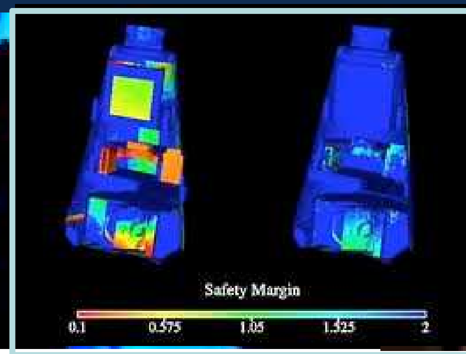
SAND2013-2282P

Exceptional service in the national interest

Sandia National Laboratories



Some of the Challenges of Predictive Simulation

Dan Segalman

U.S. DEPARTMENT OF ENERGY

NNSA

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Sandia National Laboratories: 60 Years of *Exceptional Service in the National Interest*

- Born of the atomic age
- Heritage of engineering and production
- Science mobilized for national security
- A legacy of industrial management
- Six key mission areas:
  - Nuclear weapons
  - Nonproliferation
  - Assessments
  - Military technologies and applications
  - Homeland security
  - Energy and infrastructure assurance

"you have …an opportunity to render an exceptional service in the national interest." *May 13, 1949 Letter from President Truman to Mr. Wilson, President of AT&T*

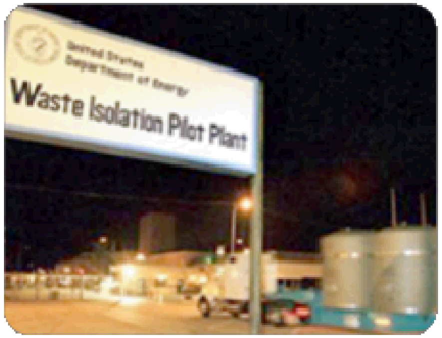
AT&T 1949-1993

LOCKHEED MARTIN 1993-Present

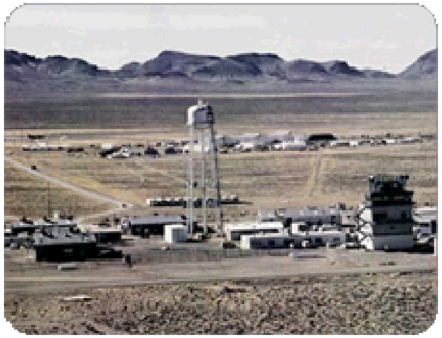
Our Highest Goal: to become the laboratory that the United States turns to first for technology solutions to the most challenging problems that threaten peace and freedom.

