 0$)**
- **maximum force: $50 < F_{max} < 150$**
- **equilibrium E2 < 8 μm**
- **maximum stress < 1200 MPa**

Optimization Under Uncertainty

Design to be Robust and Reliable

Rather than design and then post-process to evaluate uncertainty…
actively design optimize while accounting for uncertainty/reliability metrics $s_u(d)$, e.g., mean, variance, reliability, probability:



(nested paradigm)

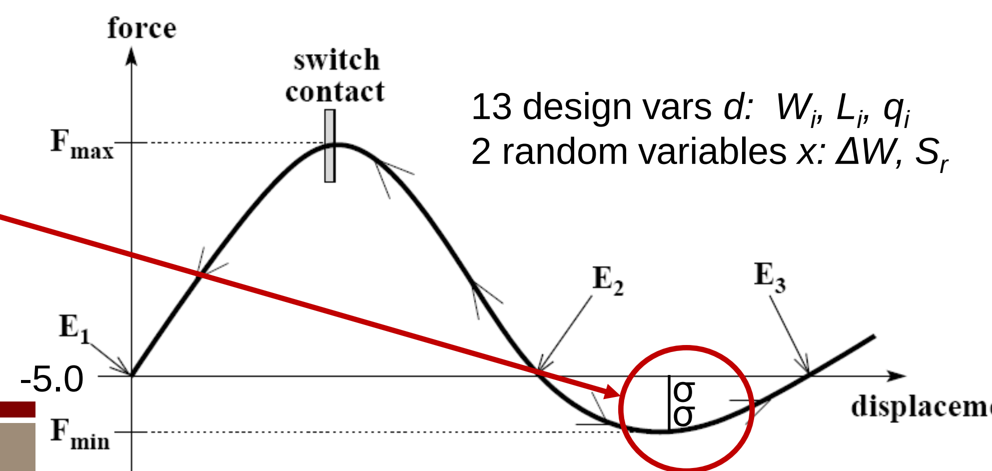
$$\begin{aligned} \text{min} \quad & f(d) + W\, s_u(d) \\ \text{s.t.} \quad & g_l \le g(d) \le g_u \\ & h(d) = h_t \\ & d_l \le d \le d_u \\ & a_l \le A_i\, s_u(d) \le a_u \\ & A_e\, s_u(d) = a_t \end{aligned}$$

Bistable switch problem formulation (Reliability-Based Design Optimization):

simultaneously reliable and robust designs

$$\begin{aligned} \text{max} \quad & & & \mathrm{E}\left[F_{min}(\mathrm{d},\mathrm{x})\right] & & \\ \text{s.t.} \quad & 2 & \le & \beta_{ccdf}(\mathrm{d}) & & \\ & 50 & \le & \mathrm{E}\left[F_{max}(\mathrm{d},\mathrm{x})\right] & \le & 150 \\ & & & \mathrm{E}\left[E_2(\mathrm{d},\mathrm{x})\right] & \le & 8 \\ & & & \mathrm{E}\left[S_{max}(\mathrm{d},\mathrm{x})\right] & \le & 3000 \end{aligned}$$

13 design vars *d*: W_i, L_i, q_i
2 random variables *x*: ΔW, S_r



Dakota Research Thrusts

- Efficient simulation-based SA, OPT, UQ
- Surrogate-based optimization and UQ
- Advanced aleatory and epistemic UQ methods
- Effective use of HPC resources
- Hybrid algorithms combining the above for robustness, efficiency

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- **Contact me with any questions: briadam@sandia.gov**

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  - Doctoral Sciences Program (DSP)
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  - MS / PhD – 3.5 +

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- Cedric Carter (BS)
- Todd Coffey (PhD)
- Steven Elliot (BS)
- Jason Jarosz (MS)
- Jordan Massad (PhD)