A Survey of Optimization Research at Sandia National Laboratories

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Optimization Applications at Sandia

- Treaty verification (nonproliferation)
- Energy
- Weapons manufacturing
  - Equipment and material reliability
  - Optimal design
  - Agile manufacturing
- Environment (geophysical inverse modeling)
- CBW defense (counter proliferation)
- Pulsed power (weapons effects and simulation)
- Agriculture (food safety)
- Civilian mine detection
- Materials and Molecular Biology (protein folding and micelle self-assembly)

Algorithmic Themes

Nonlinear Optimization

Optimization methods that refine solutions to computationally expensive engineering science problems.

Global Optimization

Optimization methods that search for the best possible solution to computationally inexpensive "black box" problems.

Combinatorial Optimization

Optimization methods that develop problem-specific methods to discrete problems for which the combinatorial structure can be studied.

Nonlinear Optimization

Algorithmic Issues

- How do we minimize the number of function evaluations needed to find a local optimum?
- How do we optimize functions with inexact or inaccurate function evaluations?
- How do we optimize nondifferentiable functions?
- How do we optimize large-scale problems with many constraints?

Nonlinear Optimization Research

OPT++

- J. Meza, T. Plantega
- A C++ library of nonlinear optimizers and pattern search methods.
- Optimization algorithms for computationally expensive engineering science problems.

DAKOTA

- M. Eldred, et al
- An optimization toolkit that provides an interface to several optimization packages
- Facilitates optimization of engineering science problems.

Miscellaneous

- W. Hart: Algorithmic development of randomized pattern search methods. W. Hart
- F. Peter: Development of a visual BASIC interface that allows interactive application of MATLAB optimization tools.

Applications

Die-Design Optimization.
W. Witkowski, K. Chen, R. Schunk

Estimation of Thermal Conductivity from Transient Temperature Measurements.
B. Blackwell, M. Eldred, R. Hogan

Optimization of CVD Reactor Design using Parallel Reacting Flow Simulation.
A. Salinger, S. Hutchinson, W. Hart

Optimal Design of Chemical Vapor Deposition Reactors
C. Moen, J. Meza, T. Plantega

Optimization in Time-Domain Electromagnetic Simulations.
M. Pasik

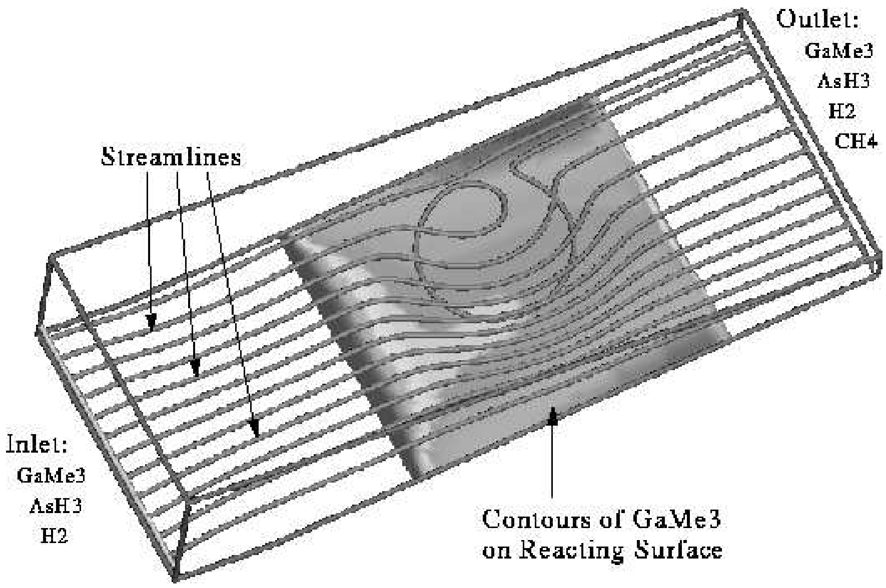
Analysis Driven Mechanical Redesign
R. Robinson

Worst-Case Fire Scenarios for Safing Devices
V. Romero, M. Eldred, W. Hart

Optimization of CVD Reactor Design using Parallel Reacting Flow Simulation.

