SAND2012-XXXX

SAND2012-0970P

Applied Mathematical Sciences at Sandia

Brian M. Adams

Optimization and Uncertainty Quantification

Applications of Mathematics Colloquium
Loyola University Chicago

February 7, 2012

Chicago, IL

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.

Personal Background

- **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:**
  - mix of algorithm development, production software
  - went for optimization focus; diversified into UQ
  - science/engineering application customers drive research and software

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Roles for Math Sciences

Goal: demonstrate the intertwined role of mathematics, statistics, computer science, and disciplinary science in executing Sandia National Laboratories' mission

- **SNL: A U.S. Department of Energy laboratory**
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SNL Core Thrust Areas Address Evolving National Security Needs

Nuclear Weapons	Defense Systems and Assessments	Energy, Climate, Infrastructure Security	International, Homeland, Nuclear Security
• Engineering lead for NW systems • Design, fabricate, test components • Simulations • Physical testing	• Information ops • Military systems • Non-proliferation • Remote sensing and verification • Space mission • Surveillance & reconnaissance	• Infrastructure Security • Energy Security • Climate Security • Enabling Capabilities	• Critical asset protection • Global security • Homeland Defense and Force Protection • Homeland Security

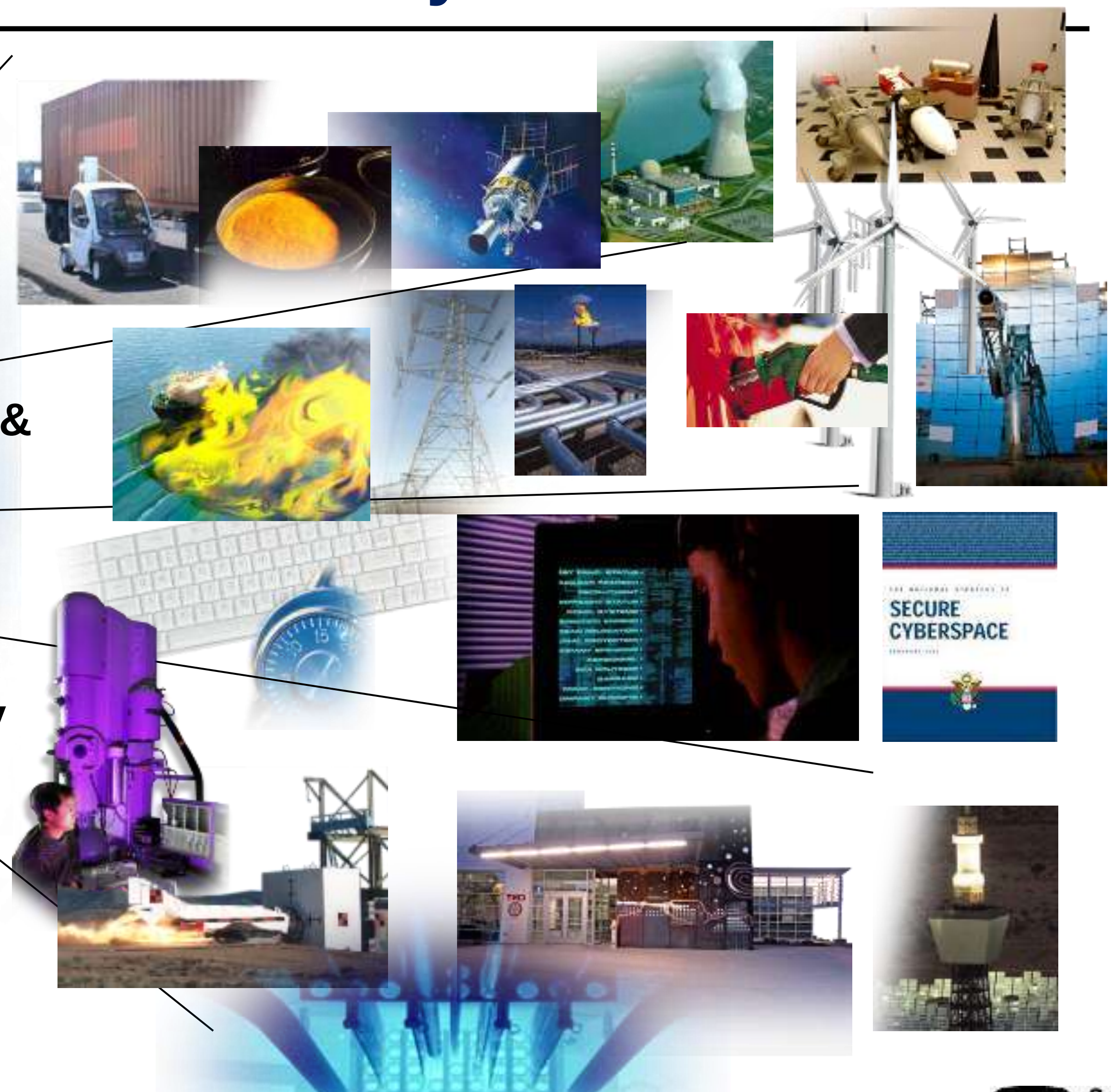
Emerging SNL
National Security Thrusts

Nuclear

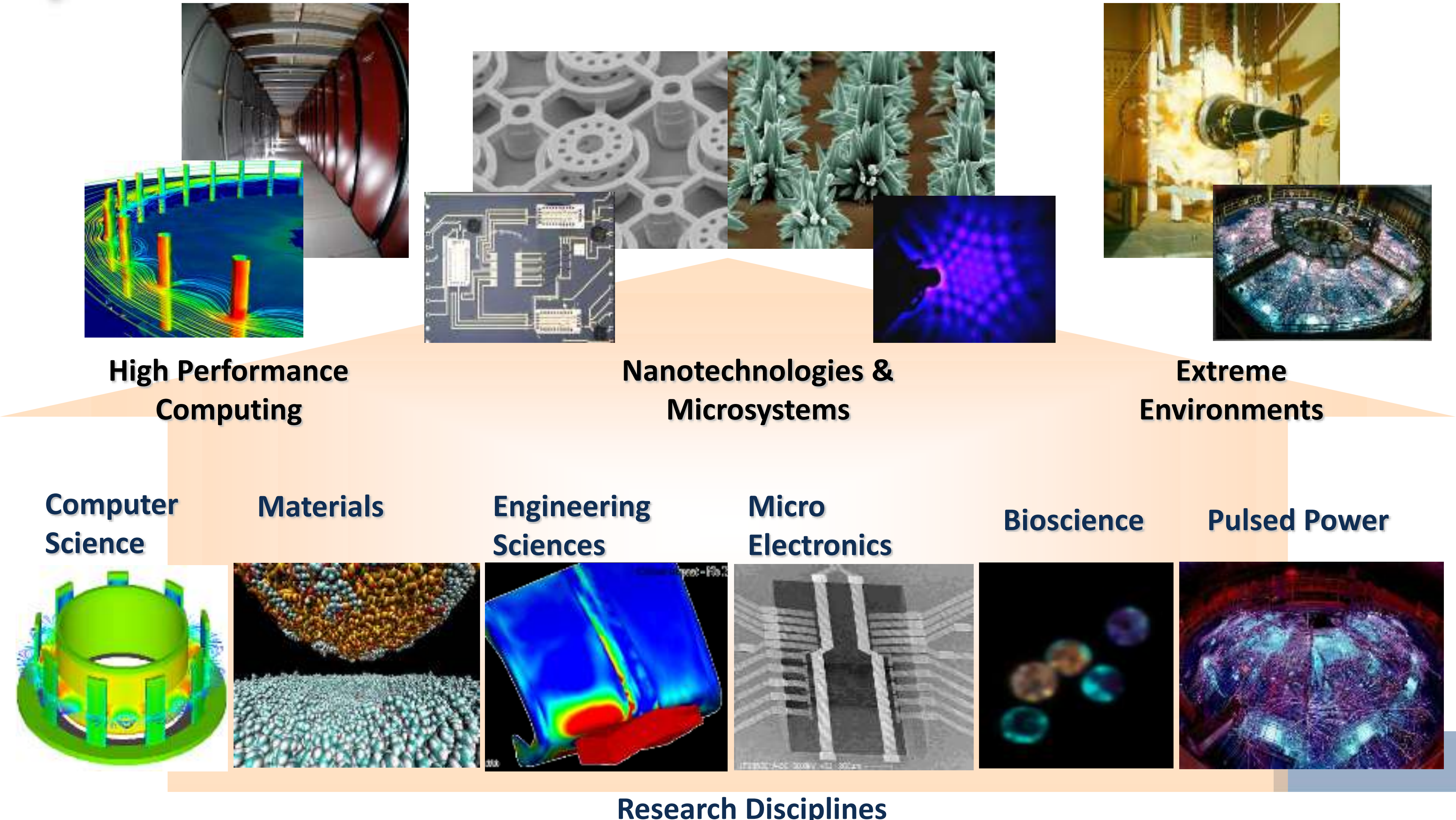
Energy &
Climate

Cyber

Science &
Technology



Fundamental Research Supports Mission Capabilities



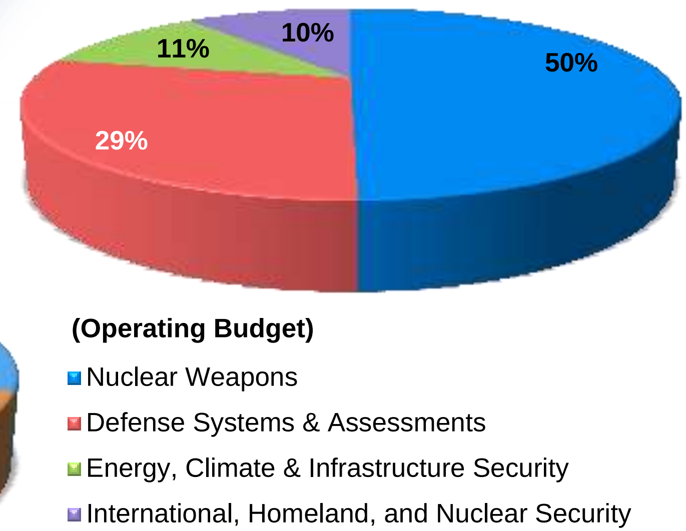
Innovation: most compelling reason to work at SNL

Staff at Five Principal Sites

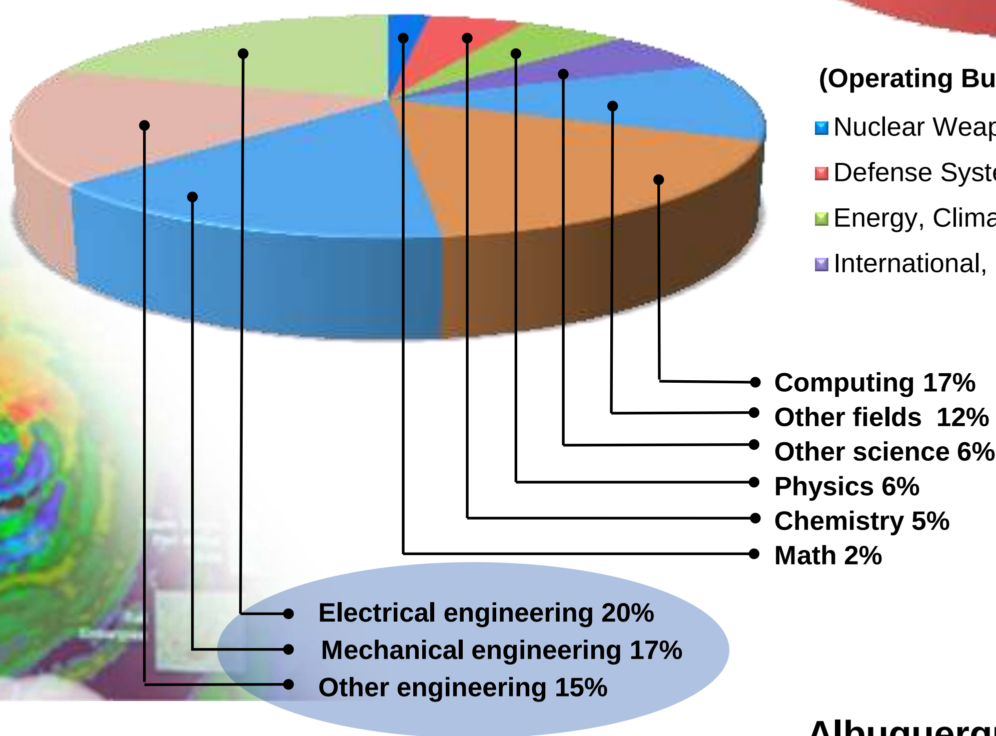
majority engineers; many with computational focus

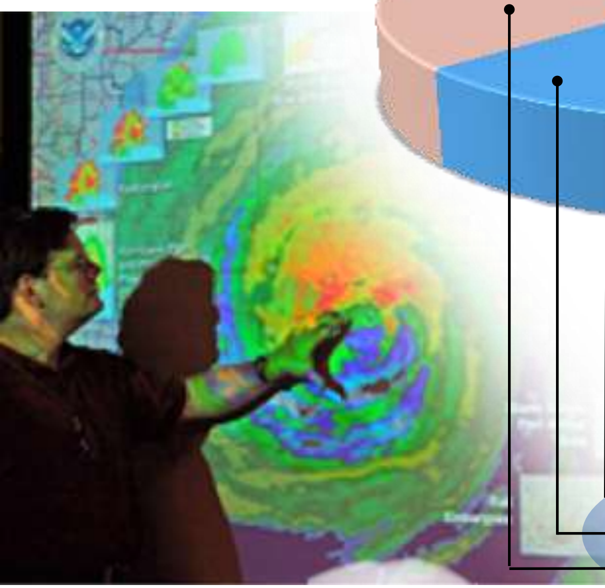
- On-site workforce: 11,876
- Regular employees: 9,122
- Gross payroll: ~$943 million

FY11 Operating Revenue
$2.4 billion



Technical staff (4,557) by discipline





Albuquerque, New Mexico

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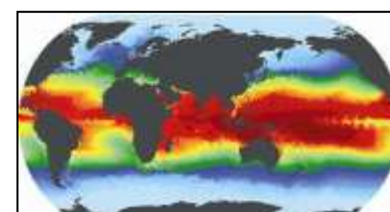
Why Computational Modeling?

