Many large-scale optimization problems can be formulated as nonlinear programming problems where the constraints represent systems governed by partial differential equations. This deceptively simple observation allows for a wealth of possibilities in the development of optimization methods applicable to such problems. This is a vast area of research on problems of importance to the nation’s environment, economy, and defense.

The work reported here had as its goal the development and evaluation of a number of different optimization strategies for problems with simulation constraints. Specifically, the work focused on applying direct search methods to and developing interior-point algorithms for problems of this form.
SOME ISSUES IN NONLINEAR PROGRAMMING ALGORITHMS FOR PROBLEMS WITH SIMULATION CONSTRAINTS

John E. Dennis, Jr.     Richard A. Tapia     Virginia J. Torczon
Department of Computational and Applied Mathematics - MS 134
Rice University
P.O. Box 1892
Houston, Texas 77251-1892

13 April 1995


Prepared for
Dr. Neal Glassman
Department of the Air Force
Air Force Office of Scientific Research
Bolling Air Force Base
Washington, DC 20332-6448
Some Issues in Nonlinear Programming Algorithms for Problems with Simulation Constraints

J.E. Dennis, Jr.    R.A. Tapia    V.J. Torczon

March 1995

1. Abstract

Many large-scale optimization problems can be formulated as nonlinear programming problems where the constraints represent systems governed by partial differential equations. This deceptively simple observation allows for a wealth of possibilities in the development of optimization methods applicable to such problems. This is a vast area of research on problems of importance to the nation's environment, economy, and defense.

The work reported here had as its goal the development and evaluation of a number of different optimization strategies for problems with simulation constraints. Specifically, the work focused on applying direct search methods to and developing interior-point algorithms for problems of this form.

2. Statement of Work

Several breakthroughs for the parallel direct search/pattern search methods were accomplished:

- began collaboration with researchers at Boeing and IBM to solve multidisciplinary design optimization problems that are not amenable to optimization techniques that require derivative information. The target application will be helicopter rotor blade design, which is a multidisciplinary design optimization (MDO) problem.

- designed a two-stage meta-algorithm for managing the use of approximation models. It is possible to guarantee convergence to a stationary point for this meta-algorithm using the theoretical properties developed for pattern search methods. This framework is sufficiently flexible to incorporate standard engineering practice as one stage.

- developed the first unifying global convergence theory for pattern search methods, a class of direct search methods for which there was either no convergence analysis or convergence could be proven only under much stronger assumptions.

- developed an extension for the parallel direct search methods that constructs an
exact penalty function to handle general constraints and yet does not require the use of derivatives. This extension has been successfully applied to a variety of problems with simulation constraints.

Included among the accomplishments for interior-point methods for linear programming:

- produced the first algorithm for linear programming that possesses both polynomial complexity and superlinear convergence.
- produced the first algorithm that is quadratically convergent and has optimal complexity under no assumption of nondegeneracy.
- developed interior-point methods for linear programming that have the property that they generate an iteration sequence which converges to the analytic center of the solution set.

The accomplishments in the area of interior-point trust-region algorithms for nonlinear programming are:

- developed first-order convergence results for trust-region interior-point algorithms for the solution of minimization problems with simple bounds.
- developed first-order convergence results for trust-region interior-point algorithms for the solution of minimization problems with equality constraints and simple bounds on some of the variables.
- extended these results to the case where the linear solvers are inexact and then used the resulting algorithm to solve an optimal control problem governed by a nonlinear heat equation and a wing design problem from Boeing.
- developed, in collaboration with colleagues at Boeing Computer Services, a taxonomy for the formulation of MDO problems, motivated by aircraft design.
- developed a solid theoretical foundation to a novel reduced subspace trust-region algorithm for nonlinear programming with equality constraints.
- developed a new approach to large-scale nonlinear programming for problems where the constraints occur naturally in blocks.

Further details follow in the sections below.

