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Workshop Report on
Large-Scale Matrix Diagonalization Methods
in Chemistry Theory Institute

held at Argonne National Laboratory

May 20–22, 1996

edited by

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Mathematics and Computer Science Division

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Introduction

The Large-Scale Matrix Diagonalization Methods in Chemistry theory institute was held on May 20–22, 1996, at Argonne National Laboratory. This interdisciplinary institute was organized by Chris Bischof and Ron Shepard and brought together 41 computational chemists and numerical analysts. The goal was to understand the needs of the computational chemistry community in problems that utilize matrix diagonalization techniques. This was accomplished by reviewing the current state of the art and looking toward future directions in matrix diagonalization techniques. This institute occurred about 20 years after a related meeting of similar size (see Report on the Workshop August 9-11, 1978, University of California, at Santa Cruz, edited by Cleve Moler and I. Shavitt and sponsored by National Resource for Computation in Chemistry). During those 20 years the Davidson method continued to dominate the problem of finding a few extremal eigenvalues for many computational chemistry problems. Work on non-diagonally dominant and non-Hermitian problems as well as parallel computing has also brought new methods to bear. The changes and similarities in problems and methods over the past two decades offered an interesting viewpoint for the success in this area.

One important area covered by the talks was overviews of the source and nature of the chemistry problems. The numerical analysts were uniformly grateful for the efforts to convey a better understanding of the problems and issues faced in computational chemistry. An important outcome was an understanding of the wide range of eigenproblems encountered in computational chemistry. The workshop covered problems involving self-consistent-field (SCF), configuration interaction (CI), intramolecular vibrational relaxation (IVR), and scattering problems. In atomic structure calculations using the Hartree-Fock method (SCF), the symmetric matrices can range from order hundreds to thousands. These matrices often include large clusters of eigenvalues which can be as much as 25% of the spectrum. However, if CI methods are also used, the matrix size can be between 10^4 and 10^9 where only one or a few extremal eigenvalues and eigenvectors are needed. Working with very large matrices has lead to the development of out-of-core methods. In 1980 during the early CI calculations, basis sets of order 10^4 were used. By the 1990s, parallel machines have been used to solve problems with 10^9 basis functions. In IVR, the basis sets, if done by brute force, are prohibitively large. In practice, a series of smaller subspaces are prediagonalized and a subset of these eigenvectors are used to form an accurate representation of the contracted basis set for the full problem. The smaller subspaces can be represented with several thousand basis functions where a few hundred to as much as 25% of the eigenvectors of each diagonalization are kept to form the contracted basis set. In the end, contracted basis sets can produce matrices as large as order a few tens of thousands. The symmetric eigensolution performed on this matrix needs to find a few tens to a few hundreds of the eigenvalues/eigenvectors near an energy of interest and are not usually extremal eigenvalues. In scattering problems, 20% eigensolutions of a matrix with several thousand basis

functions may be solved. Also, scattering and molecular dynamics problems can lead to the need to solve complex symmetric eigenproblems.

Another interesting area was the description of the properties of typical matrices. Chemists often refer to their matrices as sparse since only a few percent of the matrix elements are non-zero. However, numerical analysts refer to sparse matrices if the number of non-zeros is not proportional to the matrix size. Thus, even though the matrices have few non-zero elements, they are not sparse in the traditional matrix theory sense. Another important property of the matrices is that they are often diagonally dominant. This property can greatly simplify issues in performing the eigenproblem. For example, the diagonal elements may represent a good initial guess to the final eigenvalues of the matrix. Several speakers noted that an important goal of the computational techniques in chemistry is to produce matrices that are diagonally dominant. It is considered so important that techniques that fail in this regard are often reworked to obtain diagonally dominant matrices. Thus, chemists avoid even attempting to find eigensolutions to matrices lacking this property. (It was also noted, however, that reactive scattering problems are not diagonally dominant.) On several occasions numerical analysts commented that some of the techniques used by chemists in finding the eigensolutions were not, in general, guaranteed to produce the right answer. The chemists responded, however, that the well-behaved nature of the matrices meant that the correct solutions were found.

