Optimization Challenges and Opportunities in the ASCI Program

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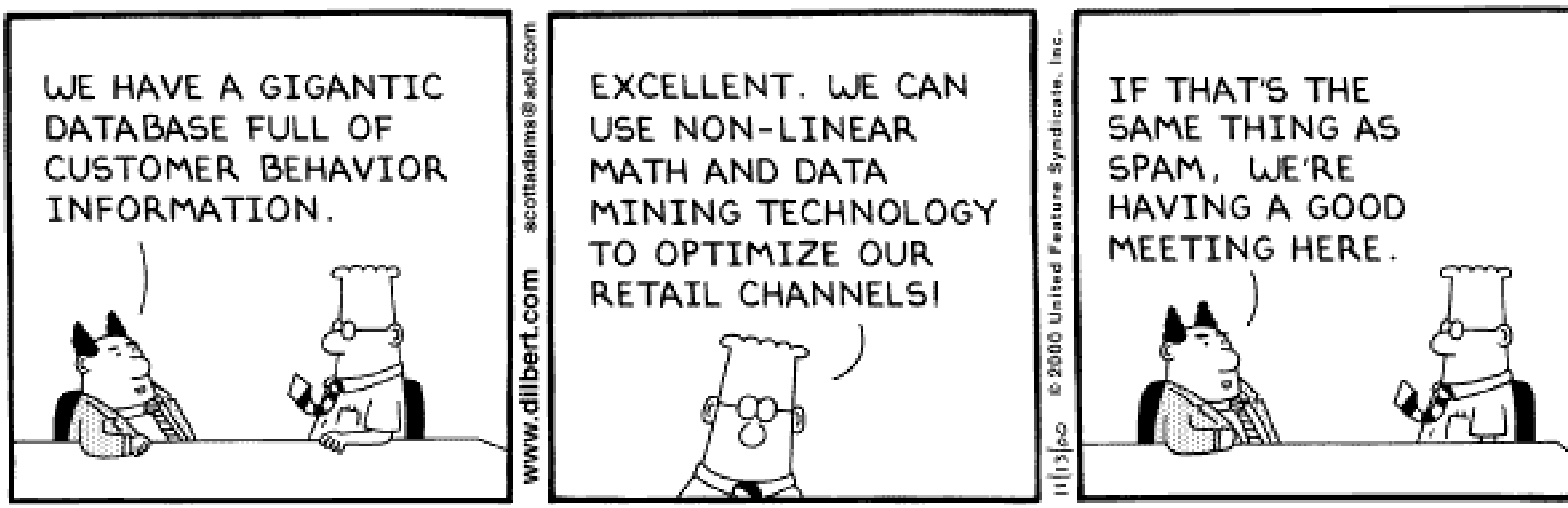
Corporate view of optimization



