

0589

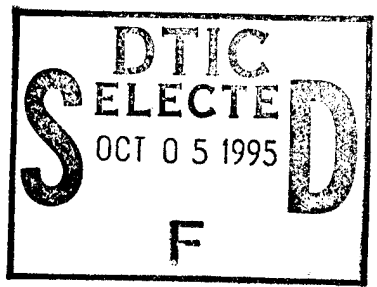
REPORT DOCUMENTATION PAGE

Public reporting burden for this collection of information is estimated to average 1 hour per response, including gathering and maintaining the data needed, and completing and reviewing the collection of information. Collection of information, including suggestions for reducing this burden, to Washington Headquarters Office, Davis Highway, Suite 1204, Arlington, VA 22202-4302, and to the Office of Management and Budget, Paperwork Reduction Project (0704-004), Washington, DC 20503.

A source of this report is Jefferson

1. AGENCY USE ONLY (Leave blank)		2. REPORT DATE	3. REPORT TYPE AND DATES COVERED FINAL/01 JAN 93 TO 30 JUN 95	
4. TITLE AND SUBTITLE WORKSHOP ON NEW OPTIMIZATION TECHNIQUES FOR LARGE COMPOUNDS			5. FUNDING NUMBERS	
6. AUTHOR(S) MARK S. GORDON			2304/DS F49620-93-1-0112	
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) IOWA STATE UNIVERSITY DEPARTMENT OF CHEMISTRY AMES, IOWA 50011			8. PERFORMING ORGANIZATION REPORT NUMBER	
9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES) AFOSR/NM 110 DUNCAN AVE, SUTE B115 BOLLING AFB DC 20332-0001			10. SPONSORING/MONITORING AGENCY REPORT NUMBER F49620-93-1-0112	
11. SUPPLEMENTARY NOTES				
12a. DISTRIBUTION AVAILABILITY STATEMENT APPROVED FOR PUBLIC RELEASE: DISTRIBUTION IS UNLIMITED			12b. DISTRIBUTION CODE	
13. ABSTRACT (Maximum 200 words) A workshop devoted to the development, testing, and applications of optimization for global and local structural optimization was supported.				

19951004 117



DTIC QUALITY INSPECTED 6

SUBJECT TERMS			15. NUMBER OF PAGES
			16. PRICE CODE
17. SECURITY CLASSIFICATION OF REPORT UNCLASSIFIED	18. SECURITY CLASSIFICATION OF THIS PAGE UNCLASSIFIED	19. SECURITY CLASSIFICATION OF ABSTRACT UNCLASSIFIED	20. LIMITATION OF ABSTRACT SAR(SAME AS REPORT)

of atoms. Examples of such systems are: (a) species which are potential new high energy fuels, such as metals with low mass embedded in solid hydrogen; (b) new nonlinear optical (NLO) polymers currently under investigation in the Wright Laboratories and by several contractors; (c) new lubricants; and (d) a variety of composite materials. Theoretical investigations are expected to play a major role in developing an understanding of such species, thereby making the development of new materials more efficient and cost-effective.

A central problem in the application of theoretical chemical methods to systems of many atoms is the determination of the stationary points (minima, transition states) on the potential energy surface. While very effective optimization methods have been developed for molecules with small numbers of atoms, these methods have limited usefulness for systems of prime interest to the Air Force. Some methods have been developed to study new drug compounds and other species of biological importance, but these methods have proved to be largely ineffective, and the potentials used in that area of research are mostly too oversimplified for our purposes.

There is therefore a critical need to develop new effective and computationally efficient methods for global and local optimizations of large species. The **specific objectives** of the proposed workshop were to:

1. Educate the optimization community regarding the specific needs of the Air Force.
2. Promote discussions among the participating scientists regarding potential solutions of the central problem.
3. Facilitate interactions among theoretical chemists, mathematicians, computer scientists, and Air Force laboratory scientists, in order to develop the broadest possible approach to addressing optimization problems.
4. Consider the role supercomputing in general and parallel computing in particular can play in solving these problems.

JANUARY WORKSHOP

The participants in the January 1993 workshop at Iowa State University were:

UNIVERSITY PARTICIPANTS

- C. Bajaj, Computer Science, Purdue University
- R. Byrd, Computer Science, University of Colorado
- J. Caruthers, Engineering, Purdue University
- A. DePristo, Chemistry, Iowa State University
- S. Elbert, Chemistry, Iowa State University
- D. Ferguson, Medicinal Chemistry, University of Minnesota
- C. Floudas, Chemical Engineering, Princeton University
- M. Gordon, Chemistry, Iowa State University
- T. Holme, Chemistry, University of South Dakota
- A. Komornicki, Polyatomics Research Institute
- L. Lasdon, Management Science, University of Texas
- T. Magee, Business, University of Colorado-Boulder
- T. Morin, Engineering, Purdue University
- J. Pekny, Chemical Engineering, Purdue University
- P. Pulay, Chemistry, University of Arkansas
- H. Rabitz, Chemistry, Princeton University
- S. Robinson, Industrial Engineering, University of Wisconsin
- B. Rosen, Computer Science, University of Minnesota
- B. Schlegel, Chemistry, Wayne State University
- B. Schnabel, Computer Science, University of Colorado-Boulder
- S. Schwartz, Albert Einstein College of Medicine
- D. Shalloway, Biotechnology, Cornell University
- J. Simons, Chemistry, University of Utah
- P. Taylor, Chemistry, San Diego Supercomputer Center
- D. Thirumalai, Chemistry, University of Maryland
- J. Weare, Chemistry, University of California-San Diego