2.1 Parallel Direct Search Algorithms for Nonlinear Programming

Research objective: develop and apply versions of the parallel direct search methods to
problems with simulation constraints.

John Dennis and Virginia Torczon began what promises to be a productive collaboration with Paul Frank at Boeing Computer Services and Andy Conn at IBM T.J. Watson Research Center, to investigate the management of approximation models for solving nonlinear programming problems. Many problems in engineering design share the feature that function evaluations are extremely expensive to compute because of the cost of running the simulations associated with the constraints to obtain values for the state variables. (For instance, a full simulation of the physics for the helicopter rotor blade design problem, which serves as the focus for the Boeing/IBM/Rice collaboration, requires several hours on a Cray Y-MP.) Consequently, a standard engineering practice is to perform the optimization on approximation models of the simulations for which values are relatively inexpensive to compute. The open question is how to manage the optimization of the approximate problem to ensure convergence to an optimal point for the true problem in an effort to reduce the overall time required to compute a solution.

John Dennis and Virginia Torczon have developed a two-level meta-algorithm to manage this process. The idea is to take some number of optimization steps on the inexpensive models that approximate the full physics represented by the simulation(s) and then use the results from the optimization of the approximation model to predict a successful iterate for the true problem. The nub of the problem is how to manage inexpensively the refinement of the model if this procedure results in a worse design.

The exciting part of this work is that, at least mathematically, one of the key analytical tools developed for the pattern search methods provides a model management strategy for which it is possible to prove first-order convergence for the two-level process.

Virginia Torczon has also developed and extended a unifying convergence theory for pattern search methods, a class of direct search methods. This theory is a natural extension of the global convergence theory for methods based on higher-order information in that one can relax the conditions on accepting a step in exchange for placing stronger conditions on the construction of the steps and yet still obtain a global convergence result as strong as the one originally given by M.J.D. Powell for trust-region globalization strategies for quasi-Newton methods—even though no explicit gradient information is used. Recent extensions of this theory include a cleaner result concerning the algebraic structure of the iterates produced by the pattern search methods (it is this structure that makes the convergence theory both for the general pattern search methods as well as for the new two-stage process possible) and a new theorem that makes clear under what conditions one can obtain the stronger result that the sequence of iterates converges to a stationary point of the function.

The unifying theory is also significant in that it introduces a structure that suggests the possibility of developing algorithms and convergence theory for nonlinear programming problems with simple bound constraints. This structure is also guiding the development of extensions for handling more general constraints.

In the meantime, Tony Kearsley, a graduate student under the direction of Richard Tapia and Roland Glowinski, has been working with Virginia Torczon to develop an algorithm for solving nonlinear programming problems without using derivatives or any higher-order information. An exact penalty function is constructed and evaluated. The extension is compatible with the parallelism enjoyed by the parallel direct search methods. This algorithm is intended for use on problems with a small number of variables and constraints. It has been applied, successfully, to such problems as the control of some friction constrained motions, the
control of a vibrating string subject to dry friction, and optimal shape problems.

Virginia Torczon continues to develop and improve the software to execute PDS, the parallel direct search methods, a particular class of direct search methods developed with John Dennis. Version 2.0 of PDS is in beta release and is being tested locally before a general release scheduled for May 1995. Feedback from many of the hundreds of users who have requested copies of version 1.0 of PDS from softlib, the electronic software library managed by the Center for Research on Parallel Computation at Rice University, has been used to improve version 2.0.

2.2 Interior-Point Algorithms for General Nonlinear Programming

Research objective: develop and apply various formulations of interior-point algorithms to nonlinear programming problems.

Considerable understanding was gained concerning the behavior of interior-point methods for linear programming. These behavior properties included both the local and the global aspects of the methods. This understanding was used to formulate a class of methods for general nonlinear programming problems. Optimal local theory was developed in the paper by El-Bakry, Tapia, Tsuchiya, and Zhang for Newton's method and in the paper by Martinez, Parada, and Tapia for quasi-Newton methods. This local theory demonstrates the validity of the formulation, since it is possible to establish local and quadratic convergence for Newton's method and local and superlinear convergence for quasi-Newton methods under the standard assumption. This leads to a satisfying local theory.