Sandia's Sites

Albuquerque, New Mexico



Carlsbad, New Mexico



Tonopah, Nevada

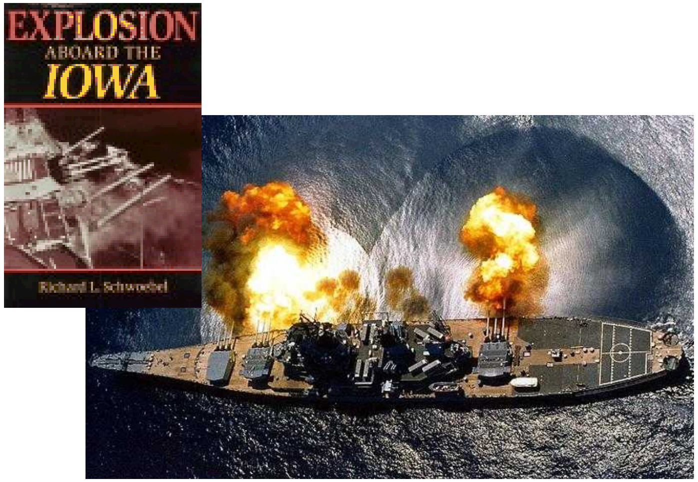
Livermore, California

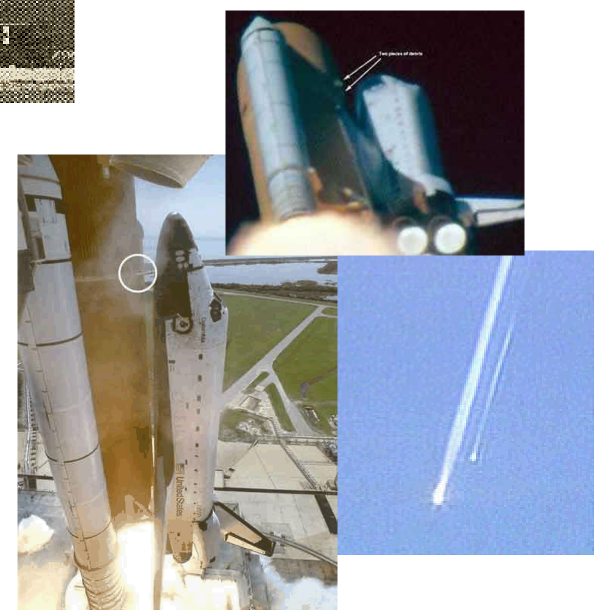
Amarillo, Texas

Kauai, Hawaii

We are often called upon to answer critical questions

Sandia National Laboratories





Columbia

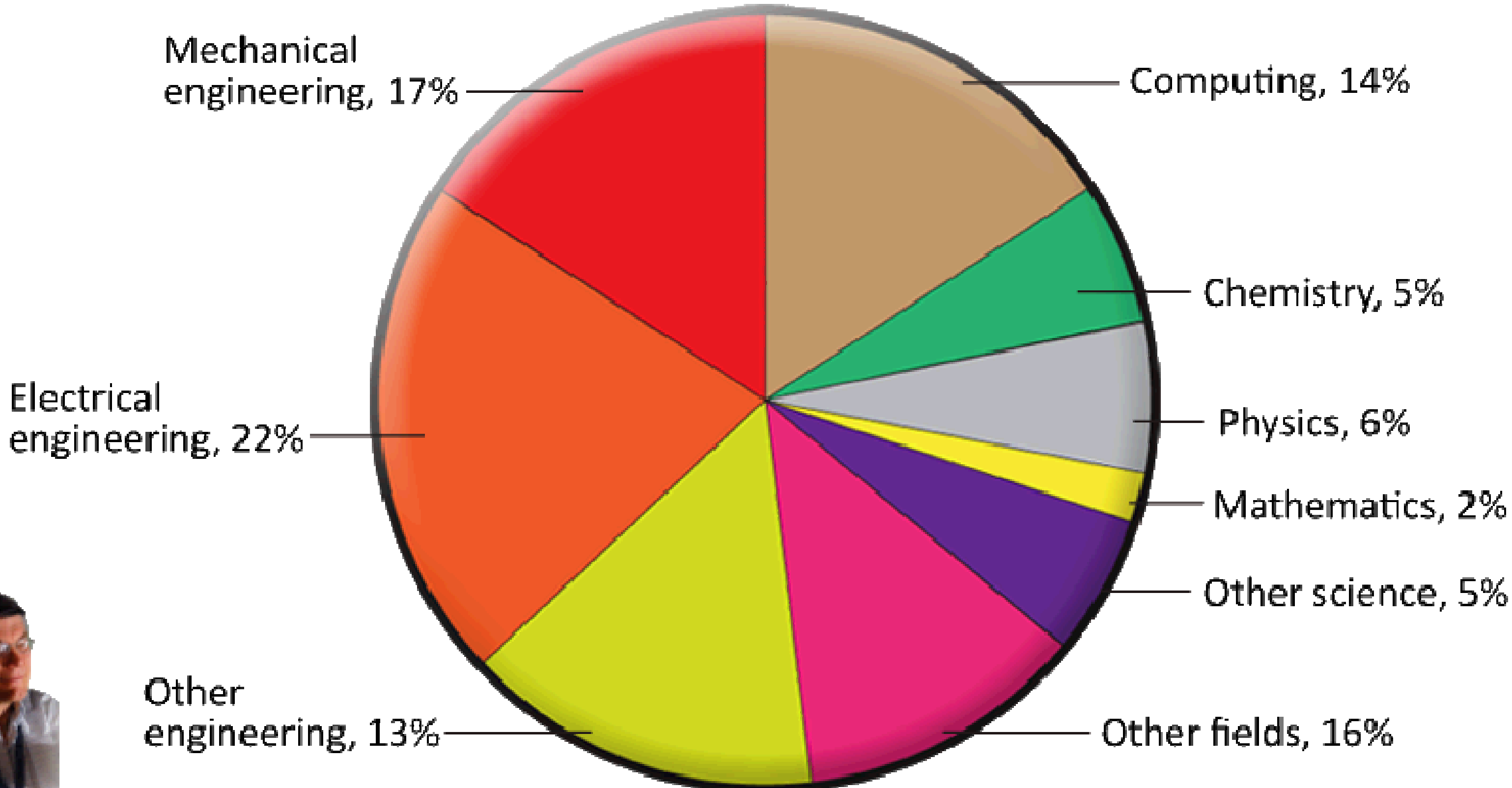
NW is now less than half the Sandia budget

Our Workforce

- Onsite workforce: 11,741
- Regular employees: 9,399
  Gross payroll: ~$369M

Data for FY13 through end of January

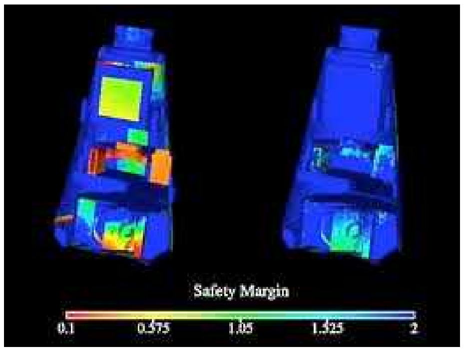
Research & Development staff(4,777) by discipline