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.

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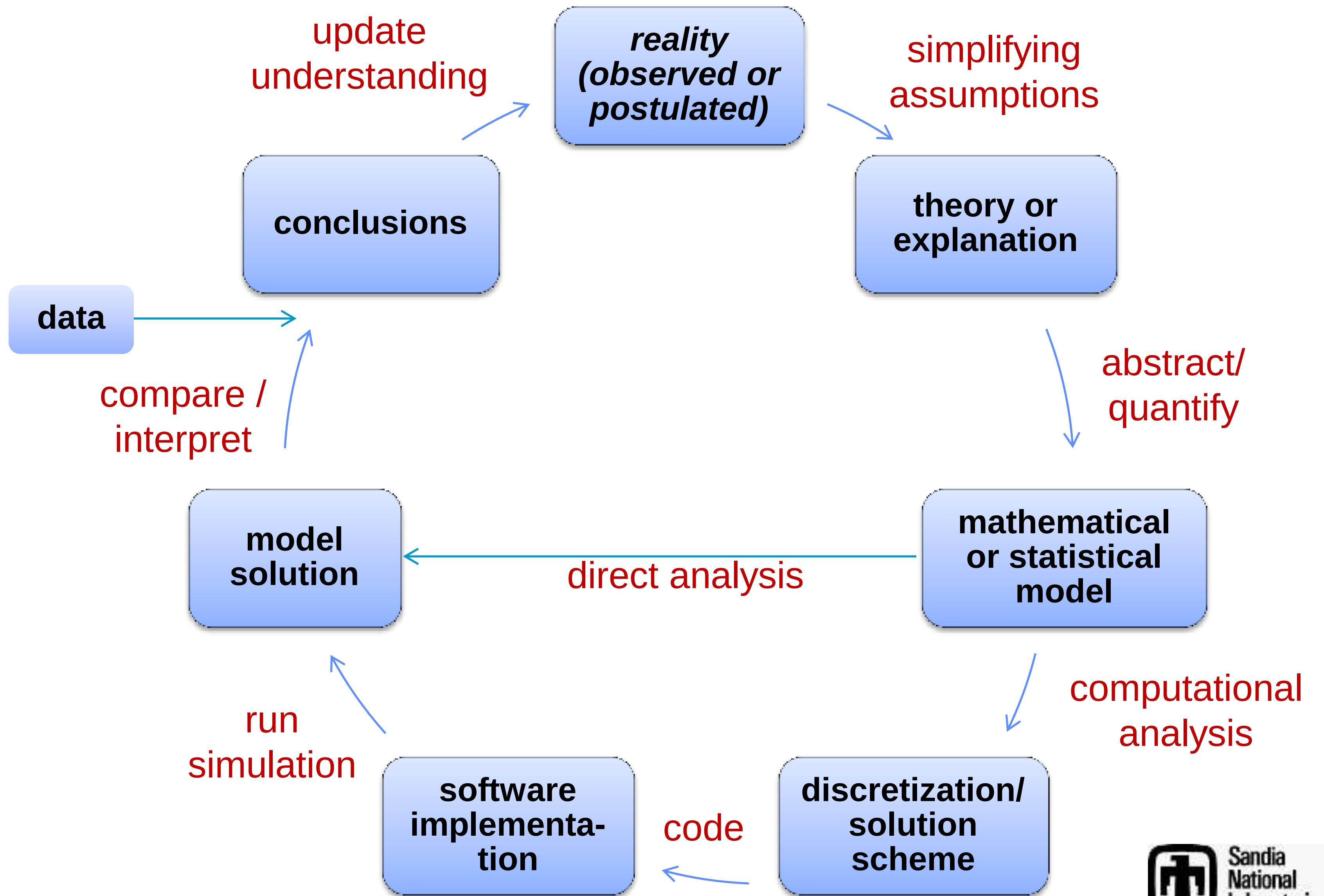
A Modeling Process



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!

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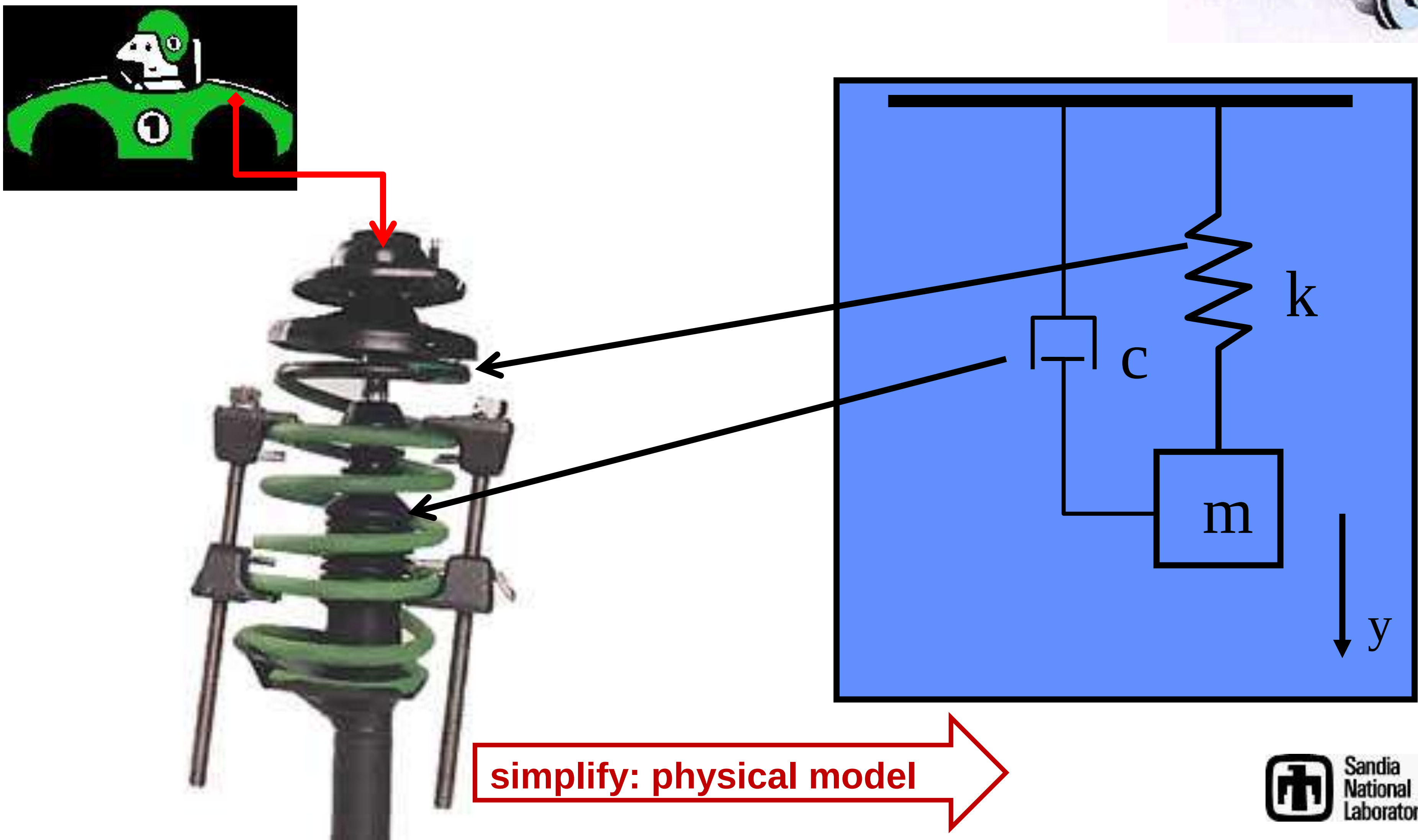
Example:
Modeling a MacPherson Strut

Goal: design a shock absorber with desired characteristics



Mathematical Model and Computation of Solution

$$m\frac{d^2y}{dt^2} + c\frac{dy}{dt} + ky = 0$$

- **Mathematical model: second-order ordinary differential equation in time**
- **Predicts displacement *y(t)***
- **For given fixed mass *m*, what *c* and *k* should one use?**
- **Discretize, program, and simulate with Matlab computer software**
- **Can see effect of *k, c* variations without building a prototype**

```
%Representative Matlab code

% define the right side of the ODE
function xdot = osc_rhs(t, x, q, f)

    m = q(1);
    c = q(2);
    k = q(3);

    xdot(1,1) = x(2);
    xdot(2,1) = -k/m*x(1) - c/m*x(2) +
interp1(f(1,:), f(2,:), t)/m;

% solve the ODE
q = [m c k];
f = [0, 0.1, 0.11, 100;
     0*[1000, 1000, 0, 0]];

x0 = [fac,0];

[t,x] = ode15s(@osc_rhs,[0:0.1:10],
x0,[],q,f);
```

see Matlab demo…

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Simple System May Give Insight in Diverse Scenarios

- automobile suspension
- shock-absorbing truck seats
- recoilless firearms, artillery
- seismograph (amplify oscillations)
- structures of linked oscillators; many mechanical and chemical structures
- structure stability: Tacoma Narrows Bridge, cadence on bridges, John Hancock tower
  - building swayed back-and-forth, exhibited snake-like bending; famous glass shedding
  - used spring—mass—dashpot to control; two 300-ton weights installed on 58-th floor, attached with springs and shock absorbers.
  - added 1,500 tons of steel braces to stiffen

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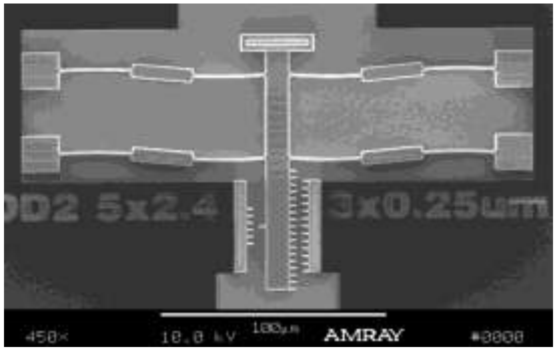
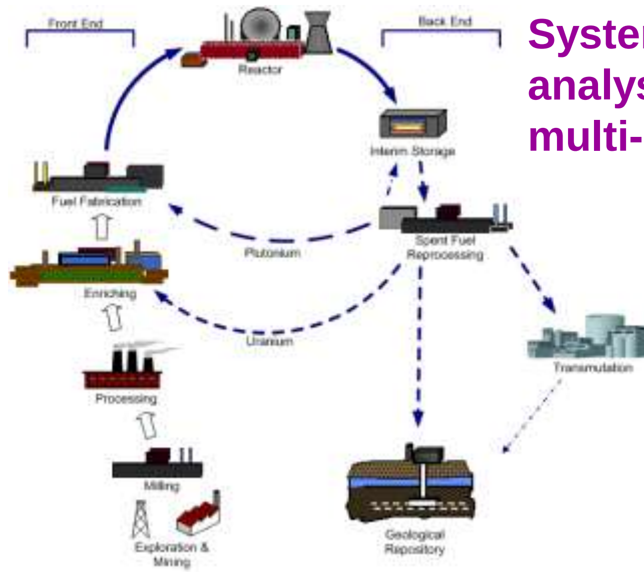
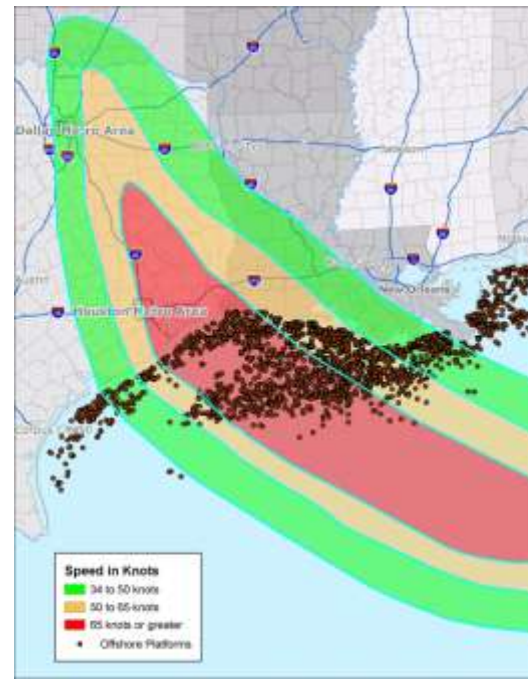
SNL Examples of Computational Simulation