2.3 Interior-Point Trust-Region Algorithms for Nonlinear Programming

Research objective: develop theory and software for trust-region interior-point algorithms to solve nonlinear optimization problems with equality constraints and simple bounds on the control variables.

Many engineering applications lead to large constrained optimization problems for a system governed by partial differential equations (PDE). The central theme in the work of John Dennis and his collaborators is to treat the discretized PDE as equality constraints that must be satisfied in order to yield a physically sensible answer. Rather than compute an accurate simulation at each optimization iteration, they effectively compute a simulation sufficiently accurate only to enable the optimization to proceed. In the equality constrained optimization formulation, they accomplish this by allowing infeasible iterates until convergence to the solution. To implement this approach, John Dennis and Luis Vicente have developed software with Matthias Heinkenschloss of Virginia Polytech Institute for both the optimization and PDE components of this problem.

John Dennis and Luis Vicente first concentrated on solving optimization problems with equality constraints. To that end they constructed, implemented and analyzed two trust-region interior-point algorithms. The first is for the solution of minimization problems with simple bounds. The first algorithm is more usual in that the trust region and the local quadratic model are consistently scaled. The second algorithm uses an unscaled trust region. A first-order convergence result for these algorithms has been developed and dogleg and conjugate-gradient
algorithms to compute trial steps has been implemented. Numerical examples show the advantages of the second algorithm.

John Dennis, Luis Vicente and Matthias Heinkenschloss then developed trust-region interior-point algorithms for the solution of minimization problems with equality constraints and simple bounds on some of the variables. These nonlinear programs arise from the discretization of optimal control problems with bounds on the control variables, which is a standard assumption for many optimal control problems. This collaboration was the result of conversations with Matthias Heinkenschloss at the AFOSR workshop at Virginia Polytech Institute in April 1994. The algorithms that have resulted maintain strict feasibility with respect to the bound constraints and use trust-region techniques to ensure global convergence. First-order convergence of these algorithms has been proven under very mild conditions on the trial steps. These convergence results include as special cases current results both for equality constraints and for simple bounds.

Most recently, John Dennis, Luis Vicente and Matthias Heinkenschloss extended these results to the case where the linear solvers are inexact. The trust-region interior-point (TRIP) algorithms have been used to solve an optimal control problem governed by a nonlinear heat equation. This problem controls the heating process of a probe inside a kiln and in its discretized form has a few thousand variables. The TRIP algorithms took only a few iterations to solve this problem.

3. New Discoveries, Inventions, or Patent Disclosures

- Not applicable.

4. Additional Statements

- J.E. Dennis, Jr. was elected Chair of the Mathematical Programming Society.
- R.A. Tapia was awarded the A. Nico Habermann inaugural award by the Computing Research Association for his work with women and minority student programs that benefit those underrepresented groups, Snowbird, UT, July, 1994.
- R.A. Tapia was selected “Professor of the Year” by the Association of Hispanic School Administrators, Houston Independent School District, Houston, TX, 1994.
- V.J. Torczon was a member of the organizing committee for the Seventh SIAM Conference on Parallel Processing for Scientific Computing.
- V.J. Torczon was invited to be a member of the Supercomputing '95 Tutorials Committee.
V.J. Torczon was invited to be a member of the Organizing Committee of the 8th SIAM Conference on Parallel Processing for Scientific Computing.

V.J. Torczon was elected Secretary, SIAM Activity Group on Supercomputing, 1994-1996.

Over 100 copies of PDS, the software for executing the parallel direct search methods on either sequential or parallel machines, has been distributed via {softlib@cs.rice.edu}, which is administered by the Center for Research on Parallel Computation.

Please see attached letters on the use of this research in corporate settings.