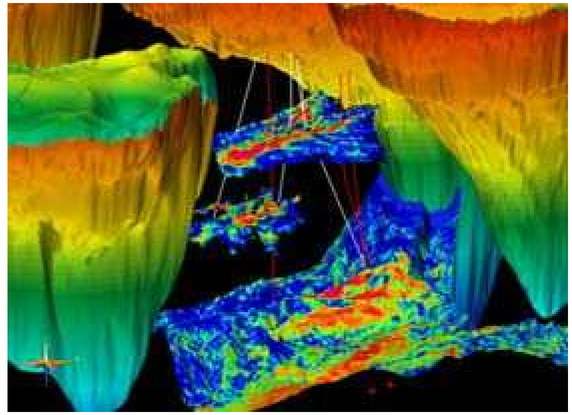


Our Mission Focus Relies on Strong Science and Engineering

Five Research Foundations

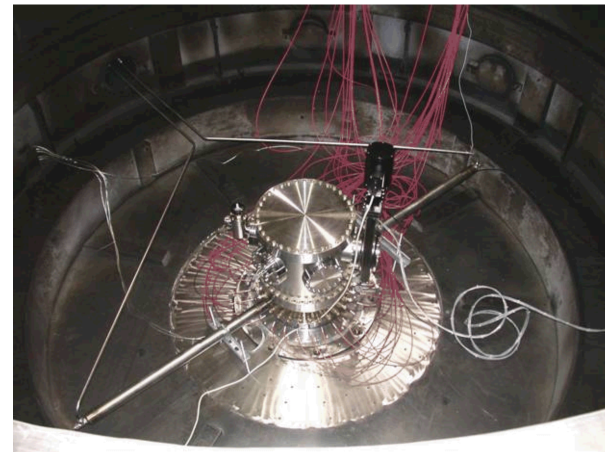
Engineering Sciences

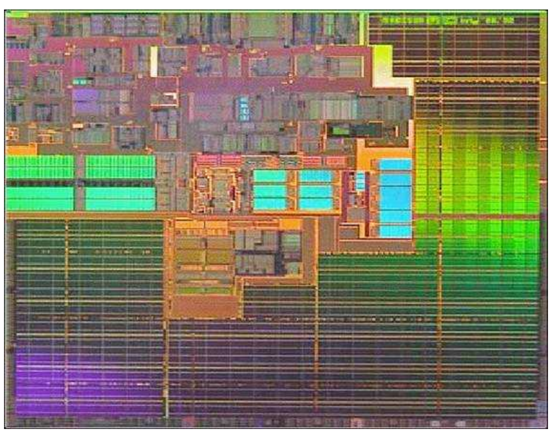




Geoscience

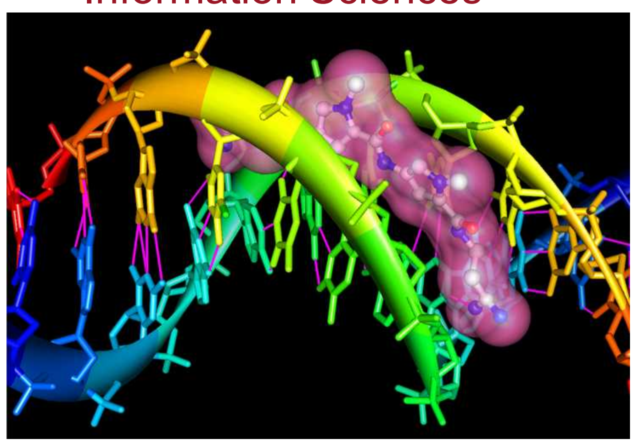
Pulsed Power Sciences

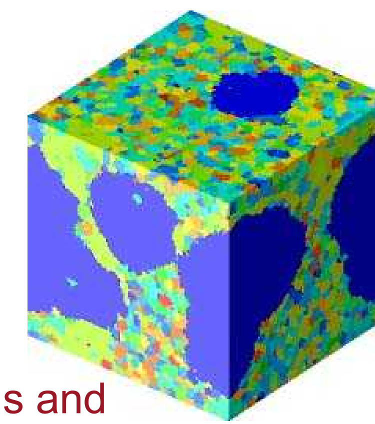




Microelectronics and Photonics Sciences

Computational and Information Sciences

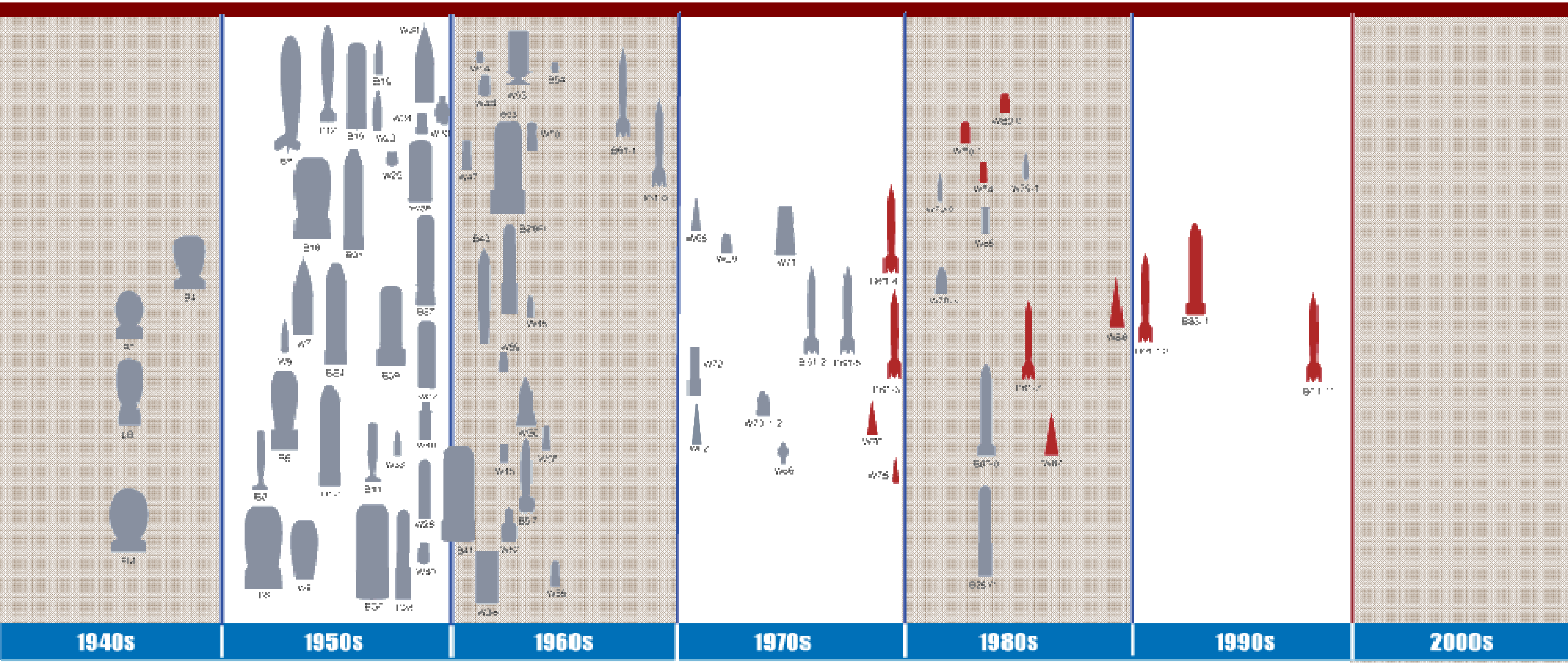




Materials and Process Science

Some Comments on the Challenges of Predictive Simulation

Motivation: Our Aging & Shrinking Nuclear Weapons Stockpile



Retired Weapons

Enduring Stockpile

The cold war is over

The last new weapon was the W88, designed in 1970s

Last U.S. nuclear test was in 1992

Even the budget for conventional testing is much smaller

How do we maintain these aging weapons?

Sandia is not in this alone!

Physics Laboratories,
Responsible for the Physics of Nuclear Explosive Package

- Los Alamos National Laboratories
- Lawrence Livermore National Laboratories

Engineering Laboratory,
Responsible for Weaponization (Arming, Fusing, Firing, Packaging, Use Control, ….)

- Sandia National Laboratories, 2 main sites

Oversight: National Nuclear Security Administration (NNSA), Part of Department of Energy