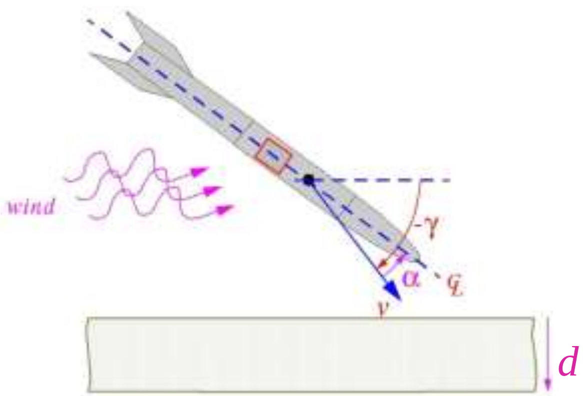
Micro-electro-mechanical systems (MEMS): quasi-static nonlinear elasticity, process modeling



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

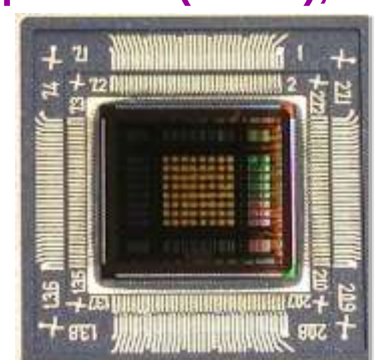


Hurricane Katrina: weather, logistics, economics, human behavior



Earth penetrator: nonlinear PDEs with contact, transient analysis, material modeling

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



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Computing Research at SNL

- How does our group support use of simulation?
- 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
- 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

We perform research and development for next-generation computing hardware and the software and algorithms to efficiently utilize them for mission-critical applications.

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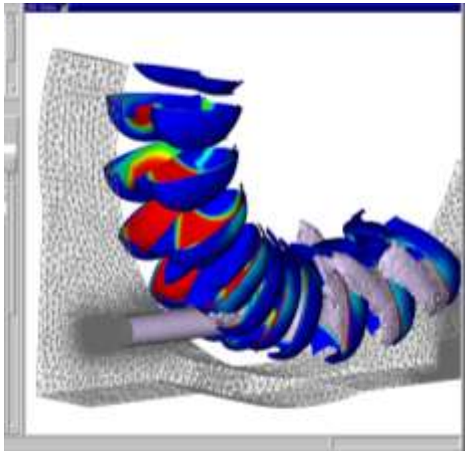
Computing Research at SNL:
Architectures, Algorithms, Applications

Cielo
142272 cores
6^{th} on TOP500

Enable simulation with:

- **Extreme-scale Computing:**
  quantum devices, scalable architectures, supercomputer operating systems
- **Computational Sciences and Math:**
  scalable algorithms: numerical PDEs, solvers optimization, uncertainty quantification; simulation of shock physics, electrical devices and circuits, nuclear power
- **Information and Cognitive Science:**
  large data handling and visualization, discrete math / complex systems, cognitive modeling and systems
- **For more information:**
  - **http://www.cs.sandia.gov/highlights/CCIM_Highlights_2009.pdf**
  - **http://www.cs.sandia.gov/**



Paraview visualization

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High Performance Computing: Sandia Systems and Software


CM-2
1988


nCUBE-2
1990


iPSC-860
1992

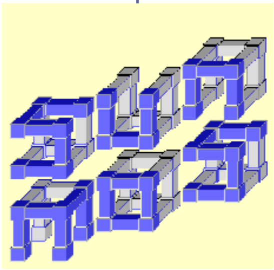

Paragon
1993

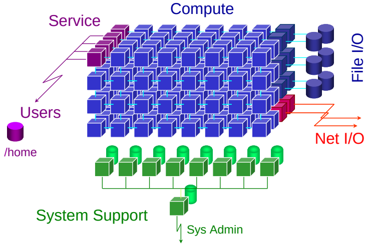

ASCI Red
1996


Cplant
1998


Red Storm
2005

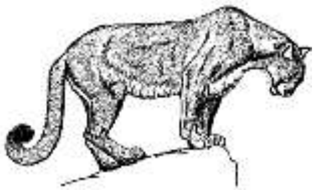
1987 1988 1989 1990 1991 1992 1993 1994 1995 1996 1997 1998 1999 2000 2001 2002 2003 2004 2005


SUNMOS
1990 - 1997



Partition Model
1990 –

Portals
1992 –


Puma, Cougar, Catamount
1993 –

Cplant
1997 – 2005

FASTOS
2004 -

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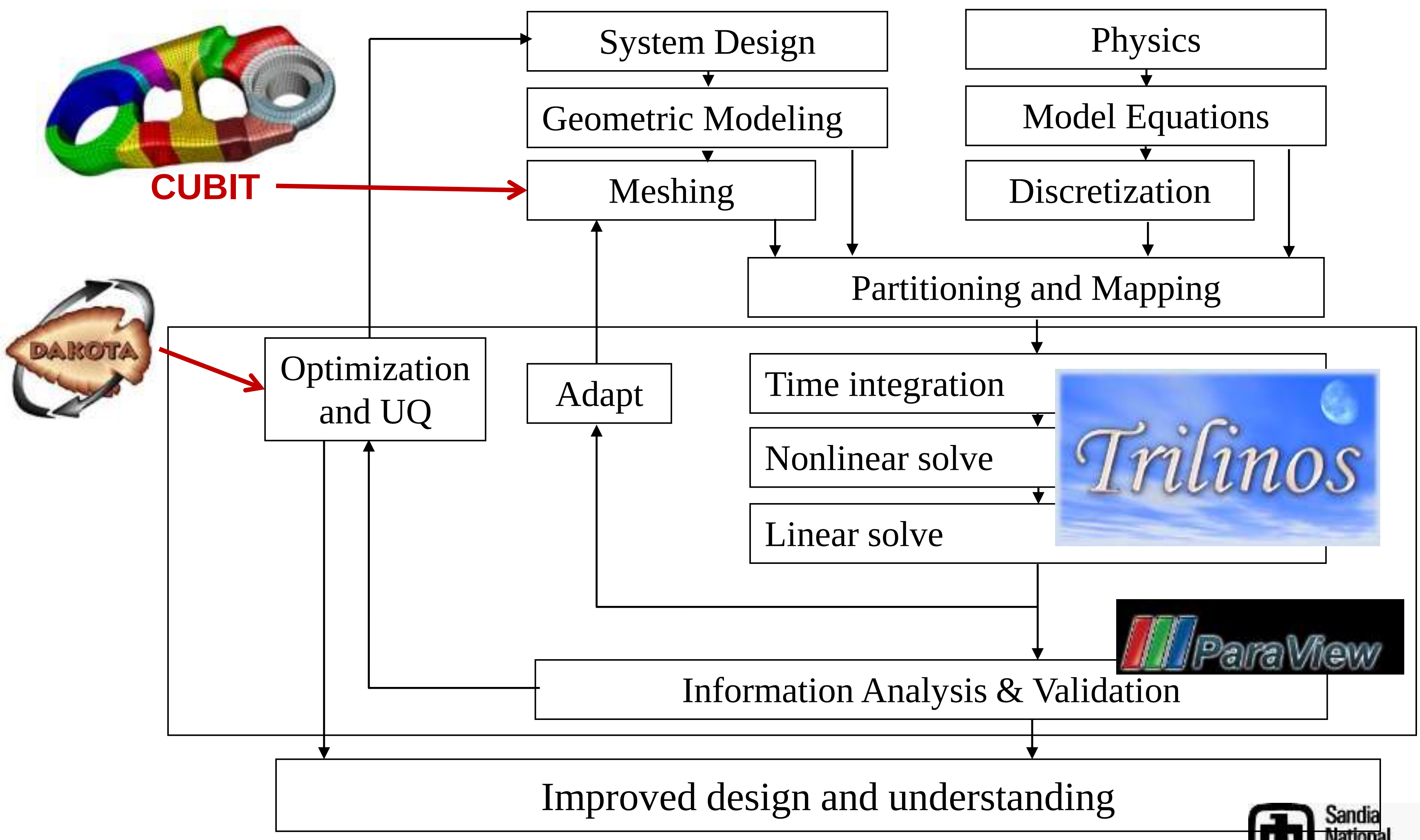
Algorithm R&D Transforming Computational Modeling & Simulation



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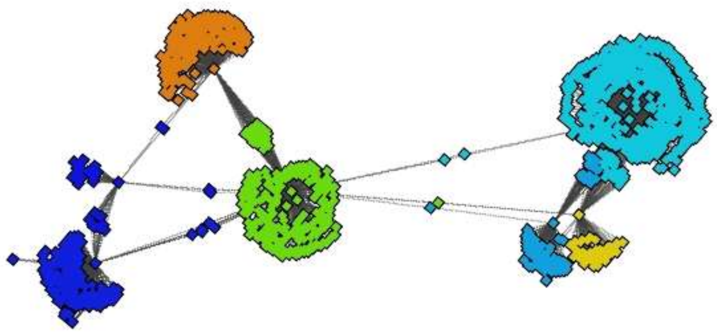
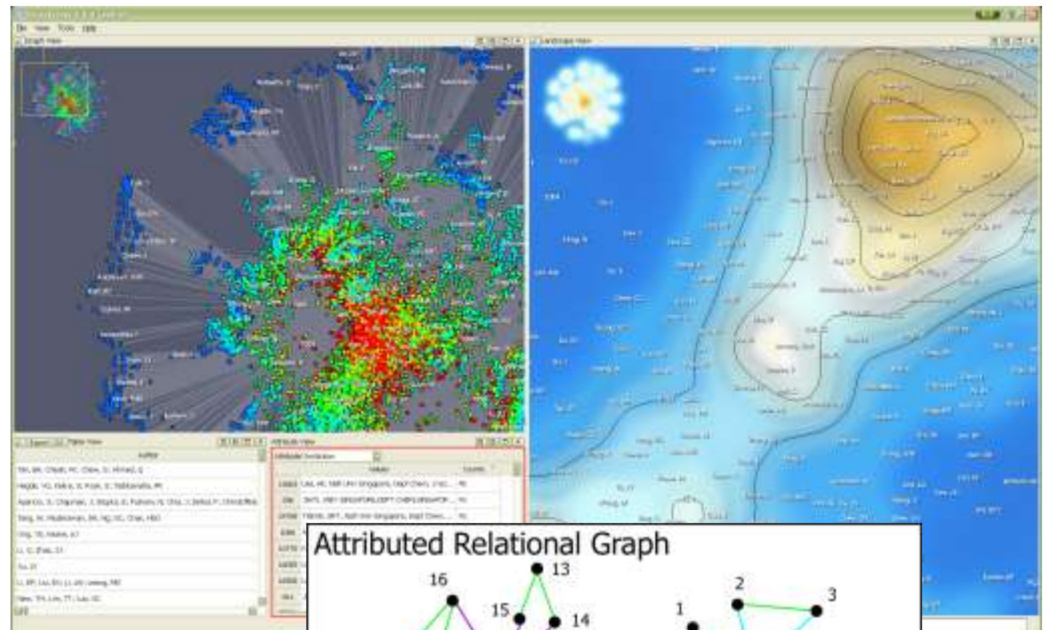
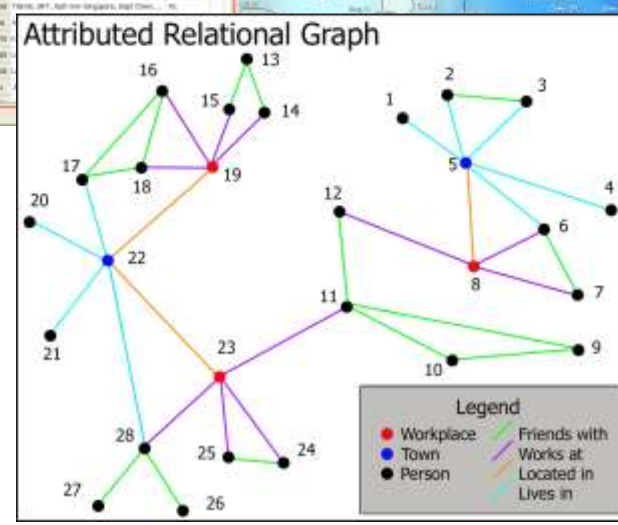
Scalable Informatics and Visualization

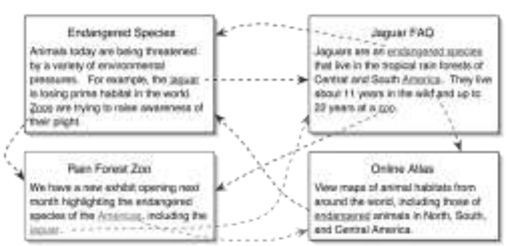
Advanced Graph Analysis: Community Clustering focuses on a smaller subset of interest.