Another important aspect of the institute was the overviews of the computational techniques used for solving eigenproblems. Several speakers noted the interesting coincidence that this year is the 150th anniversary of the publication of Jacobi's method for the eigenproblem. As noted above, many computational chemistry problems, especially in SCF, involve finding only a small subset of the spectrum. When a good preconditioner is available, as is the case in a symmetric diagonally dominant matrix, chemists typically use the Davidson method invented by Ernest Davidson, who attended the institute. Alternative methods are also available which apply to a greater range of problems and applications. Several numerical analysts discussed eigensolvers which do not necessitate diagonally dominant matrices thus avoiding the need to formulate the problem in this way. Implicitly restarted Arnoldi methods can be used to solve both symmetric and nonsymmetric problems. The Jacobi-Davidson method and a truncated RQ algorithm allow for preconditioning. Both these methods seek to generalize Davidson's method to matrices that are nonsymmetric as well removing one of its drawbacks. That is, if the perfect preconditioner is used, namely the inverse of the matrix, the Davidson method stagnates. Another technique discussed was Lanczos which is applicable to non-Hermitian problems. The numerical analysts discussed the relationships between these various methods. In contrast to the above sparse methods, a number of speakers gave presentations on dense techniques. A key difference between sparse and dense techniques is that the latter ones require order n^2 storage, where n is the order of the matrix. The standard technique is to use the QR method though bisection is becoming increasingly popular due to the search for parallel methods. Alternative methods,

such as the Invariant Subspace Decomposition Algorithm (ISDA), were also presented.

Several talks focused on software available for performing the eigenproblem. ARPACK implements the Arnoldi method for symmetric, nonsymmetric, and complex cases. ABLE is a matlab program which uses the Lanczos approach for the non-Hermitian eigenvalue problem. For dense problems, LAPACK, the follow-on to EISPACK, has both symmetric and nonsymmetric eigensolvers. For parallel computations, PeIGS implements bisection for finding the eigenvalues and uses inverse iteration to get accurate eigenvectors. PRISM eigensolvers use the ISDA approach to find the complete eigensolution. The ScaLAPACK and PRISM projects are both working on parallel nonsymmetric eigensolvers. P_ARPACK, a parallel version of ARPACK, was also discussed. With a vision toward to future, the upcoming joint NSF/ARPA initiative for Optimized Portable Application Libraries (OPALs) which will use mathematical descriptions and manipulations to generate algorithmic variants and codes was discussed.

The interaction during the institute lead to a number of interesting ideas and observations. One area where the numerical analysts expressed interest is in creating sample test cases that represent real chemistry problems. While the institute successfully explained the nature of the problems, having real matrices to work with would allow for realistic testing of new methods and ideas for the eigenproblem. Another area of future interest is how to incorporate the insights on the nature of the problems into general eigensolvers. For example, how can a general package include preconditioners which are as good as the physical knowledge currently applied to specific chemistry applications? It was also noted that problem formulation tradeoffs made by computational chemists are currently outside the eigensolvers. It is an interesting long term question of how to more tightly integrate these two.

Overall, the Large-Scale Matrix Diagonalization Methods in Chemistry theory institute was considered a stimulating exercise by the participants. Everyone took advantage of the unique opportunity for interaction between the often disjoint work of computational chemists and numerical analysts. The interrelationships and differences between the diverse types of computational chemistry problems and potential eigensolvers was also made clear. It seems clear that the challenging nature of the chemistry problems envisioned requires concerted efforts by chemists, numerical analysts, and computer scientists to arrive at workable solutions.