5. Publications

5.1 Published during reporting period:


5.2 To appear:


• V.J. Torczon, “PDS: Parallel Direct Search Methods for Unconstrained Optimization on Either Sequential or Parallel Machines,” ACM Transactions on Mathematical Software.

5.3 Submitted for publication:


6. Participating Professionals

6.1 Research personnel and visitors:

• Natalia Alexandrov
• Alan Carle
• Mahmoud El-Alem
• Amr El-Bakry
• Mohammed El-Hallabi
• Michael Fagan
• Matthias Heinkenschloss
• Robert Michael Lewis
• Hector Martinez
• Andrew Meade
• Juan Meza
• Doug Moore
• Stephen Nash
• Sandra Augusta Santos
• Michael Trosset
• Homer Walker
• Joe Warren
• Karen Williamson
• Hiroshi Yabe
• Yin Zhang

6.2 Graduate students:

• Natalia Alexandrov, Ph.D. 1993, "Multilevel Algorithms for Nonlinear Equations and Equality Constrained Optimization" (directed by J.E. Dennis, Jr.)
• Miguel Argaez (under the direction of R.A. Tapia)
• Debora Cores, Ph.D. 1994, "A Robust Choice of the Lagrange Multiplier in the Successive Quadratic Programming Framework" (directed by R.A. Tapia)
• Rodolfo Elizondo, M.A. 1994, "Solving Large-Scale School/Student Assignment Problems" (directed by R.A. Tapia)
• Mark Gockenbach, Ph.D. 1994 “An Abstract Analysis of Differential Semblance Optimization” (co-directed by R.A. Tapia and W.W. Symes)
• Maria Gonzalez-Lima, Ph.D. 1995 “Effective Computation of the Analytic Center of the Solution Set in Linear Programming Using Primal-Dual Interior-Point Methods” (directed by R.A. Tapia)
• Anthony Kearsley (under the direction of R.A. Tapia and R. Glowinski)
• Anne Kilgore, M.A. 1994, “Very Large-Scale Linear Programming: A Case Study in Exploiting Both Parallelism and Distributed Memory” (directed by R.E. Bixby with V.J. Torczon)
• Michael Kokkolaras
• Zeferino Parada (under the direction of R.A. Tapia)
• David Serafini (under the direction of J.E. Dennis, Jr.)
• Luis Vicente (under the direction of J.E. Dennis, Jr.)
• Pamela Williams (under the direction of R.A. Tapia)
6.3 Undergraduate students:

- Gann Bierner
- Sam Spencer

6.4 Industrial collaborators:

- E.J. Cramer (Boeing Computer Services)
- A. R. Conn (IBM T. J. Watson Research Center)
- A. Booker (Boeing Computer Services)
- P. Frank (Boeing Computer Services)
- E. Nunez (Shell Development)
- B. Tjoa (Dynamic Matrix Control Corporation)
- G.R. Shubin (Boeing Computer Services)

7. Coupling Activities

Presentations by J.E. Dennis, Jr.


- Invited speaker: “Interacting with Industry and Preparing Students for the Job


- Invited speaker: “Problem Formulation for Multidisciplinary Design Optimization, Colloquia, Departments of Mathematics and Industrial and Systems Engineering, Georgia Institute of Technology, Atlanta, Georgia, April 1994.


• Invited speaker: “Trust-Region Methods for Large-Scale Nonlinear Programming,” Colloquium, Department of Computer Science, University of Maryland, College Park, Maryland, November 1994.

• Invited speaker: “Managing Approximation Models in Optimization,”
  Boeing/IBM/Rice Workshop, Boeing Computer Services, Bellevue,

Presentations by R.A. Tapia

• Plenary session: “The Historical Development of Computational Optimization,”
  Regional meeting of the American Mathematical Society, Knoxville, Tennessee,
  March 1993.

• “Why Be a Good Student?” second grade class West University Elementary

• Keynote address: “The Value of Education,” CalTech Minority Youth Program
  Los Angeles, California, March 1993.