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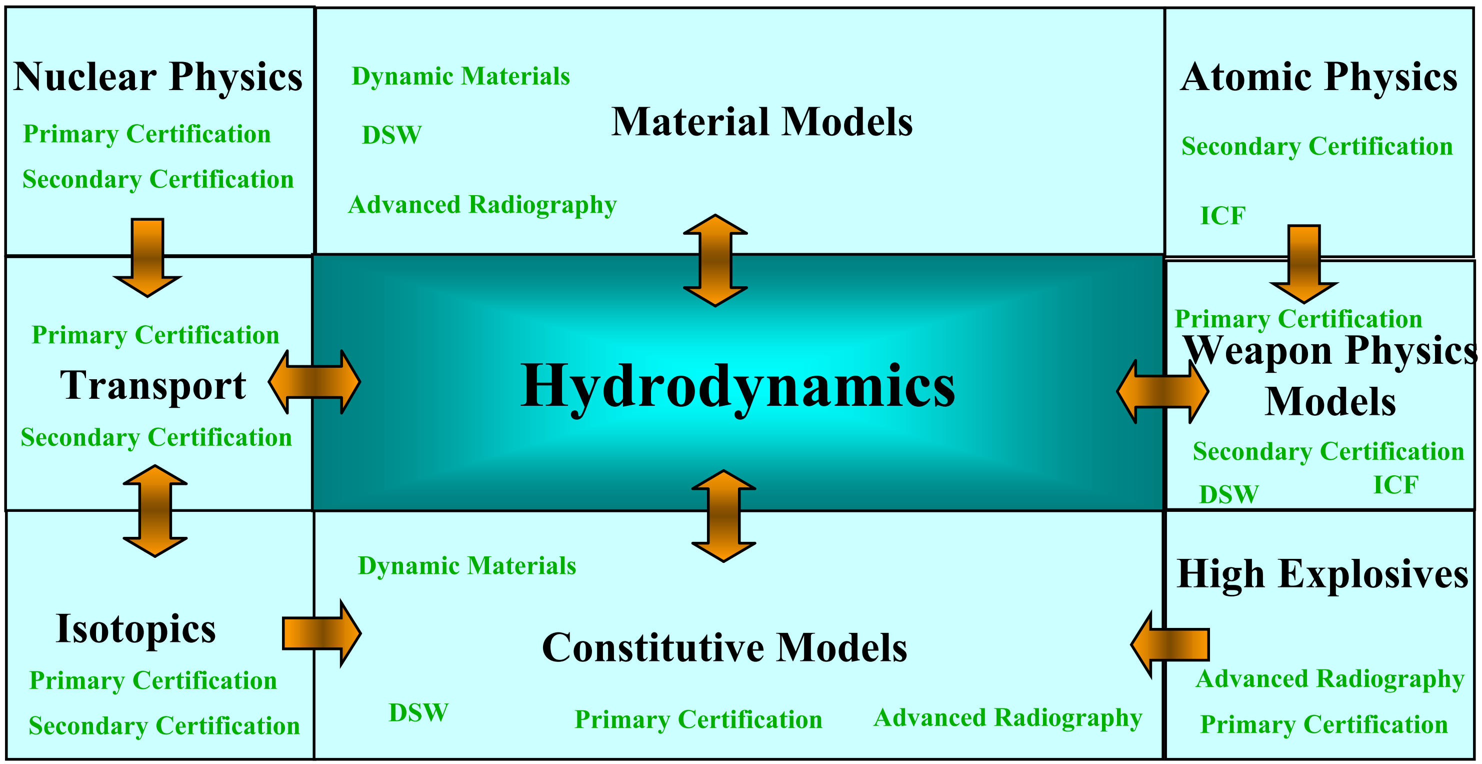
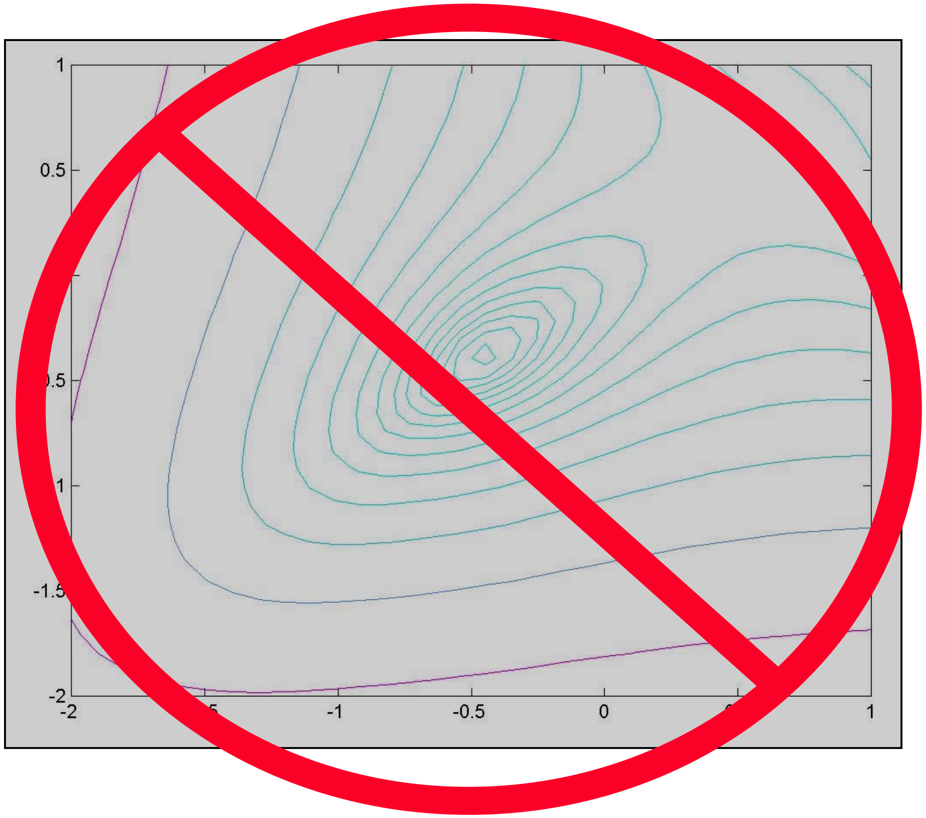
ASCI is predicated on the development of advanced, multi-physics models that will be used for predictive simulation



Elements of a Simulation Application

Optimization algorithms often assume many features



- Smooth function
- Functions accurate to machine precision
- Cheap functions
- Gradients and Hessians readily available

That's not an optimization problem !

