Optimization Challenges and Opportunities in the ASCI Program

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## Acknowledgments

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<th>Sandia</th>
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Corporate view of optimization
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!
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
Advances in computer technologies have allowed higher levels of structural dynamics modeling sophistication

Recent Past:
- Shellshock 2D
- NASTRAN
  - 30,000 dof

Today:
- SALINAS MP
  - >10M dof.

10 years ago:
- NASTRAN
  - 200 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

Fused silica or sapphire impactor

Fused silica or sapphire window

VISAR data

u

t
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
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

- 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

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

- 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)

Balance is important
Optimization Framework
R&D Activities

❖ **DAKOTA** - **D**esign and **A**nalys**i**s **K**it for **O**p**T**imiz**A**tion
  - optimization methods (SAO, PICO, OPT++, SGOPT, APPSPACK)
  - multilevel parallel execution of analysis codes for optimization
  - parameter identification and sensitivity analysis methods

❖ **IDEA** - **I**ntegrated **D**esign, **E**xploration, and **A**nalys**i**s
  - 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
Many different optimization approaches were used for Applications Milepost

**Dakota Framework**

- Gradient-based Opt.
- Opt. Via Pattern Search
- Latin Hypercube Sampling

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

Exploration: Design of computer experiment

Model building

Screening

Analysis
  Main Effects

Design of new experiment
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
Many areas open for collaboration (soon to be published ASCI Technology Prospectus)

## Road Map

### Scalable Solvers

<table>
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<tr>
<th>Functional Area</th>
<th>1999</th>
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<td>Linear Solvers</td>
<td>Linear solver package for 1B structured mesh</td>
<td>Linear solver package for 100M unstructured mesh</td>
<td>Parallel algebraic Multigrid (MG) codes</td>
<td>Eigensolver package for systems with 30M DOF</td>
<td>Scalable algebraic MG for 1B unstructured mesh</td>
<td>Eigensolver package for systems with 300M DOF</td>
<td>Linear solver package for 10B unstructured mesh systems</td>
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<td>Nonlinear Solvers/Optimization</td>
<td>Parallel optimization toolkit for model-based design</td>
<td>Nonlinear optimization library for 8000+ processors</td>
<td>Constrained optimization toolkit for systems with 100M DOF</td>
<td>Optimization under uncertainty toolkit</td>
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**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