A. Salinger, S. Hutchinson, W. Hart

Problem: determine best process parameters for a Chemical Vapor Deposition reactor



Method:

- use MPSalsa to simulate a CVD reactor; use DAKOTA to perfom optimization with the inlet concentration, inlet flow rate and rotation rate of reaction disk.
- DAKOTA executes on a workstation and is coordinated with MPSalsa (through shell scripts), which runs on a Paragon (using 256 processors)

Global Optimization

Algorithmic Issues

- How do you balance the need for global search (to insure that the global optimum is found) and local refinement (to generate the global optimum)?
- How do you terminate such that you can guarantee that a global optimum is found?
- How can we compare the performance of optimization algorithms, when we want to find both optimal and near-optimal solutions quickly?
- How should we coordinate a global search among independent optimization processes that are executed in parallel?

Global Optimization Research

SGOPT

- W. Hart, et al
- A C++ library of stochastic global optimization algorithms (especially evolutionary algorithms).
- Research includes evolutionary pattern search algorithms and evolutionary hybrids that use local search.

Miscellaneous

- J. Meza, R. Judson: Developed a parallel genetic algorithm that is included in OPT++.
- J. Wagner, L. Painton, R. Eisler: Application-specific implementations of genetic algorithms.

Applications

Reducing Component Fatigue and Reliability-Based Optimal Circuit Card Layout
David Robinson

Optimization of the Reliability of Macro Systems
Laura Painton

Vibration Isolation
E. Ponslet, M. Eldred

The Use of Parameter Estimation And Optimization to Provide Laser Weld Schedules
R. Eisler

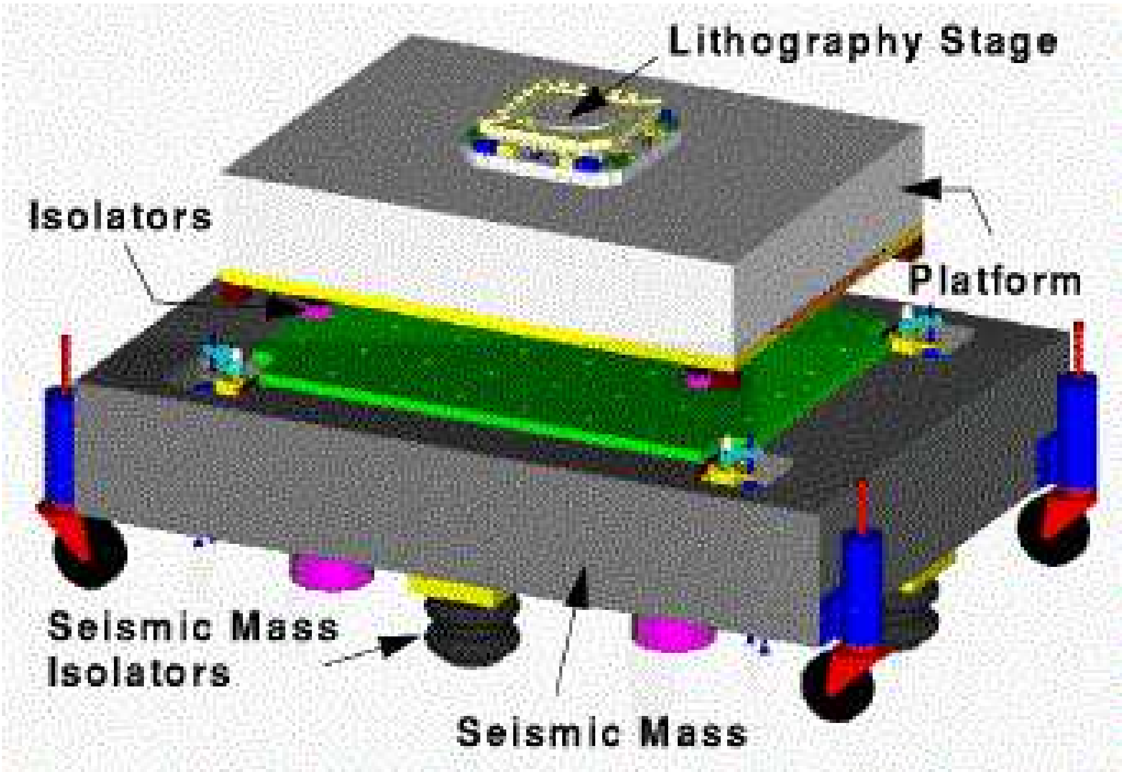
Optimization of Commercial Nuclear Reactor Fuel Management
Mark Lenard