Agenda

MONDAY: Building 200, Room J183

- 9:00 Introduction (C. Bischof, R. Shepard)
9:15 E. R. Davidson “Finding a Few Eigenvectors of Very Large Matrices”
- 10:15 *Break*
- 10:30 D. C. Sorensen “Algorithmic Foundations of Iterative Eigenvalue Solvers”
11:30 G. I. Fann “Current Issues in Parallel Eigensolver in Computational Chemistry”
- 12:00 *Lunch*
- 1:15 P. J. Knowles “Configuration Interaction in Molecular Electronic Structure”
2:00 A. Edelman “Interdisciplinary Scientific Computing Can Work”
- 2:45 *Break*
- 3:15 J. Olson “The Configuration Interaction Method in Electronic Structure”
4:00 Xiaobai Sun “Scaling and Squaring in Invariant Subspace Decomposition Methods”
4:30 A. Tsao “Can Application Libraries be Optimized AND Portable?”
- 5:00 *End of Sessions*
6:30 *Dinner at the Weinkeller Microbrewery*

TUESDAY: Building 200, Room J183

- 9:00 G. Schatz “Time Independent Scattering Calculations”
9:45 Z. Bai “Invariant Subspace Decomposition Method and Lanczos Method for Large Scale Nonsymmetric and Complex Symmetric Eigenvalue Problems”
10:15 R. Wyatt “Computation of High-Energy Eigenstates”
- 10:45 *Break*
- 11:00 P. Pulay “Three-Term Recursion Relations for Large Eigenvector Problems”
11:30 S. Huss-Lederman “MPI: Why It’s Different”
- 12:00 *Lunch (Cafeteria Room 1)*

1:15 R. J. Van De Geijn “Towards Usable and Lean Parallel Linear Algebra Libraries”
 2:00 E. L. Sibert “Highly Excited Vibrational States”
 2:30 V. Ortiz “Diagonalization Techniques in Electron Propagator Theory”

 3:00 *Break and move to MCS Bldg. 221*

 3:30 R. J. Harrison “Experiments with Multilevel Diagonalization”
 4:00 J. C. Light “DVR’s and FBR’s: Sparse vs. Full Representations”
 4:30 S. K. Gray “Iterative Diagonalization and Wave Packet Dynamics”

 5:00 *Cave Demo & Drinks in Interaction Room*
 7:00 *Conference Dinner at Connie’s Pizza*

WEDNESDAY: Building 200 Auditorium

9:00 C. Bischof “Parallel Orthogonal Matrix Reduction Techniques”
 9:30 T. Carrington “Calculating the Vibrational Energy Levels of Three- and Four-Atom Molecules with the Lanczos Algorithm”
 10:00 A. F. Wagner “Quantum Dynamics Studies”

 10:30 *Break (Group Photo outside Bldg. 200)*

 11:00 R. Shepard “The Subspace Projected Approximate Matrix (SPAM) Modification of the Davidson Method”
 11:30 R. B. Lehoucq “ARPACK: General Purpose Software for the Large Scale Eigenvalue Problem”

 12:00 *Lunch (Cafeteria Room 1)*

 1:15 J. Cullum “Matrix Eigenvalue Problems: Arnoldi versus Nonsymmetric Lanczos Algorithms”
 1:45 H. Dachsel “An Efficient Data Compression Method for the Davidson Subspace diagonalization Scheme”

 2:15 Open Discussion: “Where Are We and Where Do We Go?” led by I. Shavitt
 3:00 *Meeting Adjourns*