• “A Primal-Dual Interior-Point Method for Large-Scale Linear Programming,”

• In-service presentation: Hispanic Heritage and Awareness, Hispanic
  Awareness Week, West University Elementary School, Houston, Texas, May
  1993.

• Keynote speaker: “The Mayan Connection,” Association for the Advancement
  of Mexican Americans, Cinco de Mayo Celebration, Houston, Texas, May
  1993.

• Speaker: Hispanic Awareness Week, Poe Elementary School, Houston,
  Texas, May 1993.

• Keynote speaker: Jackson Middle School, First Annual Girl's Athletic

• Keynote speaker: King Middle School, Cinco de Mayo Celebration, Crosby,
  Texas, May 1993.

• Invited speaker: “The Changing Role of Mathematics and National Agenda
  Issues,” Rice University School Mathematics Project, Houston, Texas, June
  1993.

• Invited speaker: Graduation Ceremony, (MS)2 Middle School Math and

• Invited speaker: Math/Science Institute Mini-Graduation, Kincaid High School,
  Houston, Texas, July 1993.

• Special lecture: “The Health of the Nation.” Families Weekend, Rice
  University, Houston, Texas, September 1993.
• In-Service Presentations to Teachers and Students, Dibol Independent School District, Dibol, Texas, September 1993.

• Invited address: “On the Historical Development of Theoretical and Computational Optimization Theory,” XXVI National Congress of the Sociedad Matematica Mexicana (SMM), Morelia, Michoacan, Mexico, October 1993. (Selection made by President of the AMS at the invitation of the President of the SMM.)


• Invited series of lectures: Distinguished Visitor Program, Department of Mathematics, University of Iowa, Iowa City, Iowa, February 1994.


• Organize and Lead One-Day Workshop, “Say Yes to a Youngster's Future.” The workshop was held on the Rice campus and attended by approximately 120 teachers, students, and parents from Eight Avenue Elementary School (predominately Hispanic), Houston, Texas, February 1994.


• Invited speaker: “Multicultural Issues in Mathematics,” Education Department Symposium, Rice University, Houston, Texas, April 1994.


• Keynote speaker: Rice Undergraduate Minority Student Program Advance Annual Banquet, Houston, Texas, April 1994.

• Keynote speaker: Promoting Representation of Women and Minorities in Mathematics, University of Houston Clear Lake Conference, Houston, Texas, April 1994.

• Keynote speaker: Hispanic Heritage Program, University of Illinois, invited by Latino Graduate Student Association, Urbana-Champaign, Illinois, April 1994.

• Keynote speaker: Semana Latina Program, California Institute of Technology, invited by Latino Graduate Student Association, Pasadena, California, May
1994.


- One Week Mathematical and Computational Sciences Awareness Workshop for K-12 Mathematics and Science Teachers from Schools with Significant Minority Enrollment, Rice University, Houston, Texas, July 1994.


Invited speaker: "On the Retention of Minorities and Women in Mathematical Sciences Graduate Programs," 1995 American Association for the Advancement of Science, Atlanta, Georgia, February 1995.

Presentations by V.J. Torczon


- Presentation: "Very Large-Scale Linear Programming: A Case Study in Exploiting Both Parallelism and Distributed Memory," CRPC Research Symposium, California Institute of Technology, Los Angeles, California, January 1994.


October 25, 1993

To whom it may concern:

This is to verify that we have researched the use of mathematical optimization techniques to invert models of sedimentary processes. Among other findings, we have established that the multidirectional search algorithms developed by Drs. V. Torczon and J. Dennis of Rice University are particularly useful for this kind of problems.

These algorithms have directly enabled us to constrain the outcome of quantitative geologic models to honor field observations, thereby enhancing our ability to predict rock properties between and beyond data.

We believe that these methods also have great potential use in other areas of the oil industry, including seismic inversion, borehole tomography, and heat-flow model parameter estimation. Therefore, we strongly recommend support for Dr. Dennis and Dr. Torczon’s research.