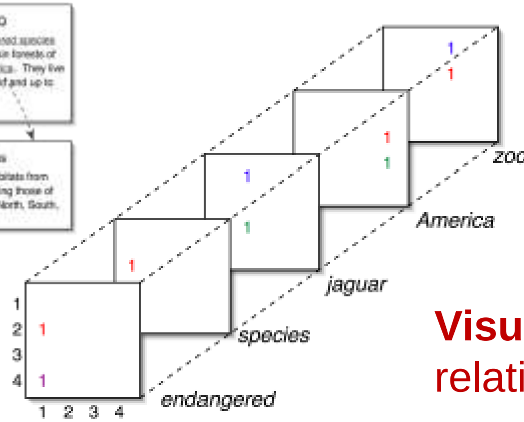






Advanced linear algebra and multi-way tensors to infer missing links and help recognize patterns





Visual Informatics: understand complex relationships; detect anomalies

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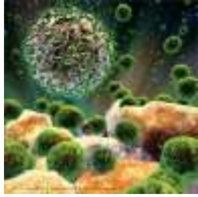
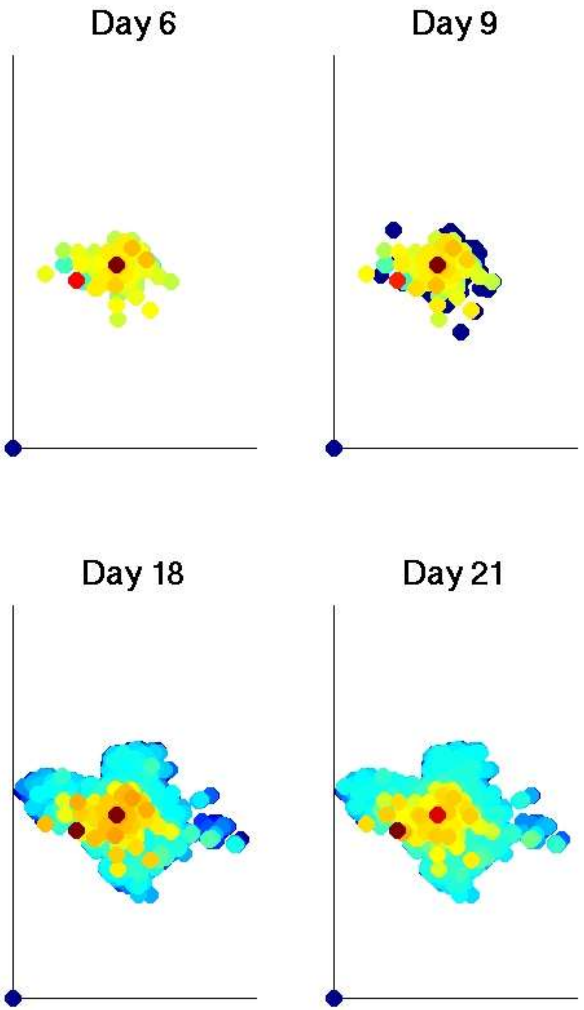
Disease Outbreak Characterization



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



- **3-year effort with Jaideep Ray (PI), Karen Devine, Youssef Marzouk, Michael Wolf (UIUC), others**
- **Bayesian inverse problem to determine initial conditions**
- **Agent-based social contact network disease propagation simulator**
  - **model geographic spread**
  - **model chain of contacts**

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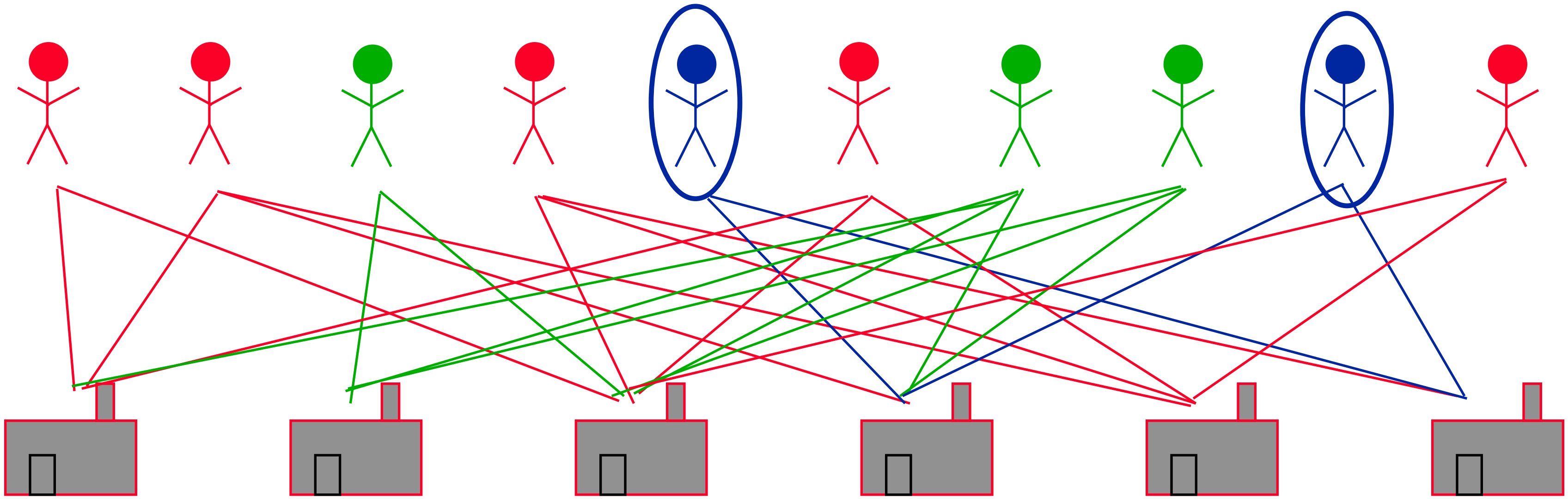
Network-based Disease Model

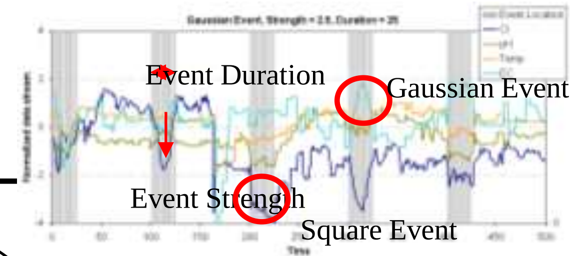
Each person's health modeled with (ordinary) differential equations; dynamic social network connecting people:



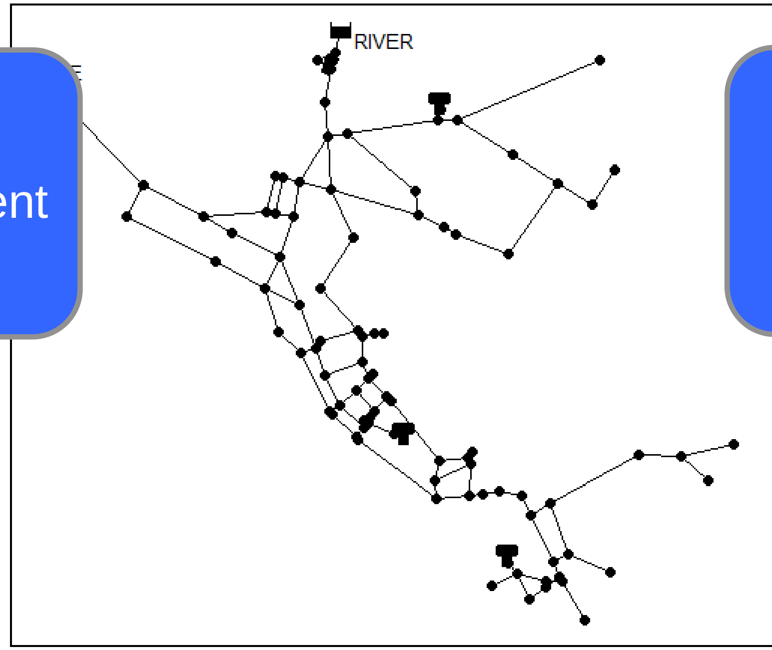
- **Graph theory for parallel partitioning and model reduction (cluster analysis on bipartite graph)**
- **Math biology for in-host disease models (pathogenesis) and transmission (epidemiology)**
- **Scalable parallelism via MPI for efficient simulations**

Water Security

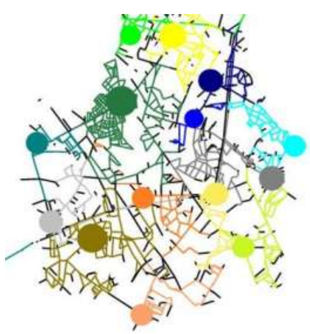
CANARY
real-time event detection



SPOT
sensor placement optimization

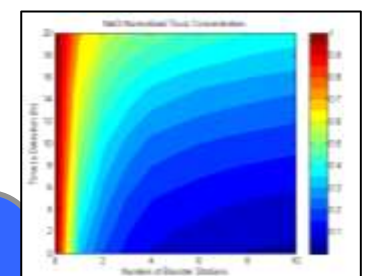


PONI
real-time contaminant source inversion



TEVA
contaminant simulation and vulnerability assessment

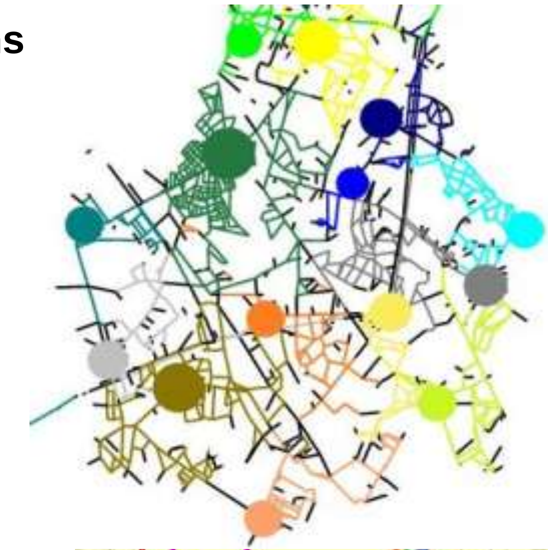
CWaRK
response protocol for isolation, flushing, and decontamination booster



courtesy Bill Hart

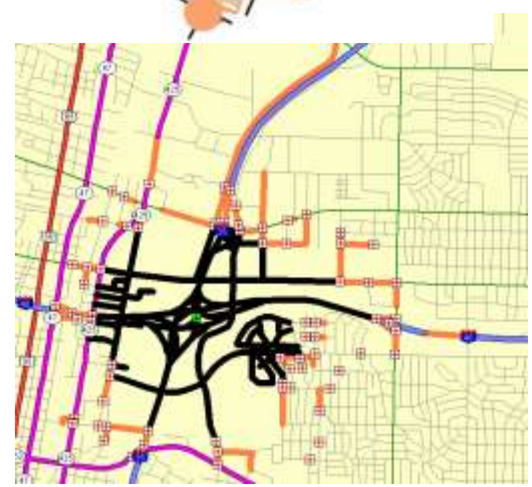
TEVA-SPOT:
Optimization of Sensor Networks

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

courtesy Bill Hart

Water Security:
Beneficial Expertise

- Civil engineering, water network design and operation
- Physics of fluid flow, electrical circuits
- Algebraic modeling of the physical processes
- Discrete optimization to place sensors (discrete math, graph theory, operations research)
- Continuous (and discrete) optimization for source inversion
- Statistics and signal processing for anomaly detection

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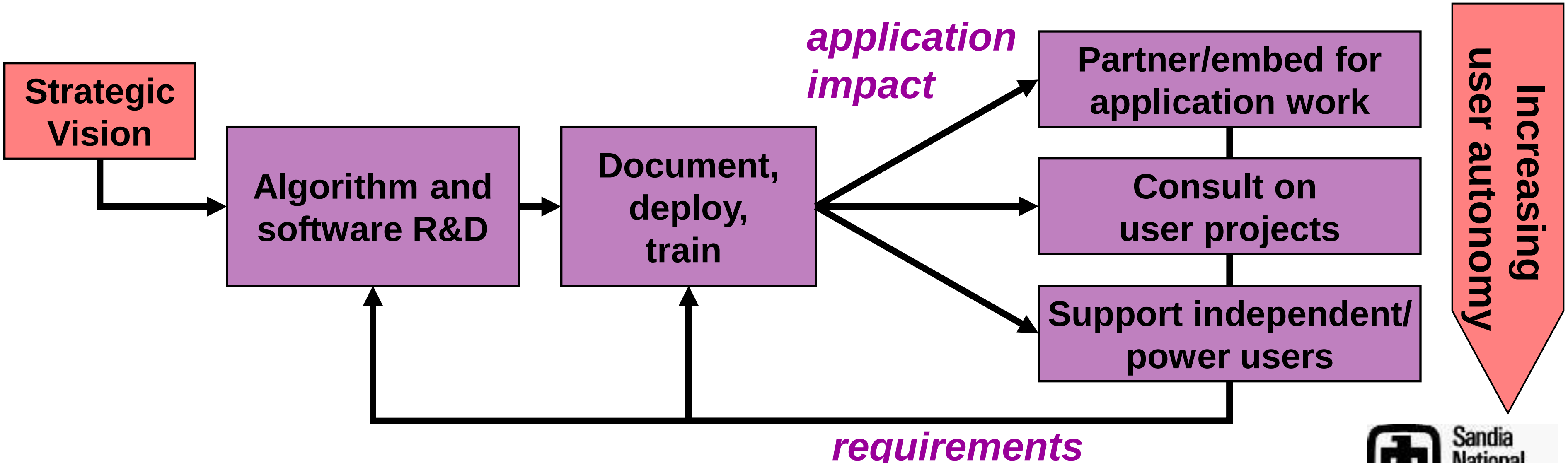
My Work Life
Largely Centers on DAKOTA