List of Attendees

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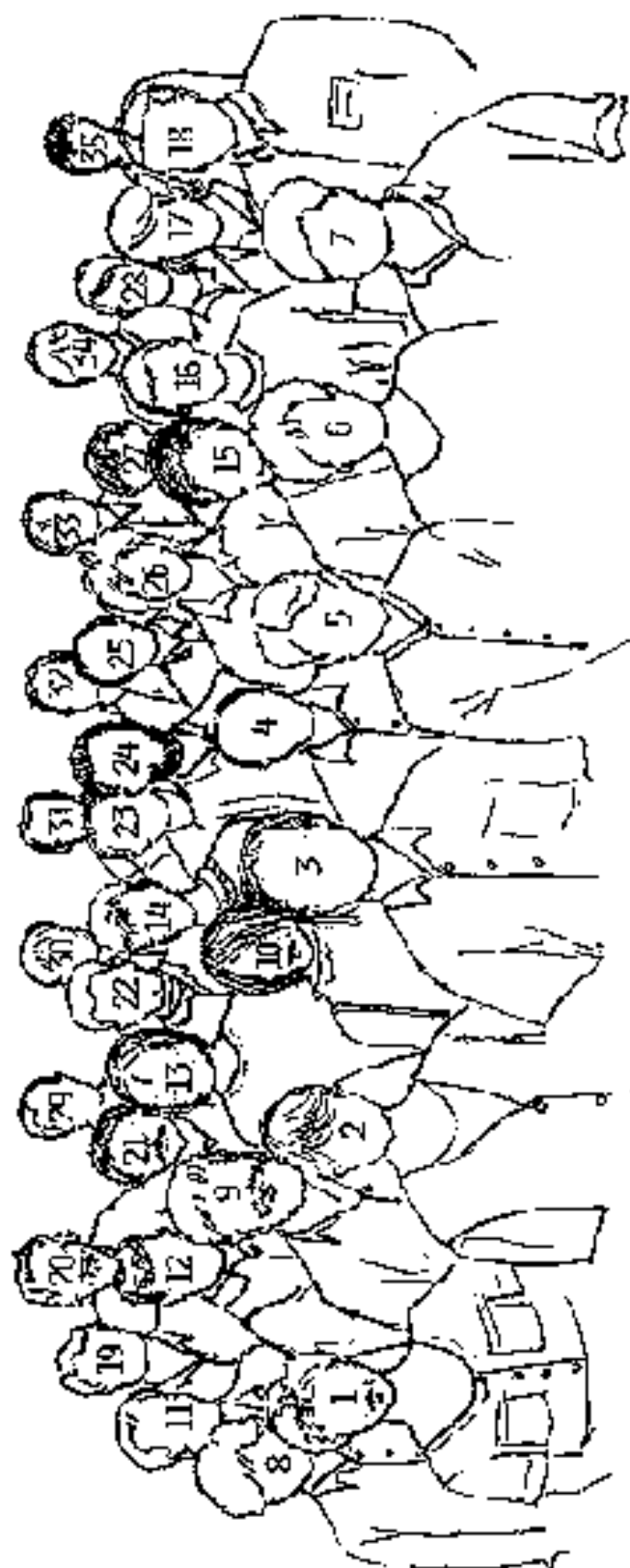
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| 2. Kristyn Naschott | 9. Darry Sorensen | 16. Y.-J. J. Wl | 23. Peter Pulay | 30. T. Carrington, Jr. |
| 3. Chris Fischhof | 10. Xiacbai Sun | 17. R. Van De Gelju | 24. Jeppe Olsen | 31. A. E. Wagner |
| 4. Zelah Shavitt | 11. Jeff Wilson | 18. Ron Shepard | 25. Robert Wyatt | 32. E. R. Davidson |
| 5. Stephen Gray | 12. C. V. Ortiz | 19. G. Kedziora | 26. E. L. Gilbert | 33. H. Dachselt |
| 6. S. Liu | 13. G. Whittier | 20. F. Sutton | 27. H. W. Jang | 34. Znsolun Sali |
| 7. D. H. Zhang | 14. P. C. Knowles | 21. K. Minkoff | 28. S. Huss-Lederer | 35. Alan Edelman |

Finding a Few Eigenvectors of Very Large Matrices

Ernest R. Davidson

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A brief history of the development of the “Davidson” method will be given along with recent attempts at improvement and analysis of convergence by other workers. Examples will be given of matrices for which it performs poorly. Suggestions will be made for improvements in the case that the number of eigenvectors desired is many greater than one, but many fewer than the squart root of the matrix dimension.

Algorithmic Foundations of Iterative Eigenvalue Solvers

D. C. Sorensen

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Recently, there have been a number of algorithmic developments in the numerical solution of large scale eigenvalue problems. The state of the art has advanced considerably and numerical software has begun to emerge for the nonsymmetric problem. Greatly improved software is also now available for symmetric and generalized problems. The algorithmic advances that have led to this improved software are based upon a better understanding of the connection between Krylov subspace projection, subspace iteration, and the QR-iteration. This talk will attempt to survey recent developments and relate them to the classic large scale iterative methods that have stemmed from the original Lanczos method.