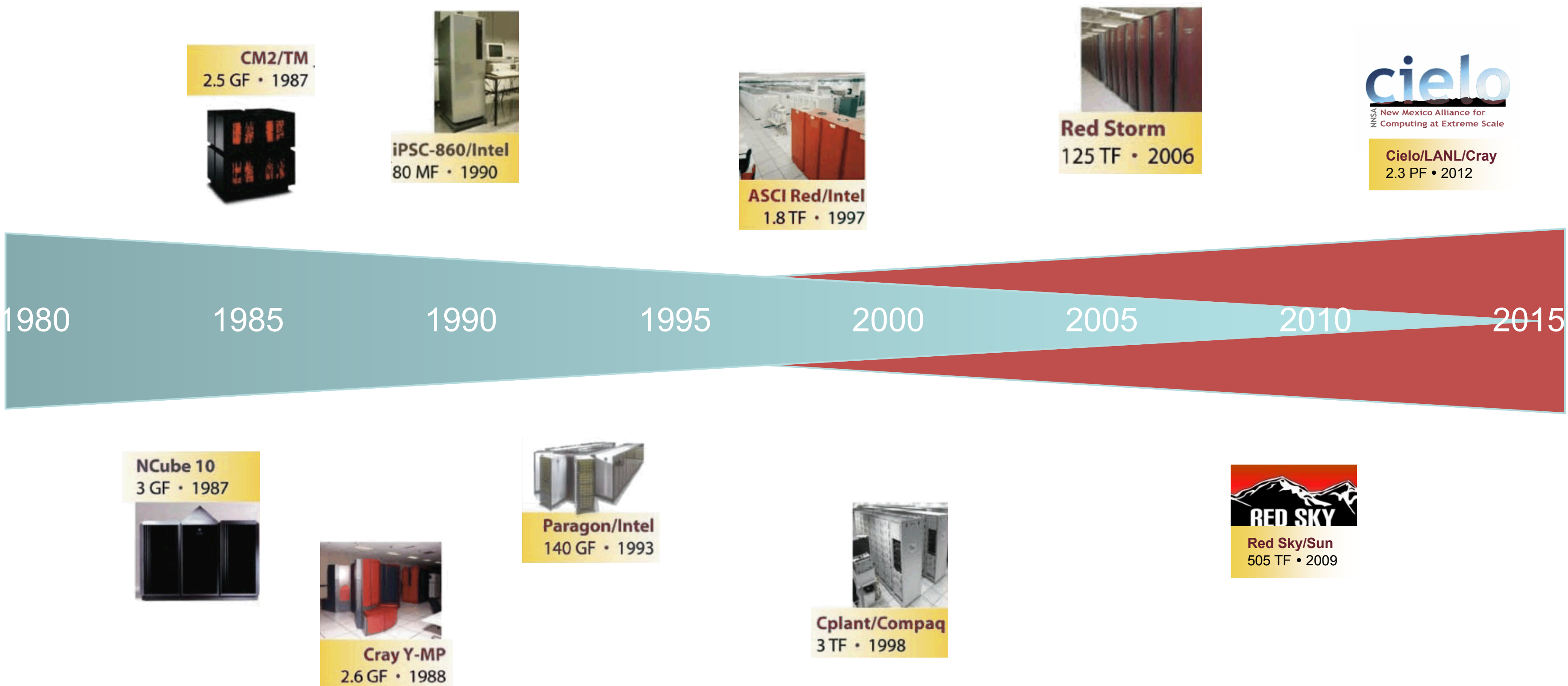
Maintaining a Shrinking Stockpile

- without underground testing,
- with minimal conventional testing
- after most of the designers have retired
  … or died

Major Part of Strategy is to Rely Heavily on Computational Simulation

- massively parallel supercomputers
- all code re-written to employ those machines
- first-principles analysis, where possible