- **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



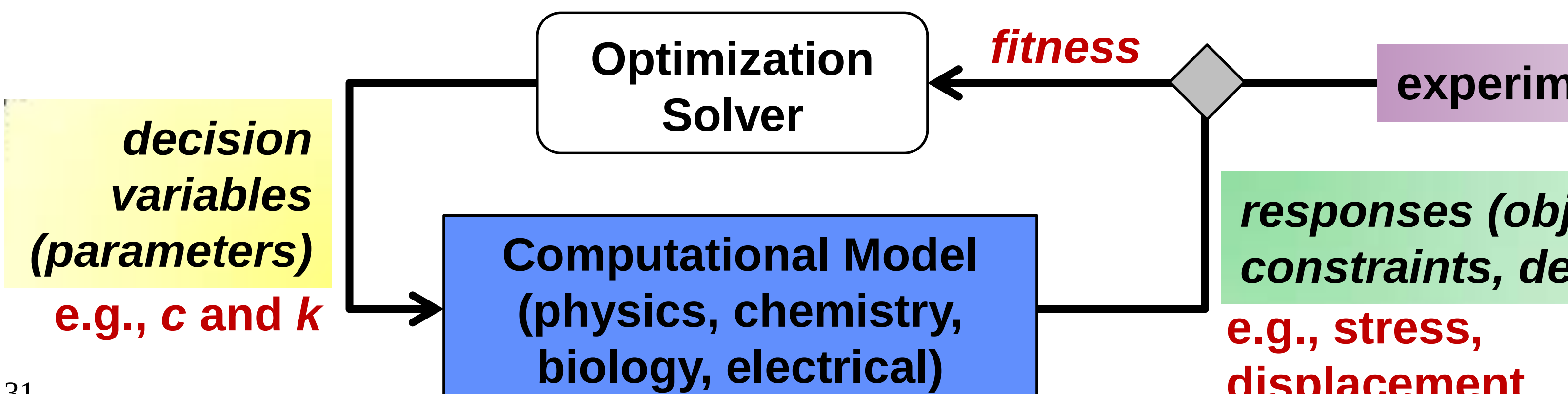
DAKOTA in a Nutshell

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-based Optimization and Calibration

- **GOAL: Vary parameters of a simulation to extremize objectives, while satisfying constraints to find (or tune) the best design, estimate best parameters, analyze worst-case surety**
- **Mapping from decision variables to objectives and constraints is (at least partially) implicit; *no explicit algebraic form***
- **Relationship is calculated by a “black box” computational model of target phenomenon (often loosely coupled to the solver)**
- **Solver iteratively evaluates the simulation and adapts based on its outputs to maximize fitness.**
- **Same process can calibrate, adjusting parameters to maximize agreement with experimental data**



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

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

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**

Determine the optimal tank shape that

- **minimizes drag for**
- **maximum range and**
- **minimizes yawing moment for separation of adjacent stores.**

Optimal design found with DAKOTA and later verified in wind tunnel experiments.

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Problem Formulation: Objectives and Constraints

Information with which to configure the solver:

Minimize:	$f(x_1, \ldots, x_N)$	***Objective function(s)****
Subject to:	$g_{LB} \leq g(x) \leq g_{UB}$	***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)
	$A_I x \leq b_I$	***Linear inequality constraints***
	$A_E x = b_E$	***Linear equality constraints***
	$x_{LB} \leq x \leq x_{UB}$	***Bound constraints***

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

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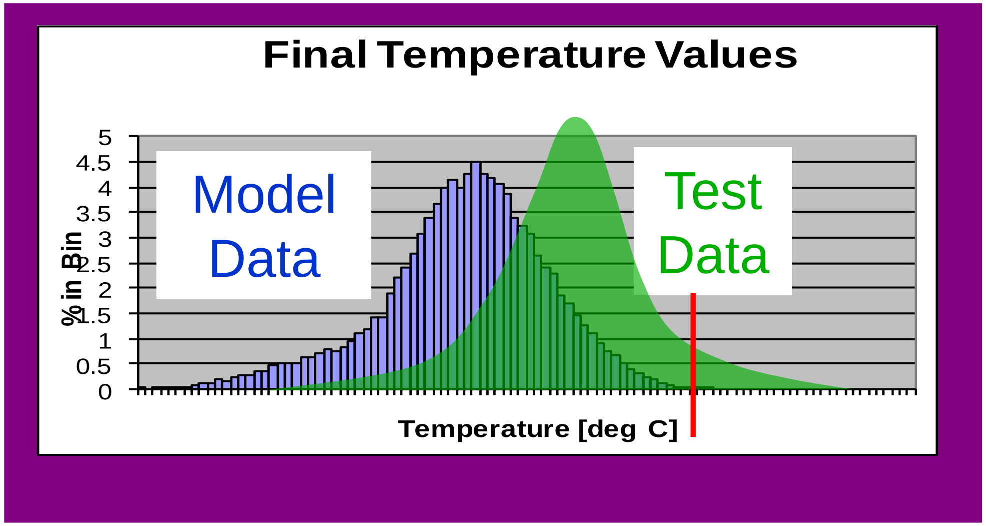
Uncertainty:
"But I wrote down and solved the equations!"

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!*

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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:***

<u>Input Variables *u*</u>
(physics parameters, geometry, initial and boundary conditions)

(possibly given distributions)

→ **Computational Model** →

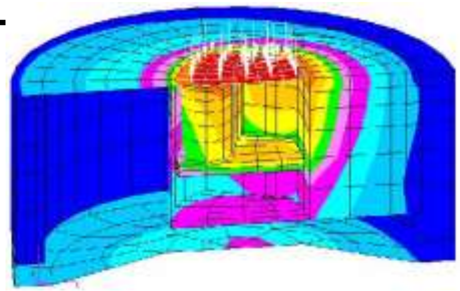
(here assumed a black-box)

Variable Performance Measures *f(u)*

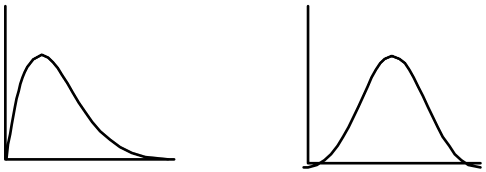
Potential Goals:

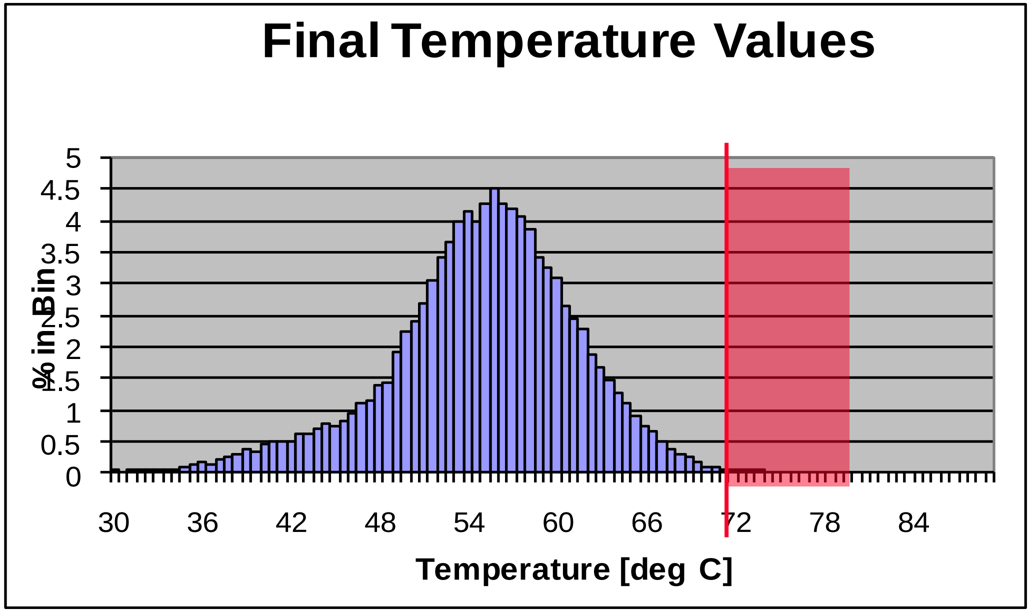
- **based on uncertain inputs, determine variance of outputs and probabilities of failure (reliability metrics)**
- **validation: is the model sufficient *for the intended application?***
- **quantification of margins and uncertainties (QMU): *how close are uncertainty-aware code predictions to performance expectations or limits?***
- ***quantify uncertainty when using calibrated model to predict***

Thermal Uncertainty Quantification



- **Device subject to heating** (experiment or computational simulation)
- Uncertainty in composition/ environment (thermal conductivity, density, boundary), parameterized by $u_1, \ldots, u_N$
- Response temperature $f(u) = T(u_1, \ldots, u_N)$ calculated by heat transfer code





Given distributions of $u_1, \ldots, u_N$, UQ methods calculate statistical info on outputs:

- Mean(T), StdDev(T), Probability($T \geq T_{critical}$)
- Probability distribution of temperatures
- ***Correlations (trends) and sensitivity of temperature***

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Assess Nuclear Reactor Crud Uncertainty

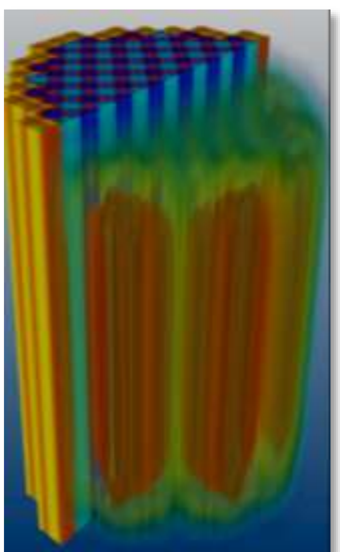
- Crud deposits form in nuclear reactors, affecting nuclear reactions
- Resulting crud-induced power shift affects reactor operation in potentially costly ways
- Induced in part by localized boiling in the core
- Key uncertainties affecting boiling predictions:
  - Operating temperature, pressure, flow rate, power
  - Radioisotope concentrations in the fuel
  - Assumptions in physical models, e.g., heat transfer rates, correlation coefficients, corrosion product release rates

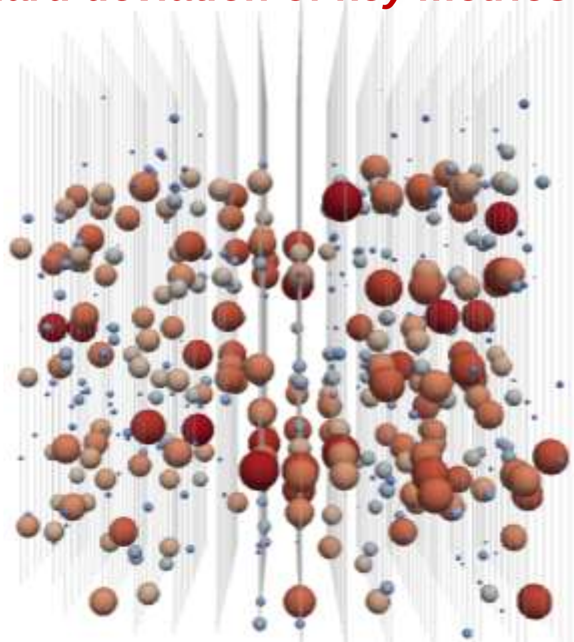
Key question: what is the likelihood of (substantial) crud formation in a nuclear reactor and where will it occur? How sure are we based on models?