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These are optimization problems

- **A recent (classified) simulation run took about 6 weeks on 2000 processors**
  - on a single processor, it would have taken over 200 years if the problem could fit into memory
  - the same run produced 11 terabytes of output
- **Sandia's Applications Milepost calculations featured an optimization problem**
  - minimize mass, subject to safety margins on stresses and/or accelerations in all FE blocks.
  - run-time on ASCI-Red was 4 days using 2560 processors
  - generated 250 GB results

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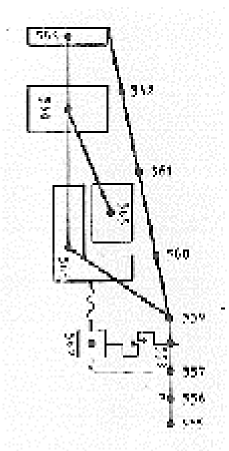
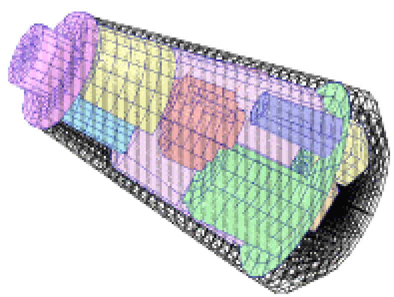
Advances in computer technologies have allowed higher levels of structural dynamics modeling sophistication