The Optimization of Neural Networks to Perform Remote Sensing
J. Wagner

Advanced Methods for Rational Drug Design
R. Judson

Vibration Isolation

Problem: determine optimal isolator configurations that minimize vibration transmission from an external disturbance



Method of Solution:

- use a genetic algorithm to identify near-optimal isolator configurations, using constraints on isolator placement, table stability and spring load.
- confirm optimization results with a laboratory experiment

Combinatorial Optimization

Problem characteristics:

- The objective function is known and often easily computed
- The parameters are discrete, with a known combinatorial structure
- The number of possible combinations of the parameters is typically exponentially large
- The parameters are often constrained

Practical Considerations:

- Exhaustive search is not possible for even moderately large problems
- Worst-case analyses are sometimes possible to demonstrate algorithmic intractability
- Performance guaranteed approximation algorithms can often be developed for intractable problems

Applications

Performance Guaranteed Methods for Scheduling
C. Phillips

Network Inhibition
C. Phillips

Assembly of DNA Fragments
D. Greenberg, S. Istrail

Optimization in Computational Molecular Biology
W. Hart, S. Istrail

Sequence Design Problems and Drug Design
W. Hart

Optimizing Assembly Sequences and Designs
R. Wilson

An Optimization Model for Agile Manufacturing
E. Kjeldgaard

A MP Mixed-Integer Programming Software Package
C. Phillips, W. Hart, J. Eckstein

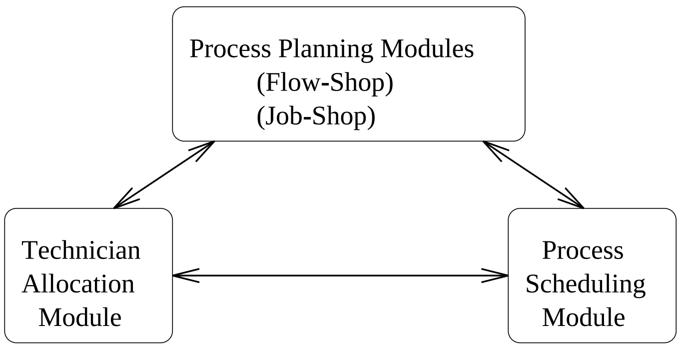
Production Planning for Agile Manufacturing

E. Kjeldgaard

Problem: quickly adapt the plan for production activities in a manufacturing environment.

- Maximize total production subject to resource limitations
- Provide solutions within a reasonable time frame with standard computational resources

Method of Solution: utilize a modular structure to allow for flexibility and to simplify the method of solution required.



Optimization in these modules involves linear programming, fast scheduling heuristics and network optimization.

SNL Optimization Web Sites

The SNL Optimization Page
http://www.cs.sandia.gov/SandiaOpt.html

Survey of Global Optimization Methods
http://www.cs.sandia.gov/opt/survey/

The DAKOTA toolkit
http://endo.sandia.gov/9234/sd_optim_dakota.html

OPT++
http://midway.ca.sandia.gov/ meza/opt++/opt++.html

Bill Hart's Research Projects
http://www.cs.sandia.gov/ wehart/proj/main.html

SGOPT
http://www.cs.sandia.gov/ wehart/proj/sgopt.html