Uncertainty in Boiling Rate for (Nuclear Reactor Quarter Core

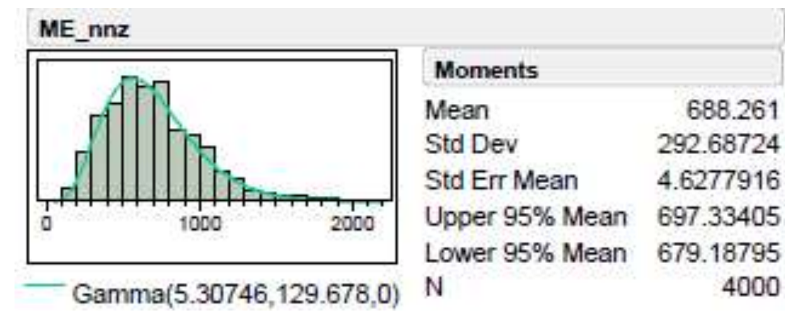
Method	ME_nnz		ME_meannz		ME_max	
	Mean	Std Dev	Mean	Std Dev	Mean	Std Dev
LHS (40)	651.225	297.039	127.836	27.723	361.204	55.862
LHS (400)	647.33	286.146	127.796	25.779	361.581	51.874
LHS (4000)	688.261	292.687	129.175	25.450	364.317	50.884
PCE (Θ(2))	687.875	288.140	129.151	25.7015	364.366	50.315
PCE (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



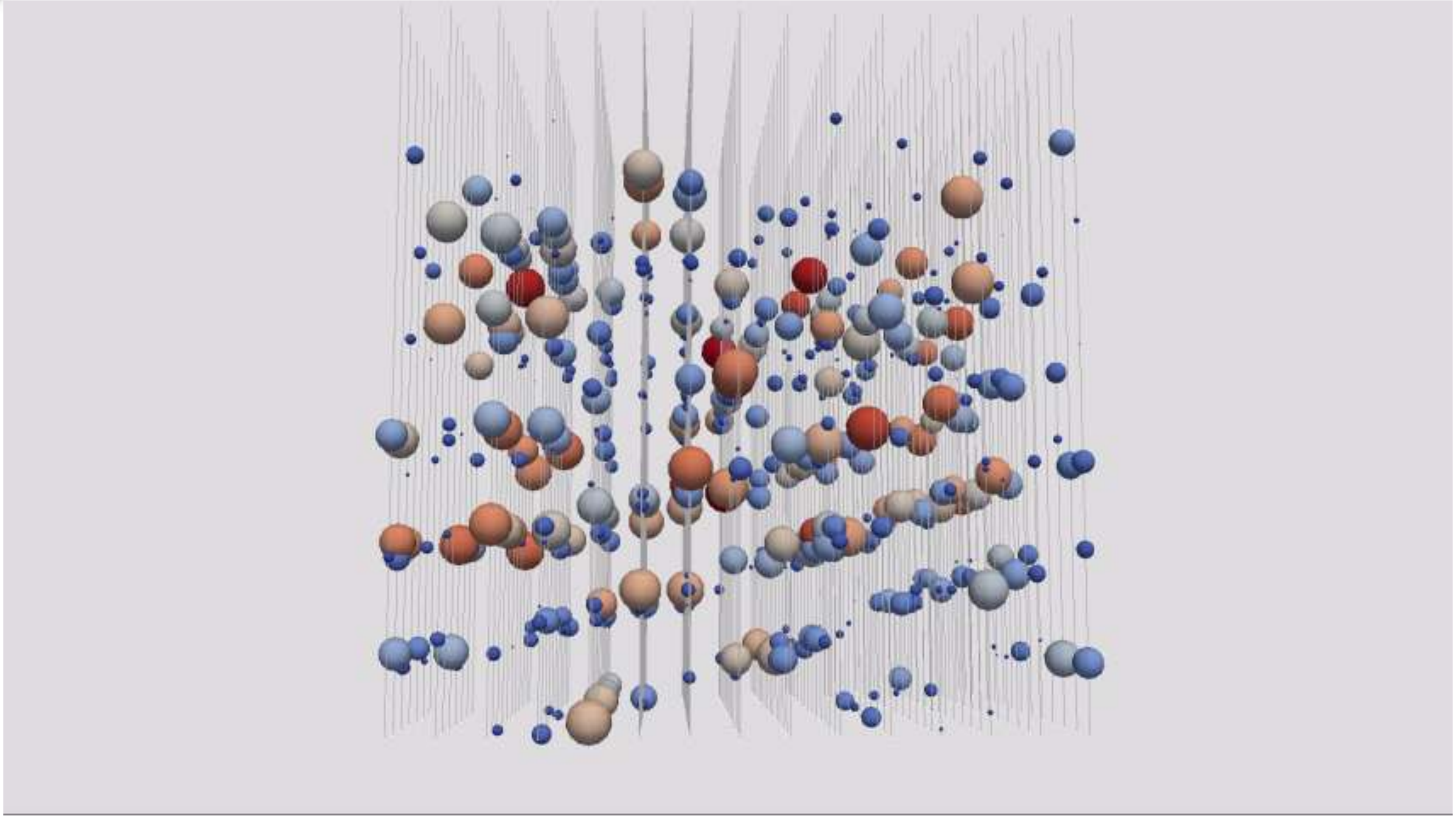


anisotropic uncertainty distribution in boiling rate throughout quarter core model



normally distributed inputs need not give rise to normal outputs…

Mass Evaporation Rate in Reactor Quarter Core



mean of boiling rate: 0 **97** **194** **291**

size indicates standard deviation of boiling rate ***($lb_m/hr\text{-}ft^2$)***

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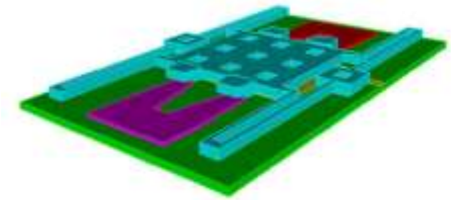
Combining Optimization and UQ

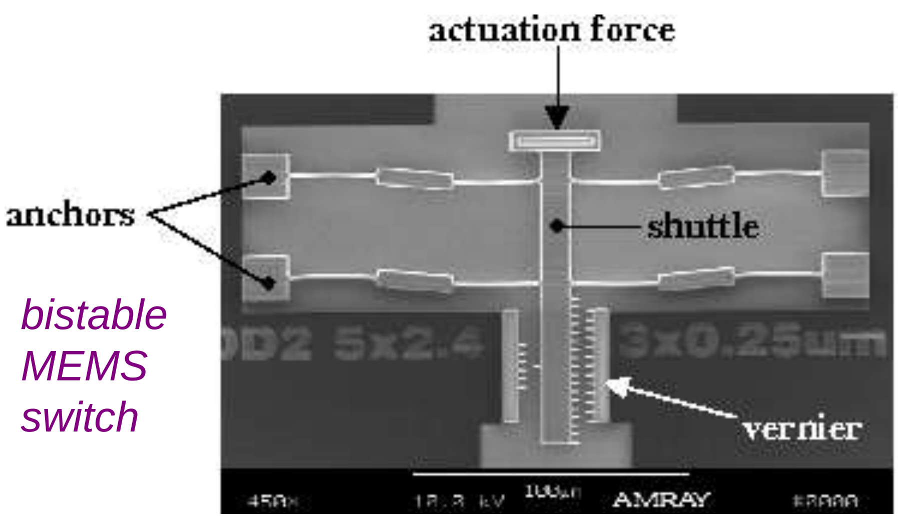
DAKOTA facilitates studies that meld opt and UQ:

- **Optimization under uncertainty**
- **Robust design**
- **Uncertainty surrounding optimal design**

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

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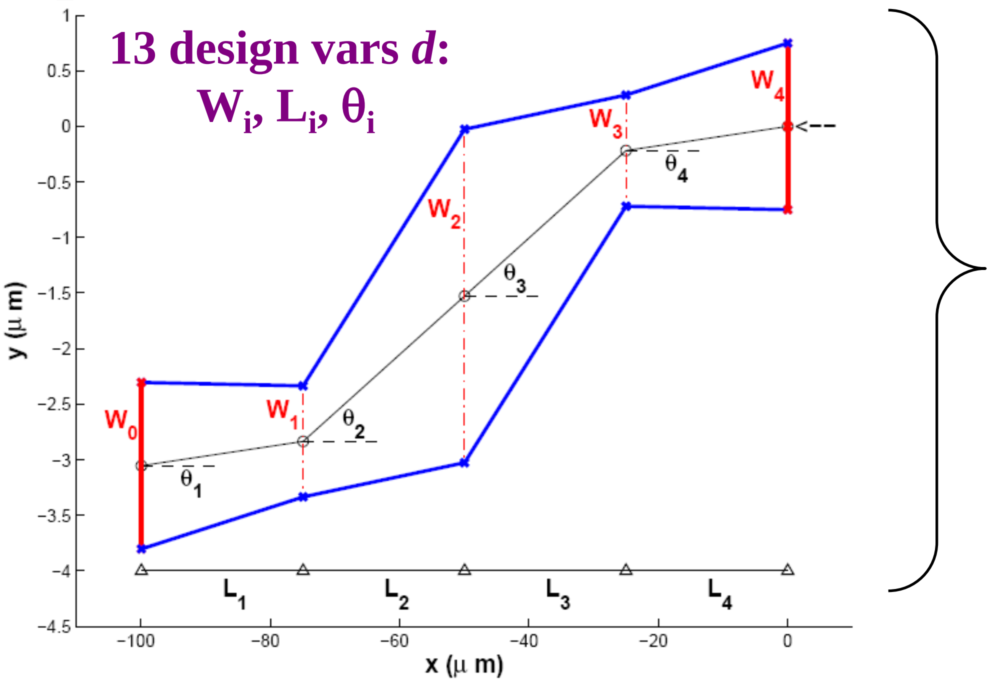
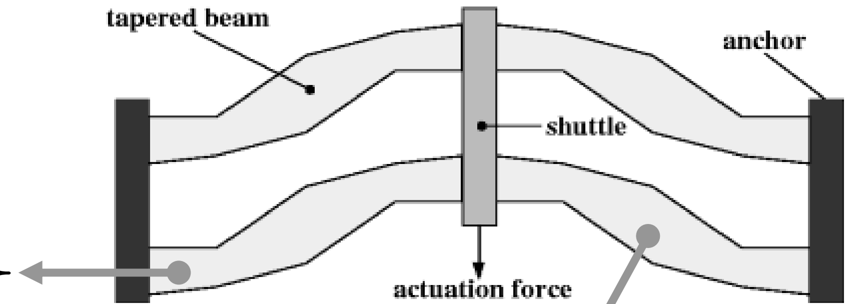
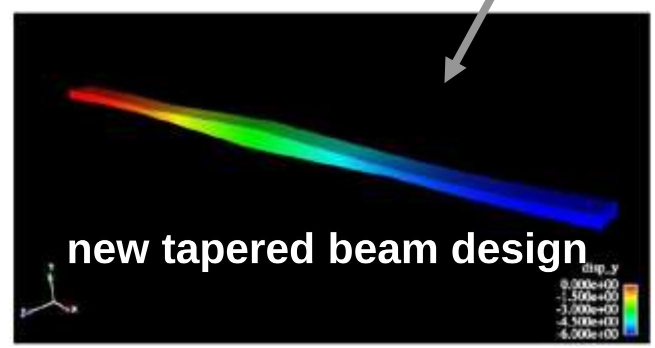
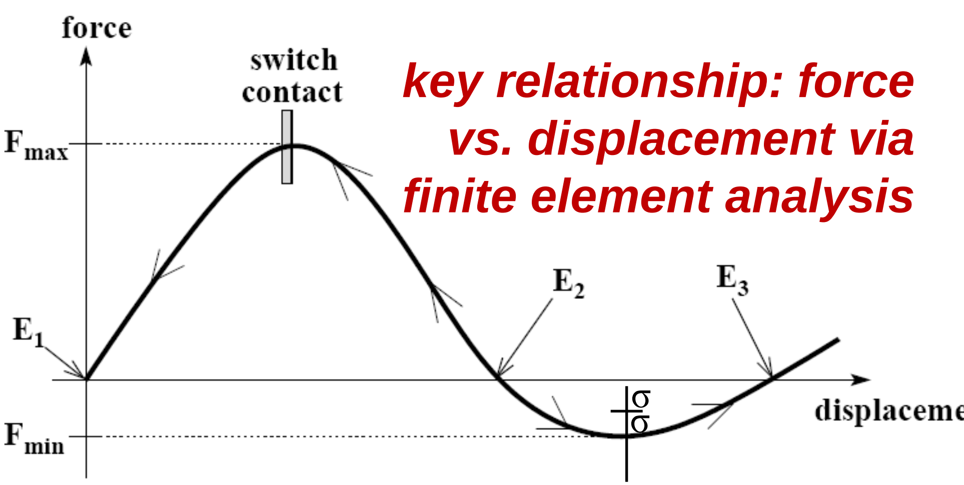
MEMS Switch Design: Geometry Optimization









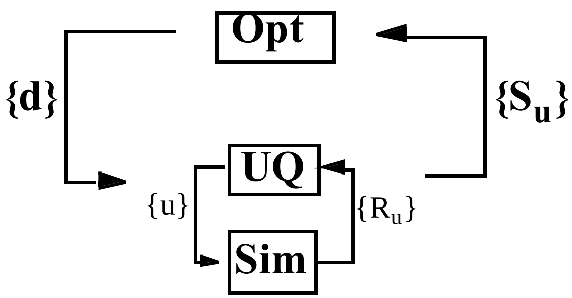
key relationship: force vs. displacement via finite element analysis

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:



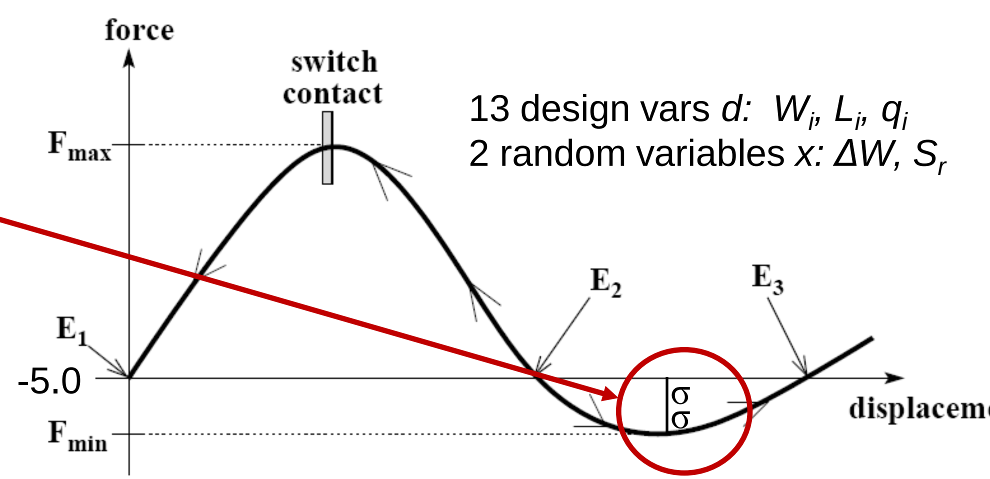
(nested paradigm)

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

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

simultaneously reliable and robust designs

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



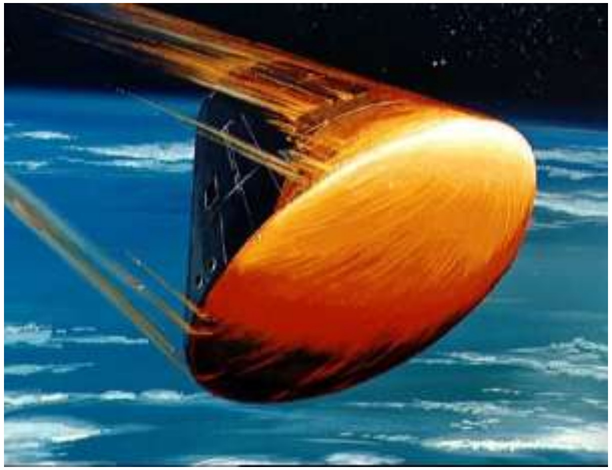
13 design vars *d*: W_i, L_i, q_i
2 random variables *x*: ΔW, S_r

Examples of UQ Challenges

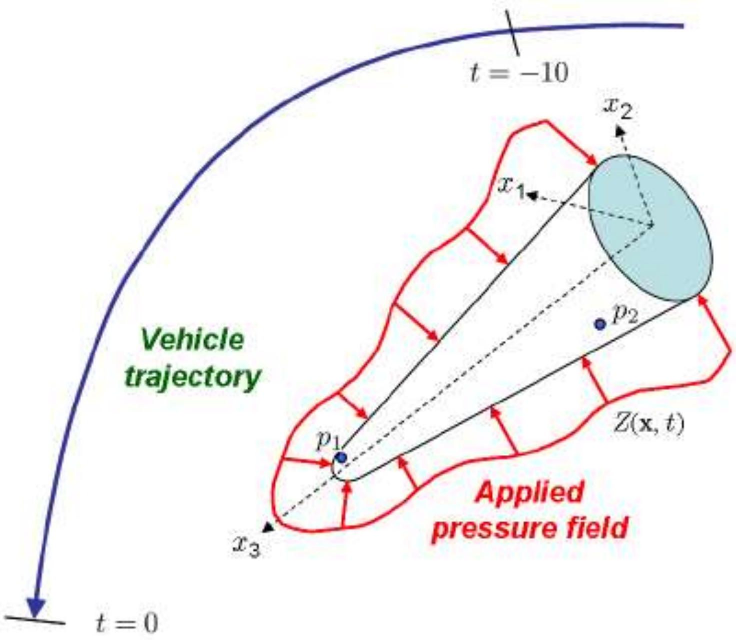
Warp to credible simulation conclusion

Challenge: UQ for Fluid-Structure Interactions

- **Atmospheric entry vehicles are subject to turbulent flow, complex chemical reactions, thermal and pressure loads.**
- **Example goal: assess uncertainty in loads imposed on structures without running costly CFD over many scenarios (typically can't afford full coupling).**
- **Need: random field characterization of uncertainty from CFD and efficient way to assess effect on structural dynamics.**

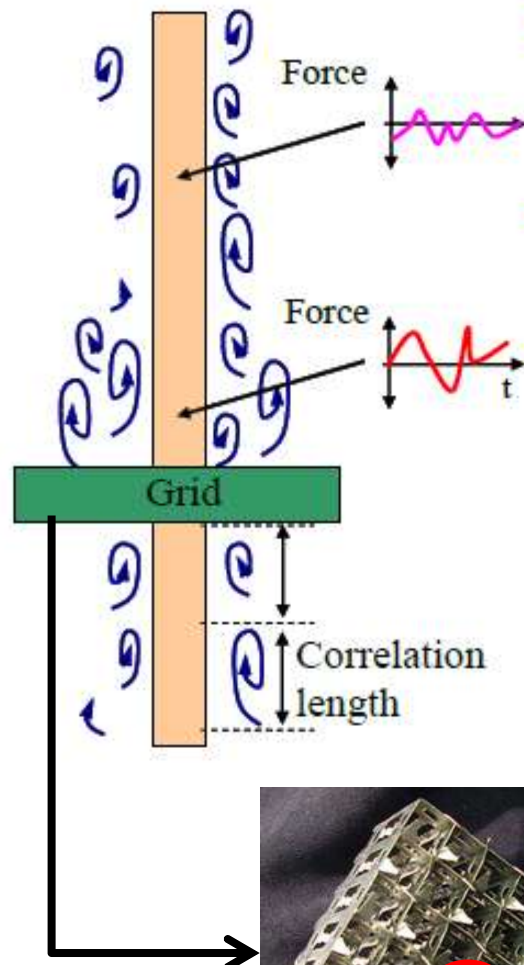


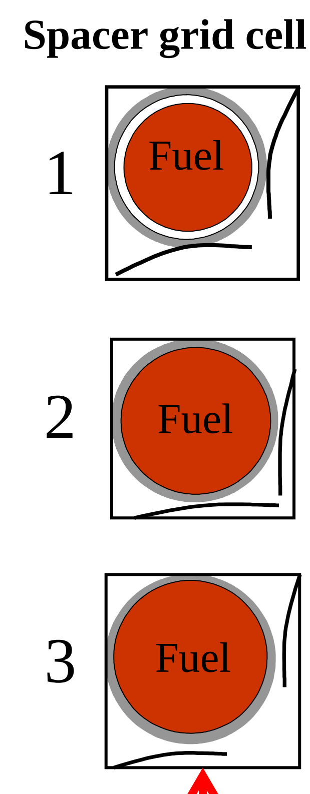
NASA (public domain)

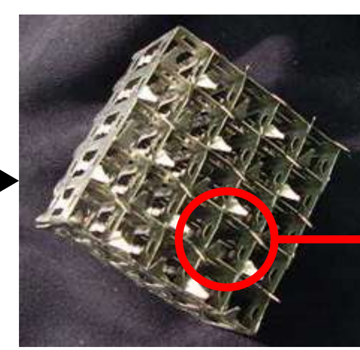


FSI: Nuclear Reactor
Grid-to-rod Fretting Failure

- **Clad failure can result from rod-spring interactions**
  - **Induced by flow vibration**
  - **Amplified by irradiation-induced grid spacer growth and spring relaxation**
- **Power uprates and burnup increase potential for fretting failures (leading cause of fuel failures in PWRs)**
- **Ideally: High-fidelity, fluid structural interaction tool to predict uncertainty in gap, turbulent flow excitation, rod vibration and wear**







Sources: CASL DOE Energy Innovation Hub, Roger Lu, Westinghouse

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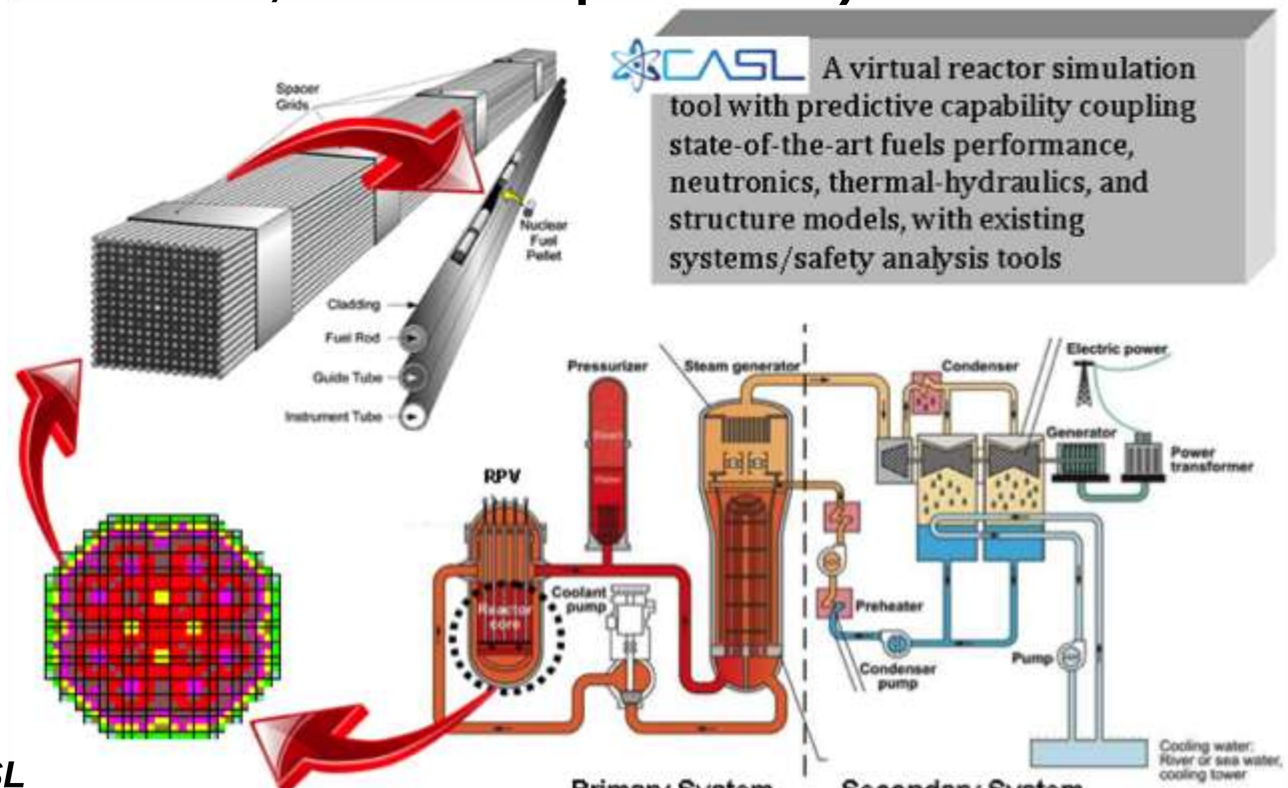
UQ for Coupled Multi-Physics

- **Can we efficiently propagate UQ across scales/disciplines?**
- **Naively wrapping multi-physics with UQ often too costly**
- **Can we invert loops and perform multi-physics analysis on UQ-enriched simulations (couple based on scalar statistics, random fields, stochastic processes)?**



Source: CASL
(DOE Energy Innovation Hub)

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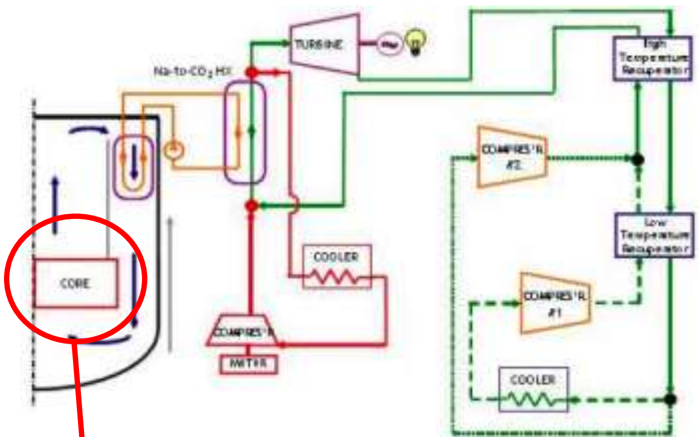
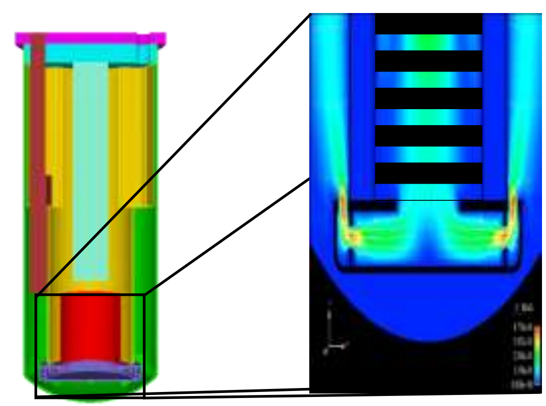
Multi-Physics, Multi-Fidelity, Heterogeneous UQ