Sandia has a long and distinguished history in massively parallel computing

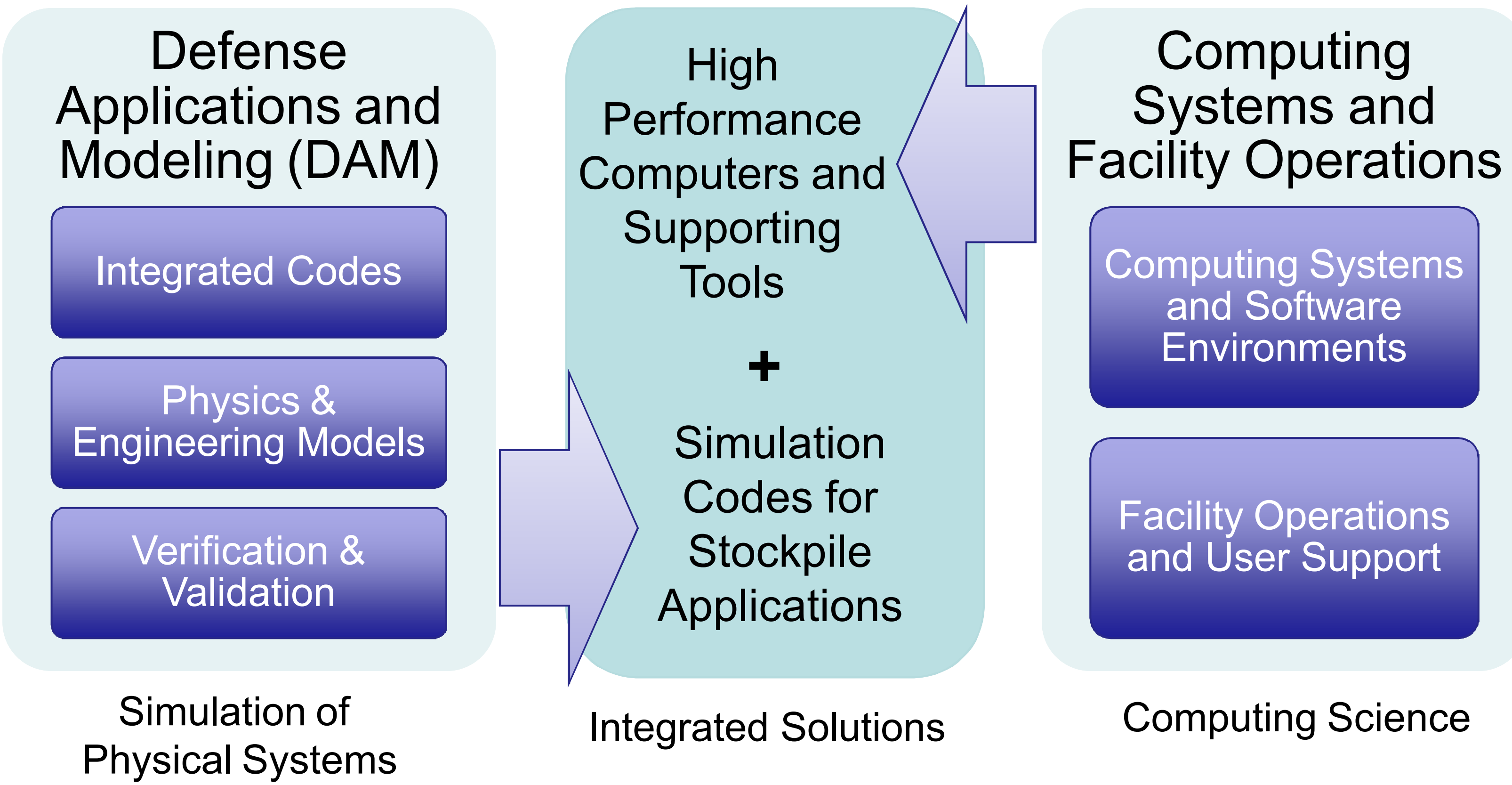


Sandia has made key contributions to computing advances for 25 years

9 R&D100 Awards, 3 Gordon Bell Awards, 3 World Records for MP speed, SC96 Gold Medal, Fernbach Award, Mannheim SuParCup

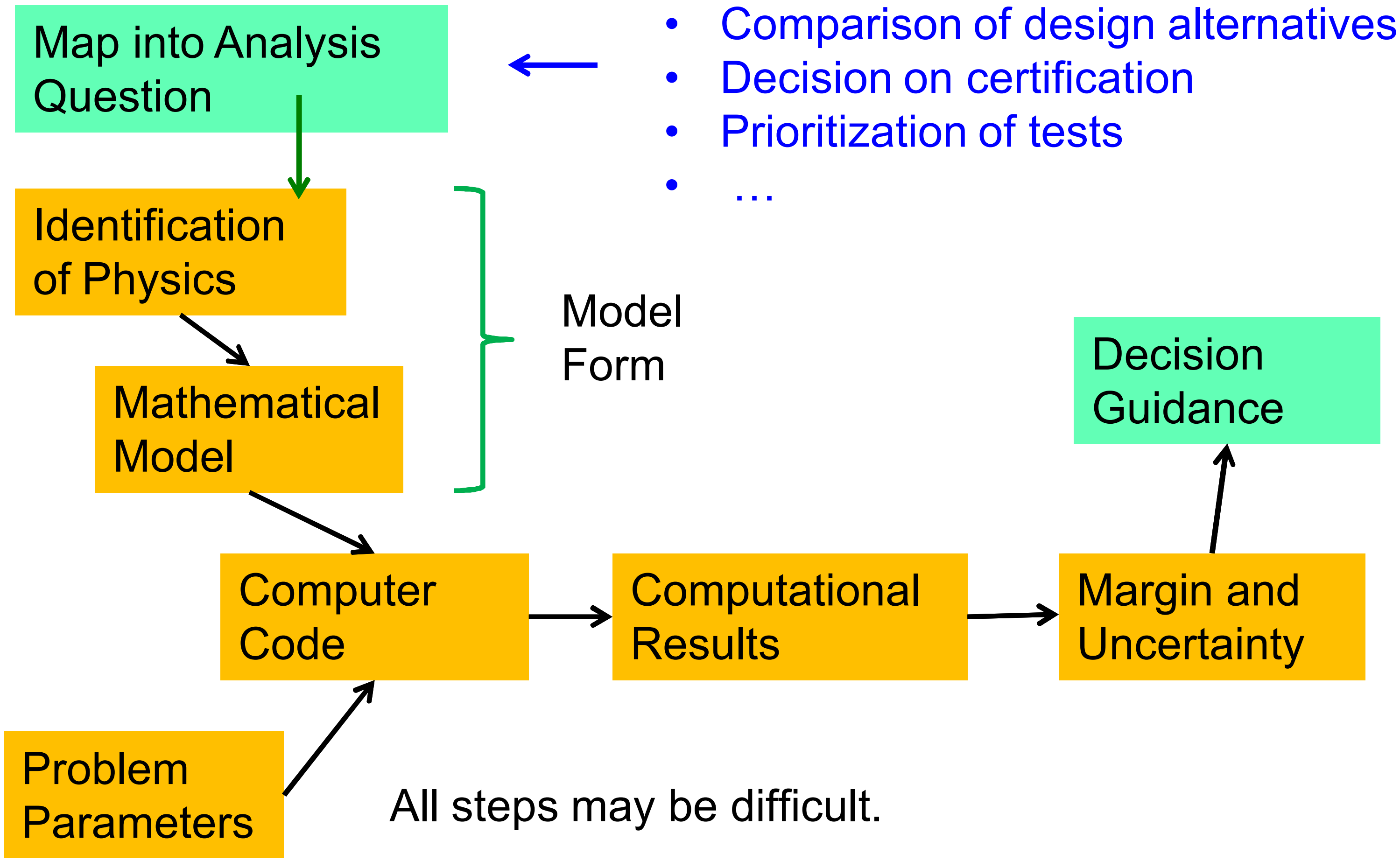
Giga=10^{9}, Tera=10^{12} , Peta=10^{15}

NNSA's
Advanced Simulation and Computing (ASC) Program



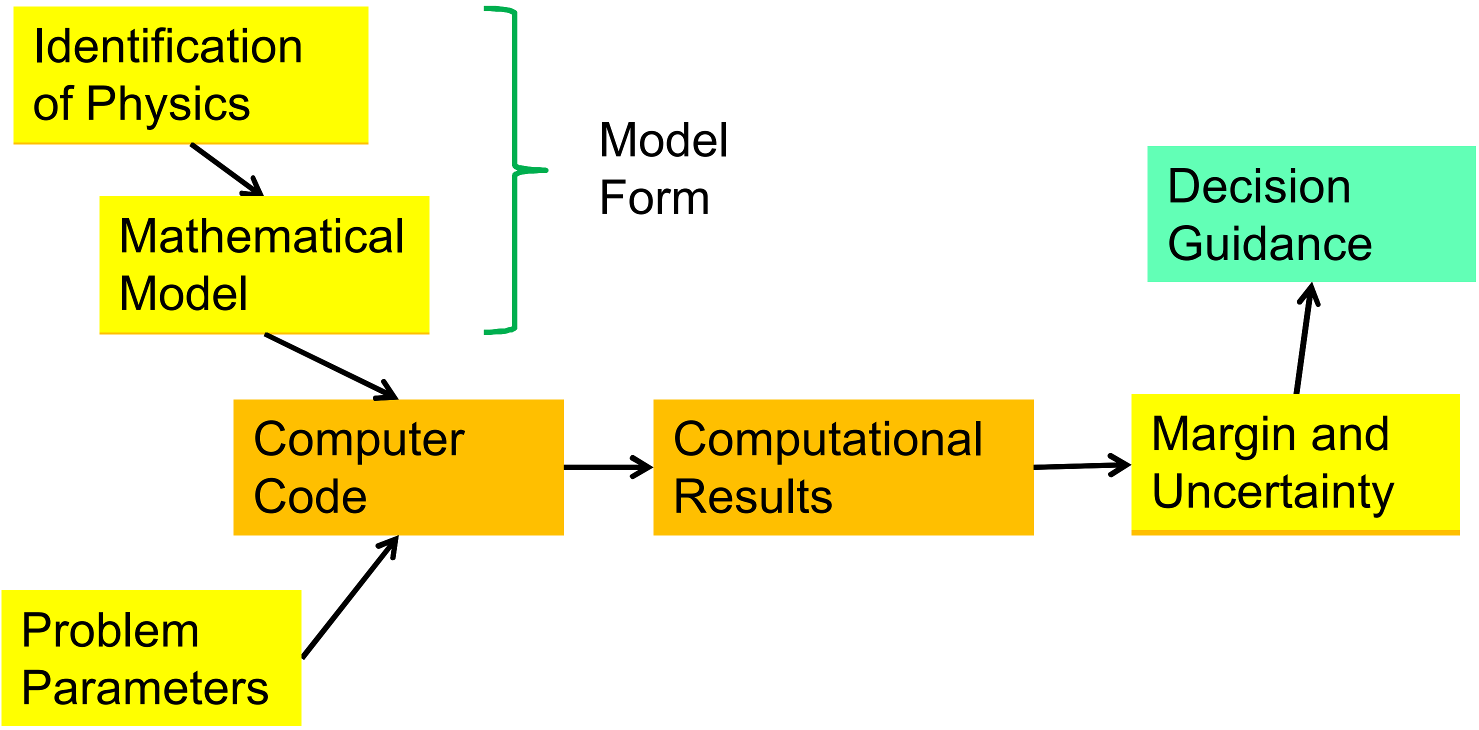
A systematic approach to incorporating high-performance computing into engineering analysis