AFOSR PARTICIPANTS

L. Burggraf, AFOSR/NC
T. Erstfeld, AFOSR/NC
N. Glassman, AFOSR/NM

PARTICIPANTS FROM AIR FORCE LABORATORIES

J. Boatz, Phillips Laboratory (AL)
M. Coolidge, Seiler Laboratory
L. Merkle, AFIT-Wright-Patterson
R. Pachter, Wright Laboratories
S. Rodgers, Phillips Laboratory (AL)

The following is the schedule of presentations at the January workshop:

SCHEDULE OF EVENTS

Friday, January 15, 1993

Spedding Hall, Room 301B, ISU Campus

Coffee, juice and rolls provided

08:30 Introductory remarks

Neal Glassman

Mark Gordon

Session 1, Ruth Pachter (WL), presiding

09:00 - 09:30 John Weare (University of California - San Diego)

09:30 - 10:00 Bobby Schnabel (University of Colorado - Boulder)

10:00 - 10:30 Tim Magee (University of Colorado - Boulder)

10:30 - 11:00 break

Session 2, Jerry Boatz (PL), presiding

11:00 - 11:30 Herschel Rabitz (Princeton University)

11:30 - 12:00 Chris Floudas (Princeton University)

12:00 - 12:30 David Thirumalai (University of Maryland)

12:30 - 14:00 lunch

Session 3, Larry Burggraf (AFOSR), presiding

14:00 - 14:30 Steven Schwartz (Albert Einstein College of Medicine)

14:30 - 15:00 David Shalloway (Cornell University)

15:00 - 15:30 Andy Komornicki (Polyatomics Research Institute)

15:30 - 16:00 break

16:00 - 16:30 Berny Schlegel (Wayne State University)

16:30 - 17:30 round table discussion

Saturday, January 16

Gateway Holiday Inn

Coffee, juice, and rolls provided

Session 4, Mark Gordon (Iowa State University), presiding

08:30 - 09:00 Ben Rosen (University of California - San Diego)

09:00 - 09:30 Steve Robinson (University of Wisconsin)

09:30 - 10:00 Chanderjit Bajaj (Purdue University)

10:00 - 10:30 break

Session 5, Neal Glassman (AFOSR), presiding

10:30 - 11:00 Leon Lasdon (University of Texas)

11:00 - 11:30 Tom Morin (Purdue University)

11:30 - 12:30 Round Table Discussion

12:30 - 2:00 lunch

Session 6, Mike Coolidge (Air Force Academy), presiding

14:00 - 14:30 Peter Taylor (San Diego Supercomputer Center)

14:30 - 15:00 Jack Simons (University of Utah)

15:00 - 15:30 Peter Pulay (University of Arkansas)

15:30 - 16:00 break

16:00 - 17:00 round table discussion

17:00 closing remarks

OUTCOMES OF JANUARY WORKSHOP

The January workshop had several positive outcomes:

- Exchange of ideas among scientists from several areas of science and engineering.
- Exposure of Air Force personnel to the current state-of-the-art in optimization methods.
- Heightening of awareness in the community of the importance of scalable computing for solving large problems.
- Development of inter-disciplinary collaborations (Schnabel-Weare, Schnabel-Schlegel)
- Focused goals of the subsequent RFP for the Initiative on Optimization

FOLLOW-UP WORKSHOP

The participants at the follow-up workshop held in Washington, DC, in May 1995 were:

Professor Alexander, University of Maryland
Professor Bajaj, University of Minnesota
Dr. Berman, AFOSR
Dr. Boatz, Air Force Phillips Laboratory
Dr. Glassman, AFOSR
Professor Gordon, Iowa State University
Professor Floudas, Princeton University
Dr. Head-Gordon, LBL
Dr. Pachter, Wright Laboratories
Professor Pulay, University of Arkansas
Professor Rabitz, Princeton University
Dr. Rodgers, Air Force Phillips Laboratory
Professor Shalloway, Cornell University
Dr. Schmidt, Iowa State University
Professor Schnabel, University of Colorado
Professor Thirumalai, University of Maryland
Professor Weare, University of California-San Diego
Dr. Yeates, Wright Laboratories

The schedule for the follow-up workshop was:

Ida and Cecil Green Building
Room Green 120
2001 Wisconsin Avenue
Washington DC 20007

Monday, May 1

8:00-8:20	Coffee
8:20-8:30	Opening Remarks (Glassman, Rodgers, Berman)
8:30-9:15	Prof Weare
9:15-10:30	Prof Pulay
10:30-10:45	Break
10:45-11:30	Prof Thirumalai
11:30-12:15	Dr Dudis
12:15-1:45	Lunch
1:45-2:30	Dr Rodgers
2:30-3:15	Prof Bajaj
3:15-3:30	Break
3:30-4:15	Prof Shalloway

Tuesday May 2

8:00-8:30	Coffee
8:30-9:15	Dr Pachter
9:15-10:30	Dr Head-Gordon
10:30-10:45	Break
10:45-11:30	Prof Floudas, Prof Rabitz
11:30-12:15	Prof Schnabel

The main purpose of the follow-up workshop was to provide a forum in which the participants in the initiative could present the preliminary results of their research. A secondary purpose was to solidify existing collaborations and to encourage new ones. Based on the enthusiastic discussions, this was a very successful meeting.