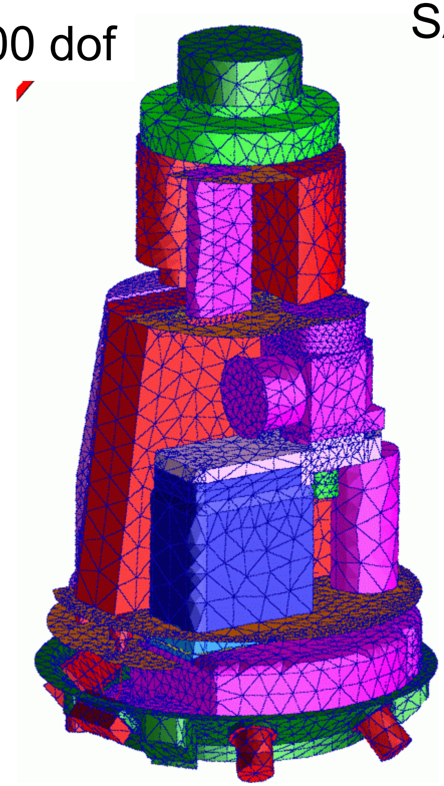


10 years ago:
Shellshock 2D
NASTRAN
200 dof



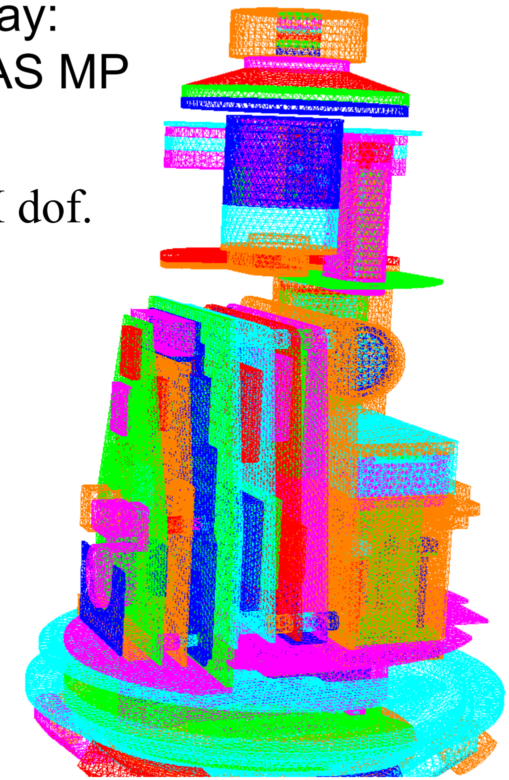
Recent Past:
NASTRAN
30,000 dof

800,000 dof



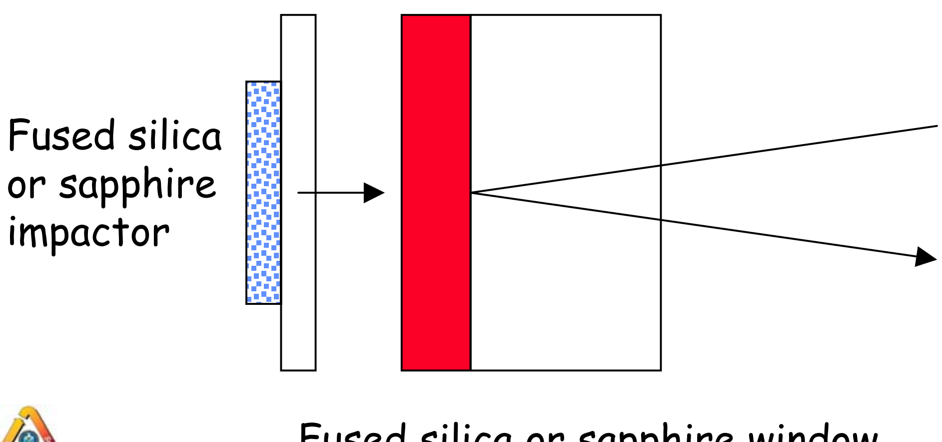
Today:
SALINAS MP

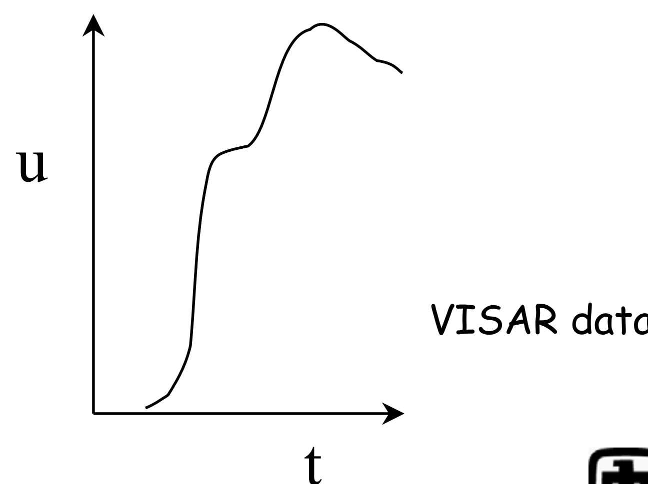
>10M dof.



Parameter Optimization of PZT 95/5

- Focuses on determining parameters for the PZT material model in ALEGRA
- Uses data from uniaxial strain impact experiments of unpoled PZT
- Model handles phase transition, pore collapse, domain distribution, plasticity



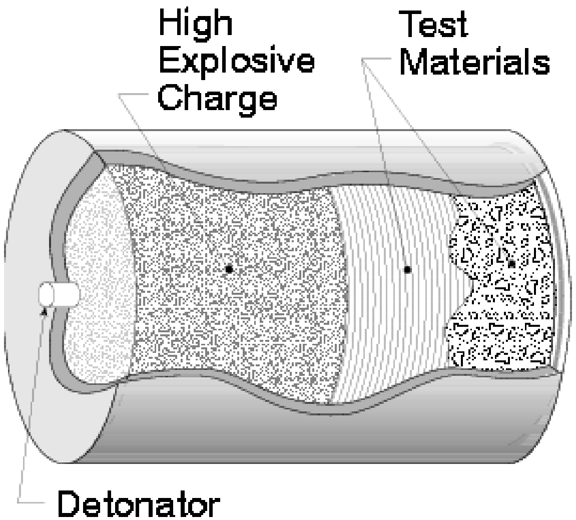


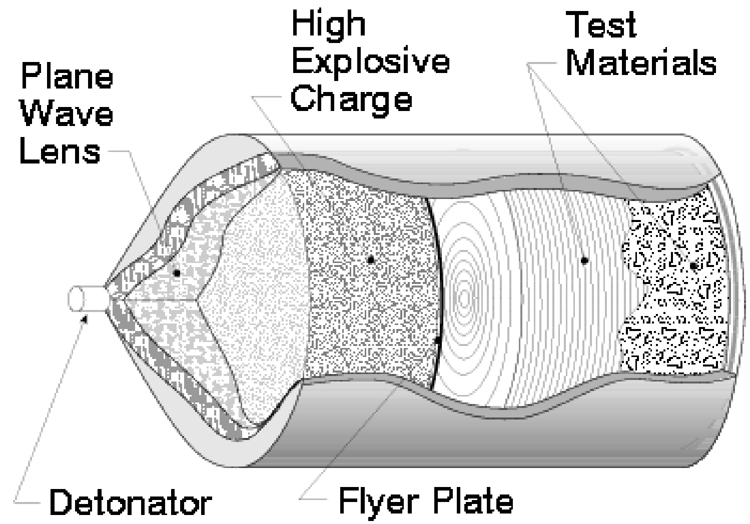
The labs are not the only ones interested in these problems (Caltech Alliance Level 1)

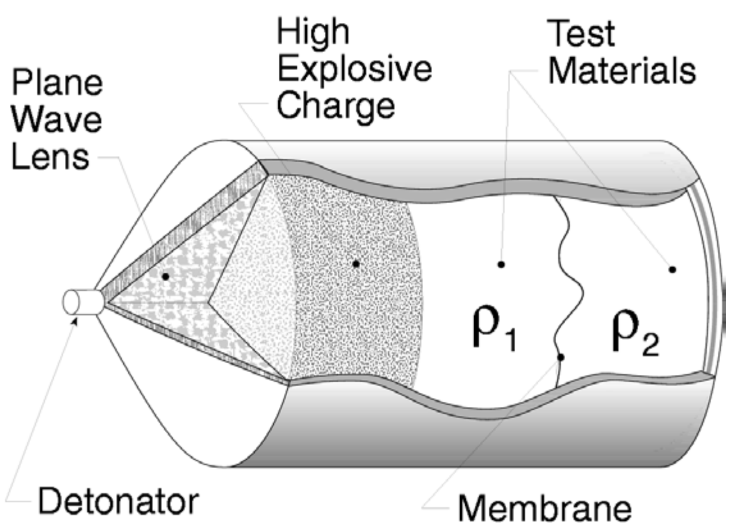
- **Shock compression science is now well-established**
  - solid mechanics
  - geophysics
  - materials science
  - computation
  - technological applications
- **Many fundamental questions remain:**
  - what is the detailed response of materials under shock loading?
  - need to develop predictive capability
  - need to develop better theories