The Predictive Process: Everything begins with a decision that needs guidance

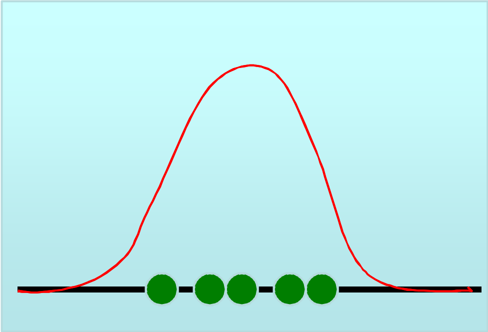


Three of the more Subtle Components

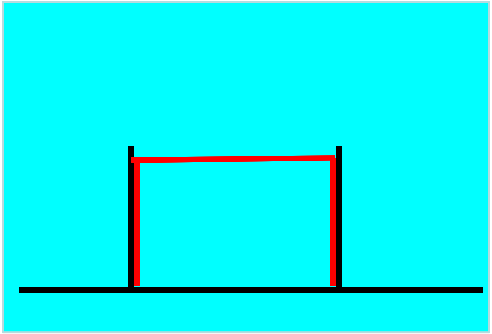
Analysis Question



Problem Parameters: There is Never Enough Data



Approach 1: Sparse Data
Fit sparse data to a standard distribution – usually Gaussian



Approach 2: No Data, Expert Opinion
Fit a distribution to the Max and Min of Expert Opinion.
At Sandia, we usually assume a uniform distribution.

There is always uncertainty in parameters and the is also always uncertainty in the nature of that uncertainty.

There is opportunity here!

Problem Parameters: There must be better approaches

There is Data from Multiple Sources

- Direct Measurements
- Indirect Measurements
- Physics-Based Bounds
- …

There must be a mathematically justifiable approach to combining this information into some meaningful probabilistic statements.

There is opportunity here!

Model Form and Model Form Error

- Should this not be EASY?
- Can we not use our super-duper computers and solve everything from First Principles?

- Rigor through “first principles” analysis can be less useful than it appears.

Physics View of Rigorous Analysis

1. Begin with some very plausible and precise mathematical descriptions of nature (postulates & assumptions).
2. Accept a few principles – such as conservation laws.
3. Employ mathematical rigor to deduce conclusions that must follow from general principles and those axioms.
4. From those mathematical conclusions, we obtain insight into the nature of nature.

Engineering is Harder than Physics

What are First Principles?
(to mechanics folk)

- Conservation of Mass
- Conservation of Momentum
- Conservation of Energy
- Objectivity

And

Here comes a strong statement

- All the rest is empiricism or assumption

Example: Navier Stokes Equation

- Conservation of Momentum

$$\rho\left(\frac{\partial v}{\partial t} + v \bullet \nabla v\right) = \nabla \bullet T + f$$

- Conservation of Mass

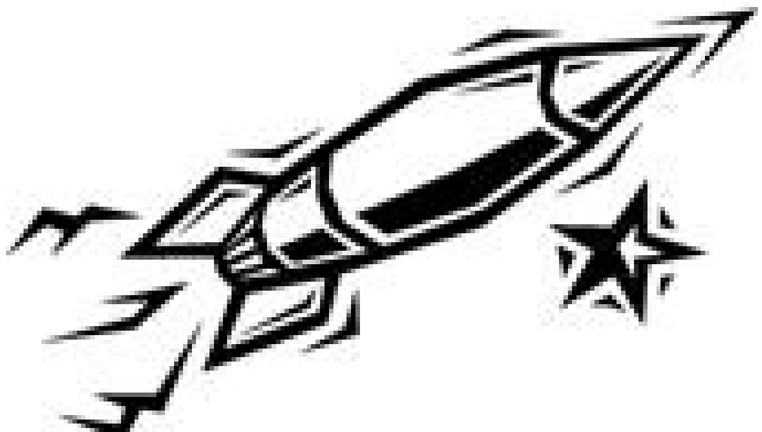
$$\frac{\partial \rho}{\partial t} + \nabla \bullet \left(\rho v\right) = 0$$

- Constitutive Equations – empirical: $T = -pI + T_D$

where $\left(\frac{1}{\beta}\right)\dot{p} = \nabla \bullet v$ **and** $T_D = \frac{\mu}{2}\left(\nabla v + \nabla v^T\right)$

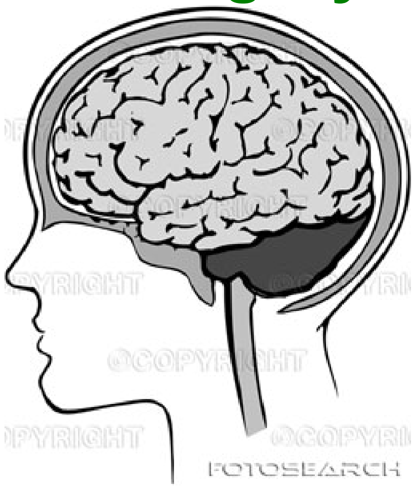
Features of Rocket Science and Brain Surgery

The Hard Engineering Problems are Like Brain Surgery



Rocket Science

- A few fundamental principles (conservation laws).
- A small number of simple approximations (rigid body motion).
- Represented succinctly by a few ODEs
- Competent practitioners produce similar results



Brain Surgery

- Fundamental principles are less helpful
- Huge reliance on empiricism and experience.
- Who the practitioner is makes a tremendous difference in outcome.