Very truly yours,

D.M. Tetzlaff

DR. DANIEL M. TETZLAFF,
Project Scientist
Scott H. Lamson  
General Electric Company  
Corporate Research and Development  
P.O. Box 8  ES 208  
Schenectady, New York 12301  

August 31, 1993  

Professor Virginia Torczon  
Rice University  
Department of Mathematical Sciences  
George R. Brown School of Engineering  
P.O. Box 1892  
Houston, Texas 77251—1892  

Dear Dr. Torczon;  

I wanted to let you know that my implementation of your multidirectional search algorithm is incorporated in a turbine blade design program that will shortly be installed as a production engineering tool for GE Power Generation and possibly GE Aircraft Engines. It is used to fit a 6-th degree (or higher) Bezier curve to a given initial x/y curve. A somewhat innocuous sounding problem, but one on which I have spent a fraction of the last 4 years wracking my brains over. Real "geometry" experts have not achieved greater success, although none have spent as long on it. Someone even tried neural nets, and I have tried Genetic Algorithms in the past. It is interesting to note that your fundamental research in optimization algorithms has overcome one impediment to taking my own fundamental research and transfer that technology to a production status tool for use by GE engineers. Keep up the flow of good ideas and creative approaches needed by U.S. industry.  

Sincerely yours,  

Scott H. Lamson  
Computational Physicist  
Fluid Mechanics Program  

cc:
September 28, 1994

To whom it may concern:

I am writing to express my enthusiastic support for the recent optimization work being done by John Dennis and his group at Rice University.

I have been leading efforts at Boeing Computer Services for the past few years to develop improved methods and problem formulations for design optimization and, lately, multidisciplinary design optimization (MDO). I and others in the Mathematics and Engineering Analysis group here have collaborated with John Dennis and Michael Lewis at Rice in this area. We have jointly developed abstractions for reasoning about MDO and new problem formulations that look promising. Among these new formulations one, the "individual discipline feasible" (IDF) approach, has been implemented at Boeing for aeroelastic design. The framework that we have developed is proving quite useful for understanding and communicating in this exceedingly difficult technical area.

John Dennis and his team at Rice took the initiative to get involved with industrial problems at Boeing. They came here of their own accord and introduced us to the ideas that eventually became IDF. They have had other impact on our work through, for example, Virginia Torczon's search algorithm that is routinely used in a parts nesting optimization problem here. They also introduced us to the automatic differentiation tool ADIFOR, a product of Rice-Argonne collaboration; we are investigating the potential use of ADIFOR in preliminary design at Boeing. I am hard pressed to think of another optimization group that has had a similar impact on real industrial problems.

There is no doubt in my mind that the MDO community stands to gain a lot by involving professional optimization people of the high calibre of John Dennis and his group. This is not to disparage engineering people who know a lot of optimization; I've just observed that folks thoroughly involved in optimization theory, practice, and in the optimization community have much to contribute to MDO. We've found this to be the case in our interaction with John Dennis. There are many in the aerospace MDO community who think that the difficulties we face are primarily engineering in nature, and that the optimization and problem formulation issues are either secondary or even "done." They are almost certainly wrong. The interplay between optimization and engineering disciplines will undoubtedly play a key role in determining success or failure as we strive to do harder and bigger MDO problems. No one appreciates this more keenly than John.
We have recently been discussing with John the possibility of him coming to Boeing on sabbatical. Given the enthusiasm expressed above, we would obviously endorse any funding mechanism that would partially support such a sabbatical. Such a visit would significantly increase the benefit of funded work by immediately channeling it into practical application. Because John is so well connected in the applied mathematics community, a sabbatical here at Boeing would also have the effect of making the academic world much more aware of industrial problems.

I would be delighted to provide any further information that would be useful.

Gregory R. Shubin
Manager, Numerical Analysis
Org. G6412, M/S 7L-21
(206) 865-3316