Experiments normally help fill in missing pieces in models – we want to do the reverse

The Virtual Test Facility





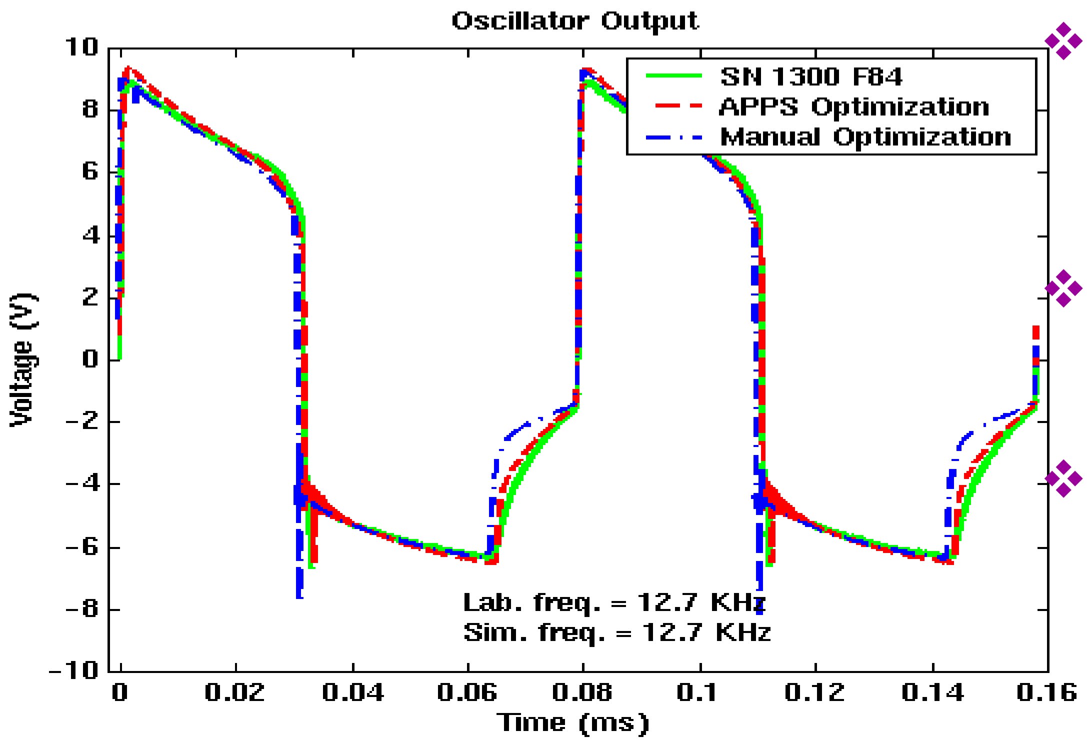


My short list of challenges in optimization for ASCI problems

- We must be able to handle very expensive function evaluations
- We need to deal robustly with variable digits of accuracy
- We must assume that gradient information is not (usually) available
- Algorithms must generate iterates that remain feasible
- We must be able to handle uncertainty in the parameters

Some approaches that we're working on to address these challenges …

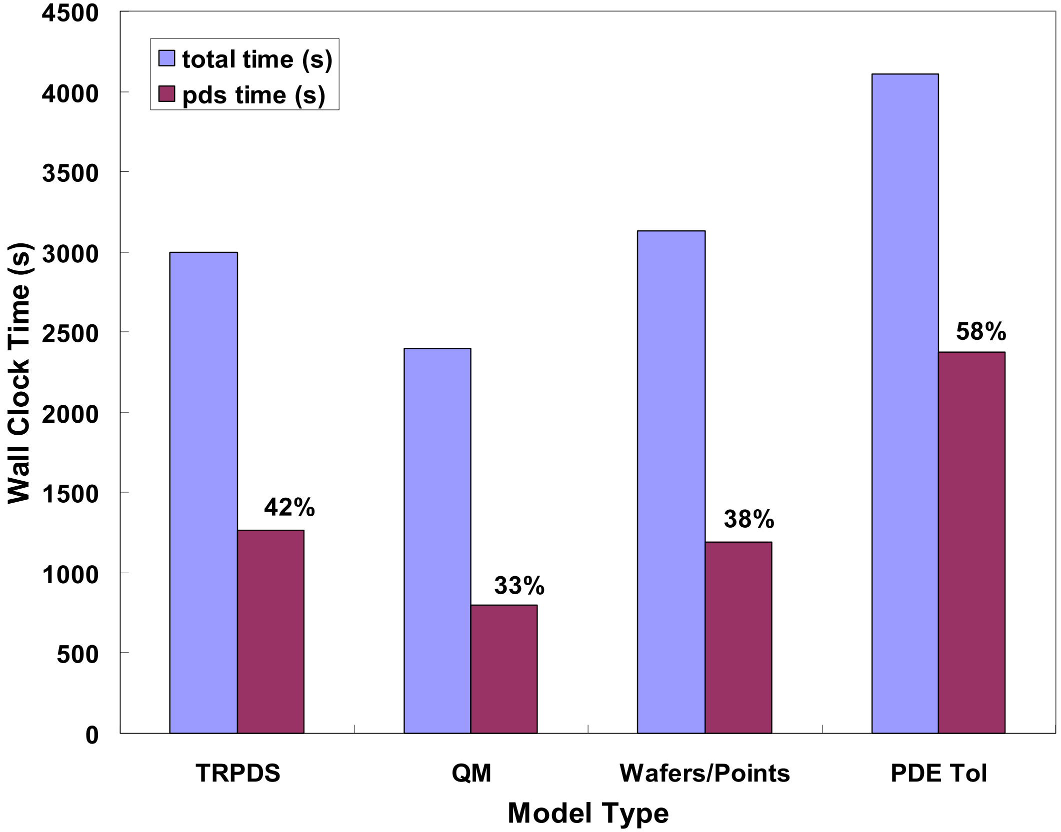
Asynchronous Parallel Pattern Search (APPS) for Nonlinear Optimization