Digression into Dissertation Topics

- Carefully chosen
- Three year chunks
- Requiring brains rather than experience
- Anticipated to be Tractable

Sounds like Rocket Science

Choose your dissertation advisor carefully.

Kinds of Idealizations We Like to Make to Make Problems Tractable

- Deterministic wherever plausible
- When there is variability, all distributions are uniform or Gaussian
- All boundary conditions are uniform, periodic, …
- Linearity wherever plausible
- Elastic Materials – at worst elastic-plastic
- Physics maps nicely from one scale to another

Much of Engineering Often Looks More Like Brain Surgery than Rocket Science

- Function of complex systems. (Such as systems that jam or have backlash.)
- Failure of complex structures. Things that fail a little at a time.
- Anything with intrinsic and unpredictable variability.
- Anything that involves wear and must still function.
- Mechanics of salt (SPR, WIPP)
- Stress corrosion cracking
- Engineering Fracture
- Predictive Structural Dynamics

Messy problems are messy in both analysis and design.

More Features that Exacerbate Model-Form Error

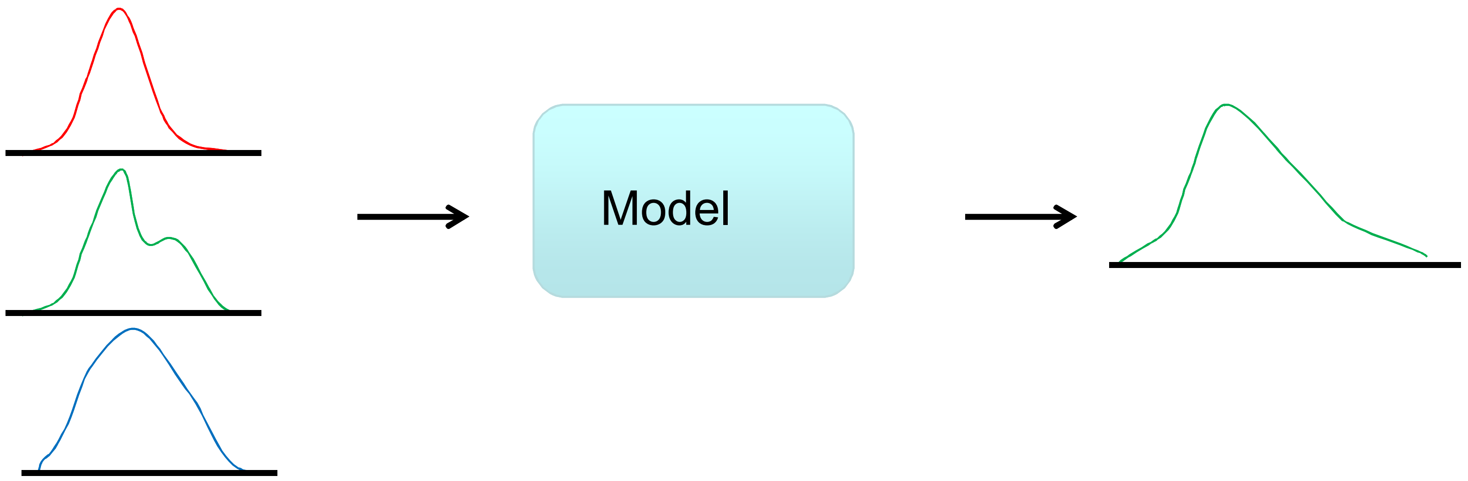
- Simultaneously multi-length-scale, multi-time-scale, multi-physics (perhaps involving complex stress balances, chemistry, diffusion and metallurgy).
- Experts in the field disagree about fundamental processes
- Though some of the processes can be modeled at the atomistic level, these efforts have yet to result in a rigorous constitutive model at the continuum level.

For such problems, one must make too many simplifying assumptions to have confidence *a priori* about any of them being correct.

We are reminded of the need to be appreciative of experimentalists.

There are tremendous research opportunities

- How to recognize clues to model form error
- How to test model form against reality
- How to quantify error and uncertainty due to model form and to accommodate into prediction uncertainty



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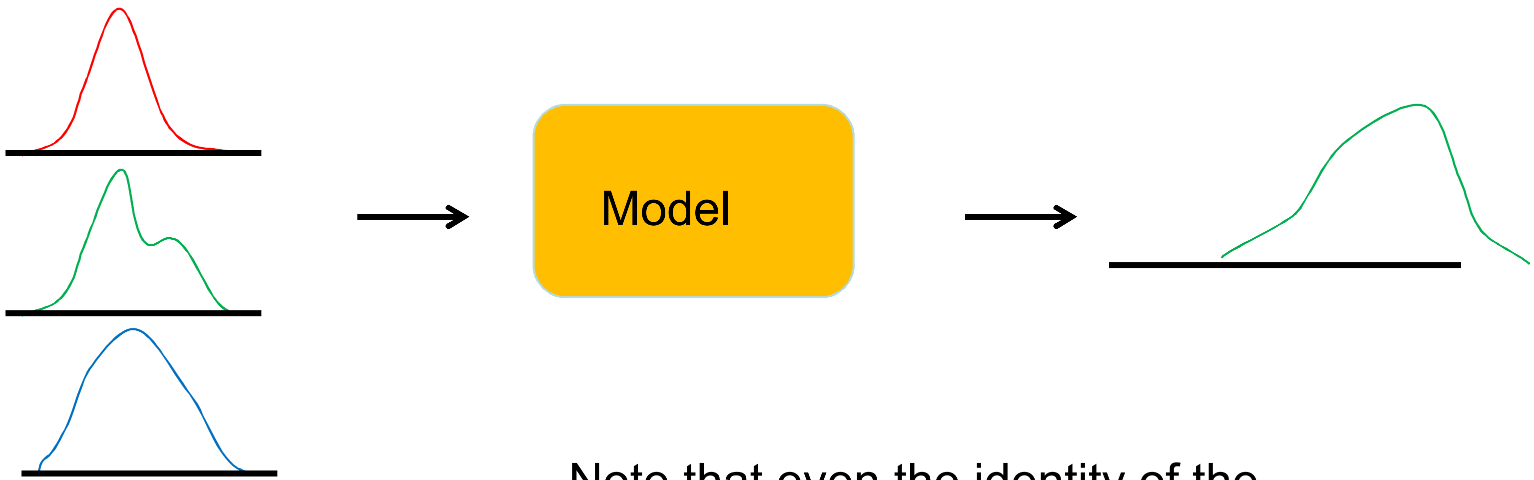


Note that even the identity of the parameters depend on model form.

