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MATHEMATICAL METHODS IN MATERIAL SCIENCE
AND LARGE SCALE OPTIMIZATION WORKSHOPS

June 1, 1995–November 30, 1996

Final Report

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ABSTRACT

The summer program in Large Scale Optimization concentrated largely on (1) process engineering, aerospace engineering (2) inverse problems and optimal design, and (3) molecular structure and protein folding. The program brought together application people, optimizers and mathematicians with interest in learning about these topics. Three proceedings volumes are being prepared.

The year in Materials Sciences deals with (1) disordered media and percolation, phase transformations, composite materials, microstructure (2) topological and geometric methods as well as statistical mechanics approach to polymers; included were Monte Carlo simulation for polymers (3) miscellaneous other topics such as nonlinear optical material, particulate flow, and thin film. All these activities saw strong interaction among material scientists, mathematicians, physicists and engineers. Approximately 8 Proceedings Volumes are being prepared.

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**MANUSCRIPTS INCLUDED IN THE 3 IMA VOLUMES
FOR LARGE SCALE OPTIMIZATION (July 10-28, 1995 workshop)**

Publisher: Springer-Verlag New York Inc.

Editors: Lorenz T. Biegler, Thomas F. Coleman, Andrew R. Conn, and
Fadil N. Santosa

Large Scale Optimization with Applications, Part I: Optimization in Inverse
Problems and Design

- A multiplier-free, reduced Hessian method for process optimization by Lorenz T. Biegler, Claudia Schmid, and David Ternet
- Experience with a sparse nonlinear programming algorithm by J.T. Betts
- The promise (and reality) of multidisciplinary design optimization by Susan L. Burgee and Layne T. Watson
- Computing sparse Hessian and Jacobian approximations with optimal hereditary properties by Roger Fletcher, Andreas Grothey, and Sven Leyffer
- Deterministic global optimization in design, control, and computational chemistry by Christodoulos A. Floudas
- Large-scale SQP methods for optimization of Navier-Stokes flows by Omar Ghattas and Jai-Hyeong Bark
- Mixed-integer nonlinear programming: a survey of algorithms and applications by Ignacio E. Grossmann and Zdravko Kravanja
- Some aspects of sequential quadratic programming methods by Walter Murray
- Numerical optimal control of parabolic PDEs using DASOPT by Linda Petzold, J. Ben Rosen, Philip E. Gill, Laurent O. Jay, and Kihong Park
- The development of the SQP algorithm for nonlinear programming by R.W.H. Sargent
- Optimization problems in model predictive control by Pierre O.M. Scokaert and James B. Rawlings
- Some recent developments in computational optimal control by Hans Seywald and Renjith R. Kumar
- Large-scale structural design optimization by Ulf Torbjörn Ringertz

Large Scale Optimization with Applications, Part II: Optimal Control and Design

- Need to scan figures to produce ps files. Santosa editor. Space mapping optimization for engineering design by J.W. Bandler, R.M. Biernacki, S.H. Chen, R.H. Hemmers and K. Madsen
- An inverse problem in plasma physics: the identification of the current density profile in a Tokamak by J. Blum and H. Buvat
- Weighting schemes and objective function formulations in sub-surface flow and transport parameter identification via inverse simulation by Martha M. Carey
- Duality for inverse problems in wave propagation by Mark S. Gockenbach and William Symes
- Piecewise differentiable minimization algorithms for ill-posed inverse problems by Yuying Li
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- Design of 3d-reflectors for near field and far field problems by Andreas Neubauer
- Optimal die shape and ram velocity design for metal forging by Linda D. Smith, Jordan M. Berg, and James C. Malas III
- Eigenvalues in optimum structural design by Ulf Torbjörn Ringertz
- Optimization issues in ocean acoustics by A. Tolstoy
- Gradient methods in inverse acoustic and electromagnetic scattering by P.M. Van Den Berg and R.E. Kleinman
- Atmospheric data assimilation based on the reduced Hessian successive quadratic programming algorithm by Y.F. Xie

Large Scale Optimization with Applications, Part III: Molecular Structure and Optimization

- CGU: An Algorithm for Molecular Structure Prediction by K.A. Dill, A.T. Phillips, and J.B. Rosen

- Potential transformation method for global optimization by Robert A. Donnelly
- Multispace search for protein folding by Jun Gu, Bin Du, and Panos Pardalos
- Modeling the structure of ice as a problem in global minimization by Jan Hermans
- Novel applications of optimization to molecule design by J.C. Meza, T.D. Plantenga, and R.S. Judson
- Issues in large-scale global molecular optimization by Jorge J. More and Zhijun Wu
- Global optimization for molecular clusters using a new smoothing approach by C.-S. Shao, R.H. Byrd, E. Eskow, and R.B. Schnabel
- Global Minimization of Lennard-Jones Potential Functions on Transputer Networks by Klaus Ritter, Stephen M. Robinson, and Stefan Schäffler
- Variable-scale coarse-graining in macromolecular global optimization by David Shalloway

**MANUSCRIPTS RECEIVED FOR THE IMA PROCEEDINGS VOLUMES
ON MATHEMATICAL METHODS IN MATERIALS SCIENCE**

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- Calculating the mechanical properties of materials from interatomic forces by Roger Haydock

PHASE TRANSFORMATION, COMPOSITE MATERIALS AND MICROSTRUCTURE, September 18-22, 1995

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- Bounding the effective yield behavior of mixtures by Tamara Olson

DISORDERED MATERIALS, November 13-17, 1995

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- Transversely isotropic poroelasticity arising from thin isotropic layers by James G. Berryman
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- Bounds on the effective elastic properties of martensitic polycrystals by Oscar P. Bruno and Fernando Reitich
- Statistical models for fracture by Lucilla de Arcangelis
- Normal and anomalous diffusions in random flows by Albert Fannjiang
- Granular media: some new results by H.J. Herrmann
- Weakly nonlinear conductivity and flicker noise near percolation by Ohad Levy
- Composite sensors and Actuators by Robert E. Newnham
- Upper bounds on electrorheological properties by Ping Sheng and Hongru Ma
- On spatiotemporal patterns in composite reactive media by S. Shvartsman, A.K. Bangia, M. Bär, and I.G. Kevrekidis
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- Enhanced nonlinear-optical responses of disordered clusters and composites by Mark I. Stockman, Lakshmi N. Pandey, and Thomas F. George

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Editor: Stuart Whittington

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