- pattern search optimizes by comparing function values at intelligently chosen points in space
- asynchrony ideal for heterogeneous computing environments
- provides high degree of fault tolerance with very little overhead

For an electrical circuit reliability parameter ID problem, we obtained a better solution and reduced the solution time by a factor of 20.

Trust Region - Parallel Direct Search (TRPDS) for Nonlinear Optimization



Preliminary results from an optimal control problem demonstrate the importance of balancing a good approximation model with the cost of its evaluation.

- uses direct search as the inner iteration of a Newton (i.e., gradient-based) algorithm
- use of computationally inexpensive models reduces cost of inner iteration
- multilevel parallelism can reduce cost of outer iteration
- available as part of the OPT++ software package

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Sequential Approximation Optimization (SAO) Strategy Development

- uses a series of surrogate (approximation) models during optimization
- surrogates eliminate nonsmooth trends in the objective and constraint function data
- inherent parallelism in the data sampling needed to build the surrogates
- provable convergence to a local minimum under mild restrictions

Computer Science issues in ASCI:
Programming methodologies

Balance is important

- **Methodologies and tools for integrating software modules**
  - to produce end-to-end simulations
  - for facilitating comparison and substitution of computational models, algorithms
  - for adding models for more faithful simulation
  - to include informational modules (visualization, I/O, storage and retrieval)

Optimization Framework R&D Activities

- **DAKOTA - Design and Analysis Kit for OpTimizAtion**
  - optimization methods (SAO, PICO, OPT++, SGOPT, APPSPACK)
  - multilevel parallel execution of analysis codes for optimization
  - parameter identification and sensitivity analysis methods
- **IDEA - Integrated Design, Exploration, and Analysis**
  - emphasis on loosely-coupled distributed computing
  - data sampling and surface fitting methods
  - parameter screening, data analysis, main effects
  - XML-based file parsing and input file GUI development

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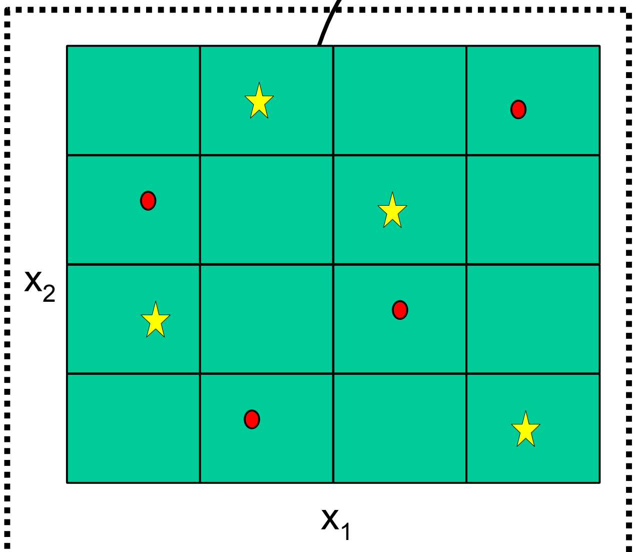
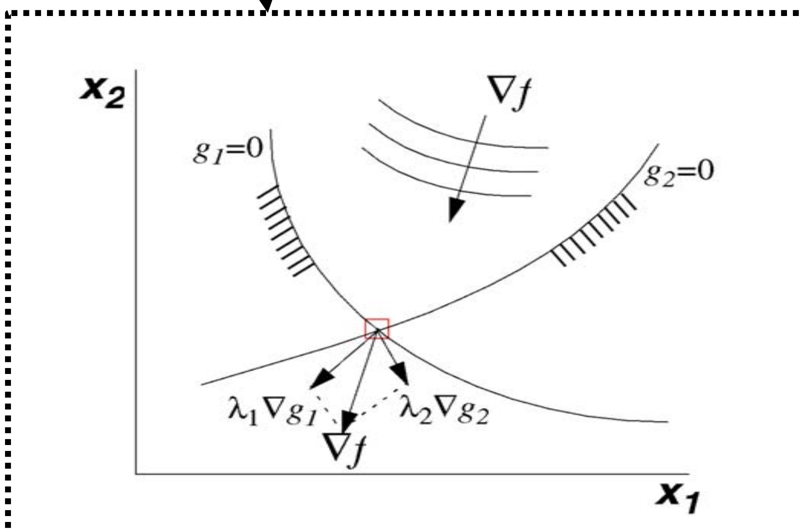
Many different optimization approaches were used for Applications Milepost