Quantification of Margin and Uncertainty

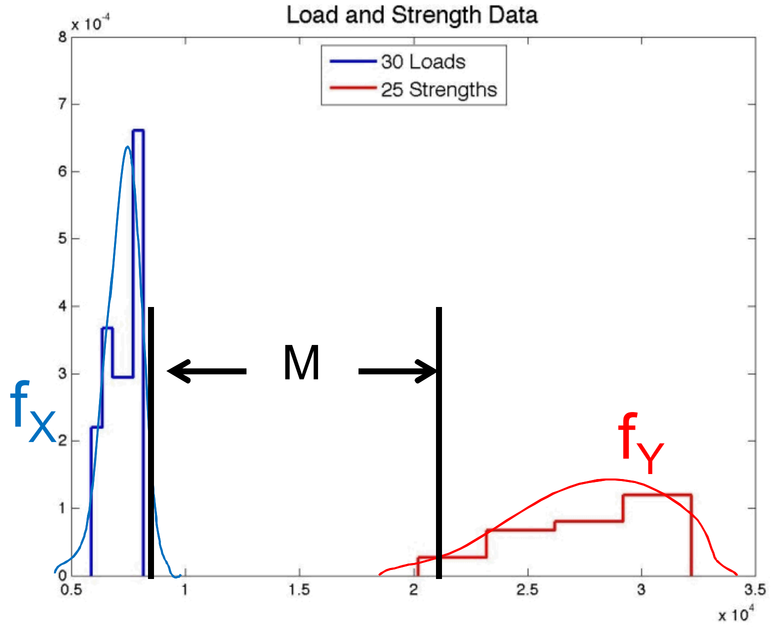
- Again, we face sparse data and major decisions
- It is an unfortunate irony of life that
  1. The less reliable a design is, the easier it is to make meaningful estimates for probability of failure.
  2. The more reliable it is, the less meaningful are efforts to quantify that reliability.

If a part has filed 50 times out of 200, then is probability of failure in the future is 25% per use

If the part has not failed yet, what is the probability of failure in future use?

Consider the usual case of conservative design and sparse simulation or experimental data

- 30 Load Predictions
- 25 Strength Estimates



How do we define Margin?

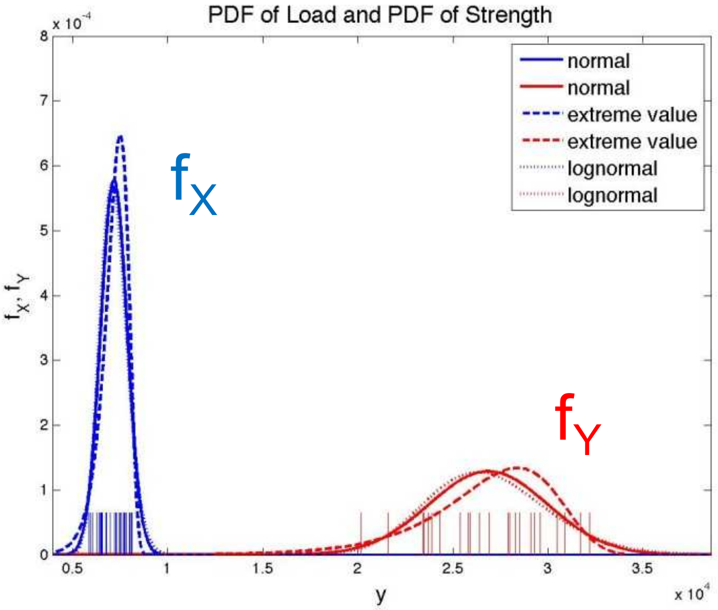
Usual Process:

Fit Distributions to the Data and Calculate Margin from those.

How to Define Margin? It should connect to the Probability of Failure.

Does large margin mean that the probability of failure (PoF) is small?

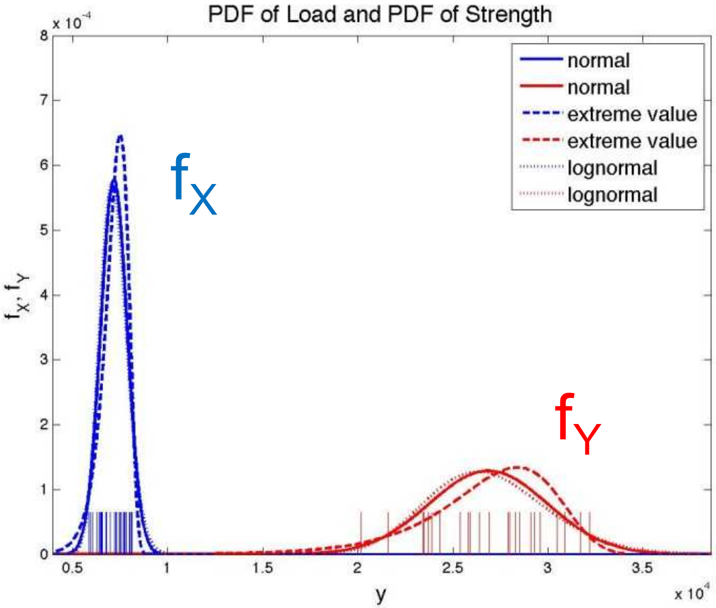
$$P_F = \int_{x>y} f_X(x)\, f_Y(y)\, dx\, dy = \int_{-\infty}^{\infty} f_Y(y) \left(\int_y^{\infty} f_X(x) dx \right) dy$$



What is the significance of which distribution form we choose?

Margin and Uncertainty

- What is the significance of which distribution form we choose?
- A Lot!



Load	Strength	PoF
extreme value	lognormal	3.7e-24
normal	lognormal	1.2e-20
lognormal	lognormal	5.8e-18
extreme value	normal	2.3e-10
normal	normal	2.8e-10
lognormal	normal	3.5e-10
normal	extreme value	4.2e-04
extreme value	extreme value	4.2e-04
lognormal	extreme value	4.2e-04

- There is opportunity here too!

Summary

- Real engineering problems are much more difficult than rocket science
- Sandia and our sister laboratories address these issues of predictive simulation as well as anybody.
- But there is still a lot of fertile room for research.

Backup Slides

Historic Relationships from the Cold War Days

Sandia is and Engineering Laboratory and we partner with two Physics Laboratories, Los Alamos National Laboratory and Lawrence Livermore National Laboratory.

The physics laboratories deal with nuclear physics
Sandia deals with everything else – arming, fusing, firing, surety, safety, …