- **Component-level uncertainty propagation via stochastic expansions**
- **Stochastic dimension reduction at component interfaces**
- **Strongly coupled solver technology for coupled stochastic problems**
- **Stochastic upscaling for low-fidelity models**
- **Stochastic sensitivities with respect to system components**



Low-fidelity Network Plant Model



High-fidelity Multi-physics Component Model (Core)

Graphics courtesy: Rod Schmidt, BRISC project

v_1

Component 1

$$v_2 = G_1(v_1, p_1) = g_1(u_1(v_1), p_1) \;\; \text{s.t.} \;\; f_1(u_1, v_1, p_1) = 0$$

v_2

Component 2

$$v_1 = G_2(v_2, p_2) = g_2(u_2(v_2), p_2) \;\; \text{s.t.} \;\; f_2(u_2, v_2, p_2) = 0$$

Nonlinear elimination

Equations

$$v_2 - G_1(v_1, p_1) = 0$$
$$v_1 - G_2(v_2, p_2) = 0$$

Newton Step

$$\begin{bmatrix} -dG_1/dv_1 & 1 \\ 1 & -dG_2/dv_2 \end{bmatrix} \begin{bmatrix} \Delta v_1 \\ \Delta v_2 \end{bmatrix} = -\begin{bmatrix} v_2 - G_1(v_1, p_1) \\ v_1 - G_2(v_2, p_2) \end{bmatrix}$$

$$\frac{dG_i}{dv_i} = -\frac{\partial g_i}{\partial u_i} \left(\frac{\partial f_i}{\partial u_i} \right)^{-1} \frac{\partial f_i}{\partial v_i}$$

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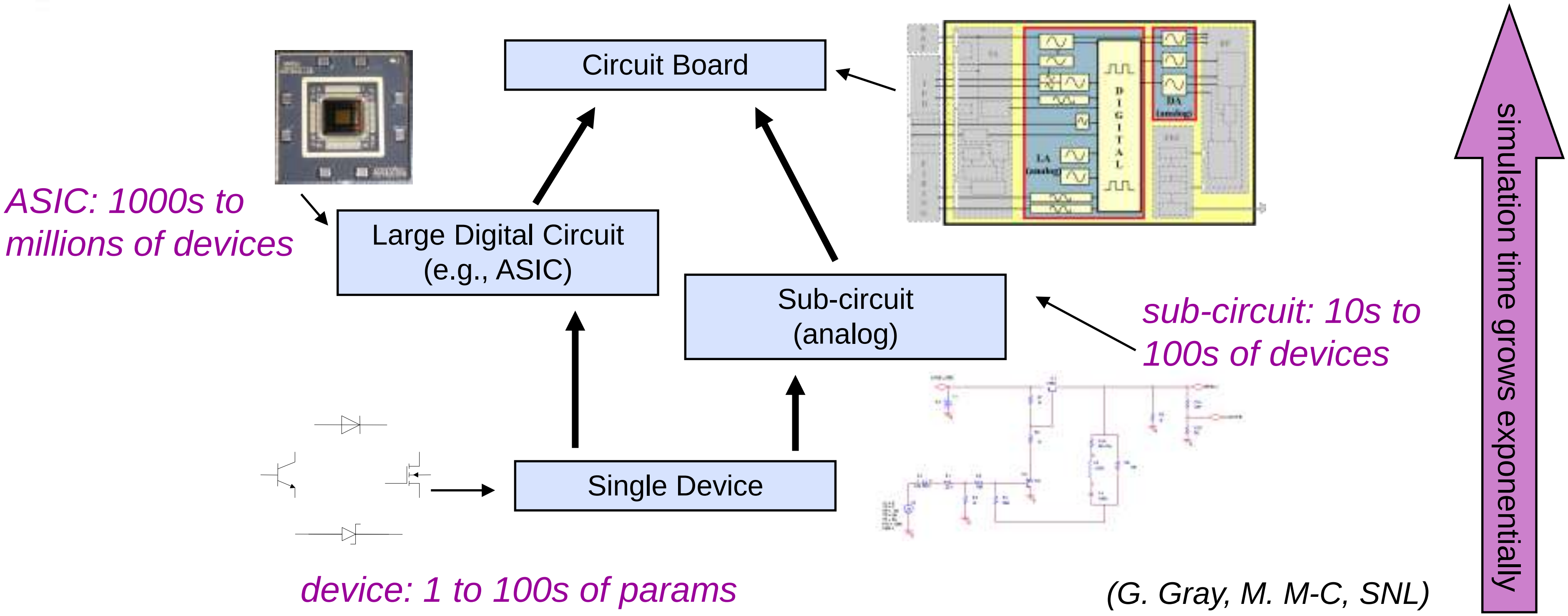
Electrical Modeling Complexity

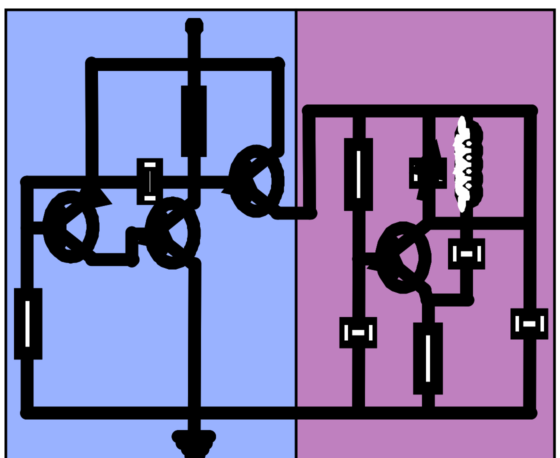


- **simple devices: 1 parameter, typically physical and measurable**
- **e.g., resistor @ 100Ω +/- 1%**
- **resistors, capacitors, inductors, voltage sources**

- **complex devices: many parameters, some physical, others "extracted" (calibrated)**
- **multiple modes of operation**
- **e.g., zener diode: 30 parameters, 3 bias states; many transistor models (forward, reverse, breakdown modes)**

Hierarchical/Network Structure

- **How can we exploit electrical systems' natural hierarchy or network structure?**
- **How does uncertainty propagate? Sufficient to propagate variance?**
- **Use surrogate/macro-models as glue between levels?**
- **Can approaches be implemented generically to apply to any circuit implemented in Xyce?**



system level
(performance metrics)

↑

circuit level
(circuit characteristics)

↑

device level
(model parameters)

↑

process level
(physical parameters)

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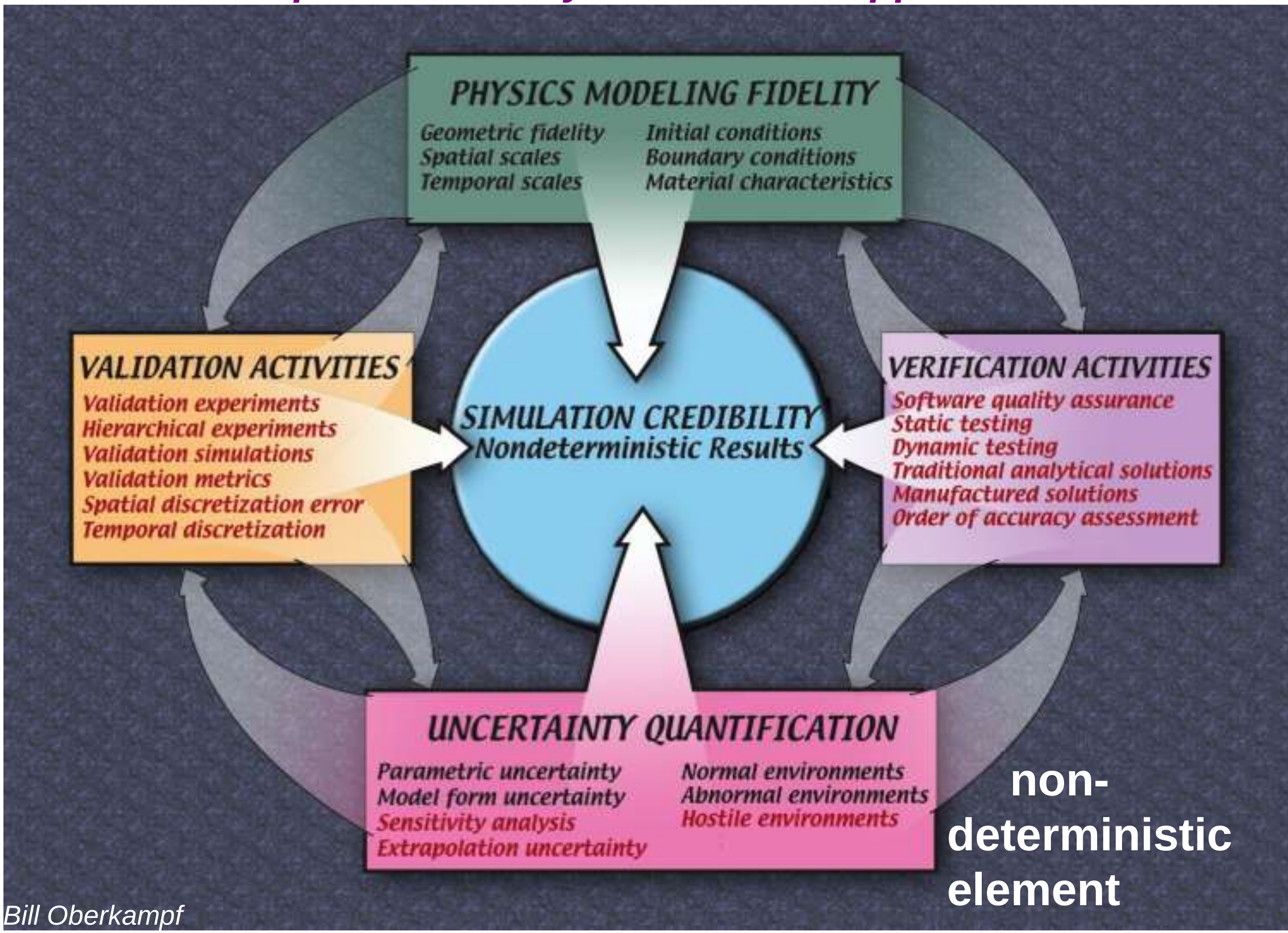
V&V, UQ, and Model Fidelity Support Credible Simulation

Insight, prediction, and risk-informed decision-making
require credibility for intended application



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Getting Started: Computational Applied Mathematics

Goal: demonstrate the intertwined role of mathematics, statistics, computer science, and disciplinary science in executing Sandia National Laboratories' mission

Helpful Training:

- **Mathematics, including statistics and probability**
- **Engineering / disciplinary science**
- **Computer science and programming skills**

Ways to Contribute:

- **New theories**
- **Analytic solutions/proofs**
- **Computational methods, iterative algorithms**
- **Software implementations**
- **Validation with experimental data**

- **See Careers in Math at http://siam.org/careers/thinking.php**
- **Contact me with any questions: briadam@sandia.gov**

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Abstract

Applied Mathematical Sciences at Sandia
Brian M. Adams
Optimization and Uncertainty Quantification
Sandia National Laboratories, Albuquerque, NM

Through this presentation I will relate my six year experience working in a mathematics and computer science research group at Sandia, a national security laboratory. The broad mission areas of the lab foster research in disciplines including engineering, materials, bioscience, energy and water, infrastructure security, scalable scientific computation, and beyond. Computational scientists support them with contributions ranging from theory and hardware to algorithms and software to solve application problems of national importance.

I will survey a number of application problems whose solution relies on mathematics, statistics, disciplinary science, and high-performance parallel computing. These are used in creating computational models (simulations) that scientists and engineers use for insight and decision making. I will also introduce optimization and uncertainty quantification algorithms and discuss their application to nuclear reactor performance assessment, water network security, micro-electro-mechanical system (MEMS) design, and disease spread modeling. I will touch on challenges of simulation credibility, or knowing that computer models are appropriate in the context in which they are used.

Bio: Brian M. Adams (http://www.sandia.gov/~briadam) is a Principal Member of Technical Staff in the Optimization and Uncertainty Quantification department at Sandia National Laboratories, Albuquerque, NM, where he has worked since 2005. He is generally interested in developing and applying algorithms and software for scientific computing. Brian's focus at Sandia has primarily been on sensitivity analysis, uncertainty quantification, and optimization of computational models (simulations). He leads the DAKOTA software project (http://dakota.sandia.gov) which addresses these problems. His recent work has also touched on surrogate (response-surface) modeling, agent-based models of disease spread, optimal electrical power flow, and nuclear reactor performance. Brian earned his B.S. in mathematics from St. Michael's College (Colchester, VT); M.S. and Ph.D. in computational applied mathematics from NC State University. His dissertation focused on HIV modeling and probabilistic calibration to patient data.

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