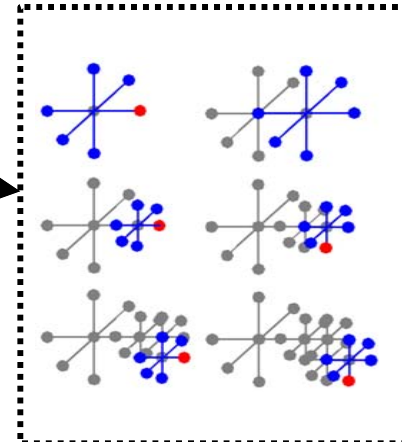
Dakota Framework



Latin Hypercube Sampling



Gradient-based Opt.



Opt. Via Pattern Search

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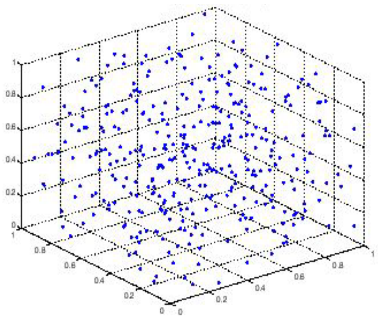
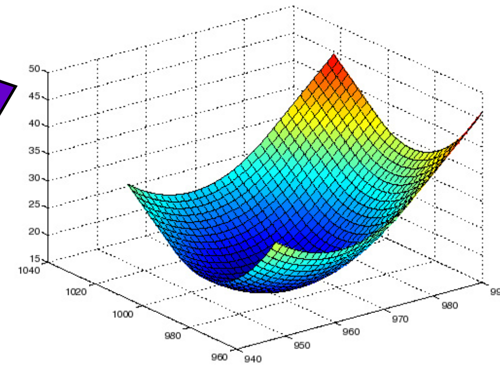
IDEA - A system to integrate a diverse set of design, exploration and analysis tools

Exploration: Design of computer experiment



Model building

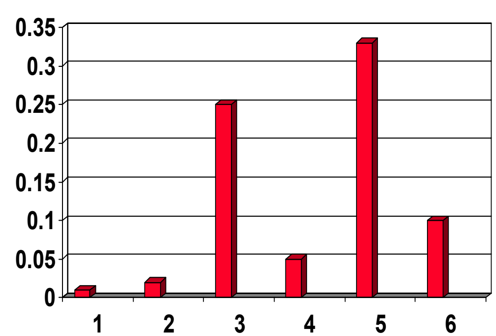


Screening

Design of new experiment

Analysis

Main Effects



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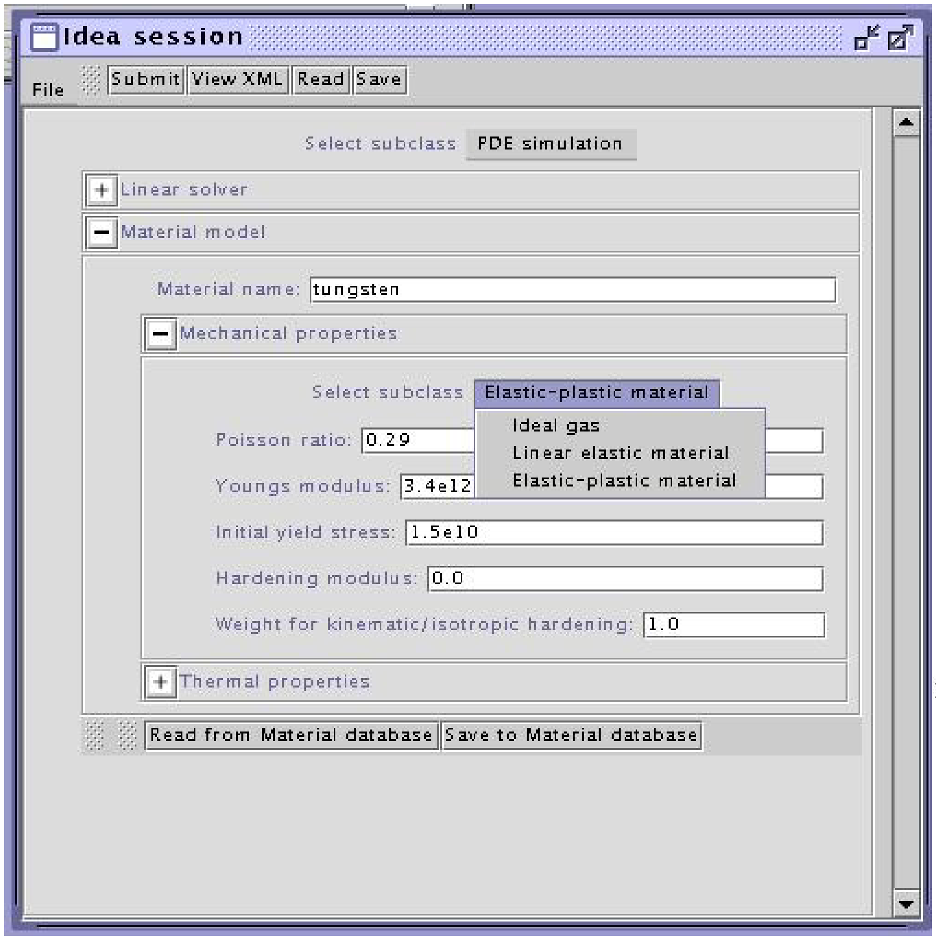
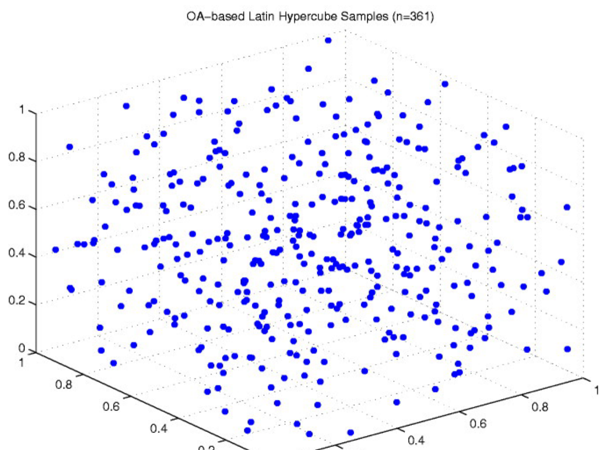
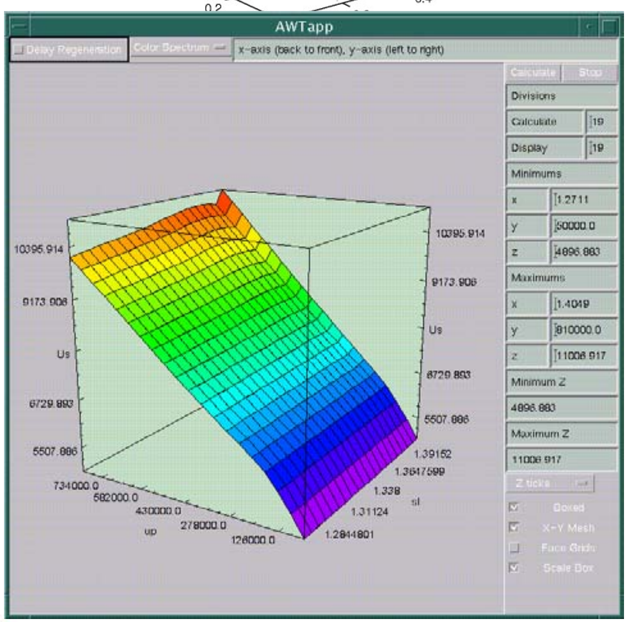
IDEA sessions are controlled from the desktop but can be distributed over many platforms



- General GUI driven by XML specification allows rapid production of new GUIs (MAUI)
- All processes can be started and controlled from the desktop
- Security accomplished by GSF

DDACE can generate random samples for determining sensitivities of parameters





- Wide variety of underlying distributions and sampling techniques
- Techniques to determine main effects
- Figure depicts results from an Alegra calculation used to estimate the sensitivity of shock velocity to the material model parameters
- Summary statistics and response surfaces can also be produced

Slope vs. shock velocity using Latin hypercube sampling

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Many areas open for collaboration (soon to be published ASCI Technology Prospectus)

Road Map
Scalable Solvers

Functional Area	1999	2000	2001	2002	2003	2004	2005
Linear Solvers	Linear solver package for 1B structured mesh Linear solver package for 100M unstructured mesh	Parallel algebraic Multigrid (MG) codes		Eigensolver package for systems with 30M DOF Scalable algebraic MG for 1B unstructured mesh		Eigensolver package for systems with 300M DOF Linear solver package for 10B unstructured mesh systems	
Nonlinear Solvers/ Optimization	Parallel optimization toolkit for model-based design		Nonlinear optimization library for 8000+ processors		Constrained optimization toolkit for systems with 100M DOF		Optimization under uncertainty toolkit

Levels of Difficulty ACCOMPLISHED PLANNED BARRIER HURDLE

Some opportunities in optimization for ASCI problems

- Algorithms for handling multiple levels of fidelity in the models
- New and better derivative-free optimization methods
- Robust interior point methods
- Techniques for handling uncertainty in the design parameters and models
- Robust, reliable, and easy-to-use optimization toolkits

The End