The survey will include the Implicitly Restarted Arnoldi, Rational Krylov, and Jacobi-Davidson methods. The latter is a generalization of the well known Davidson method. It provides a means to utilize a preconditioned iterative solution to the shift-invert equations that needn't be solved accurately. The development of this capability is a very promising area of algorithmic research that could greatly increase our ability to solve very large scale problems.

Some Current Issues in Parallel Eigensolvers for Computation Chemistry

George Fann

Molecular Science Research Center
Pacific Northwest Laboratory
Richland, WA 99352

We survey implementations and software packages for parallel computers for solving all of the eigenvalues and eigenvectors of dense, real, standard symmetric eigensystem problems. There are three methods that are in popular use: 1) Householder reduction to tridiagonal form, bisection for eigenvalues, inverse iteration for tridiagonal eigenvectors (some form of orthonormalization for eigenvectors), and back transformation of the eigenvectors; 2) block 1-sided or 2-sided Jacobi iterations; and 3) spectral methods (e.g., sign functions, invariant subspace methods).

Let n denote the dimension of the matrix. Let p denote the number of parallel processors. If $n/p > 7$ the fastest method is type 1 above, Householder reduction + bisection + inverse iteration. For degenerate clusters of eigenvalues inverse iterations using random starting vectors can produce non-orthogonal eigenvectors and some form of orthonormalization must be performed. In chemistry applications, degenerate clusters of eigenvalues occur in the Fock matrices or in the current density fitting matrices. One of the fastest and most robust solvers in this category is PNNL's PeIGS software, which performs full parallel orthonormalization for degenerate cluster of eigenvalues. Other popular solvers of this type that do not orthonormalize across processors are SCALAPACK's PDSYEVX (which orthonormalize within each processor) and Intel's EISCUBE. Performance results on the Intel Paragon and the SGI-Cray T3D will be given.

Recent works by Hendrickson and Jessup and also the SCALAPACK team show that good performance and scaling are achievable with block Householder reduction algorithms in library quality codes. Currently, the fastest and the most scalable Householder reduction code was written by Hendrickson, Jessup and Smith; however, for $n/p < 8$ with fixed n and increasing p , the speedups of all current Householder reduction algorithms stop improving on computers such as the Intel Paragon. Recently, Singh and Parlett showed that it is possible to remove orthogonalization in many cases. Orthonormalizations can consume as much as 60% of the solution time for the PeIGS code on completely degenerate eigen-problems. As a consequence of Singh and Parlett's work, faster and improved serial algorithms have also been implemented.

For $n/p < 7$, the fastest, most robust and flexible method is the 1-sided block Jacobi method from Bush of the Daresbury Laboratory.

If the ratios of computation to communication latency and bandwidth remain the same for the next generation of parallel computers then spectral methods (e.g., PRISM or the sign function methods) will be important because these methods are based on matrix multiplication. We present performance and scaling results for matrix multiplication (modified van de Geijn's `sB_BLAS`) on the NERSC's T3D and CCSC's Paragon.

Interdisciplinary Scientific Computing Can Work

Alan Edelman

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Last year, Tomas Arias (Physics) and Alan Edelman (Math. Lab for Computer Science) created the MIT Advanced Numerics Physics Team with the goal of interdisciplinary collaboration in the fields of Physics, Computational Materials Science, Parallel Computing and Mathematics. Our mission was to create a truly interdisciplinary environment where new algorithms would be created, real codes would be written on high performance architectures, and new mathematical ideas would be studied. In this talk I will discuss the results of these efforts.

Scaling and Squaring in Invariant Subspace Decomposition Methods

Xiaobai Sun

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The increasing gaps in access time to data in different levels of memory hierarchy have left the room for the development of parallel solvers for dense eigenvalue problems such as the so called invariant subspace decomposition methods. In this talk, we introduce the matrix algebra underpinning the scaling and squaring techniques used in invariant subspace decomposition methods. The theory leads to an automatic scaling scheme for the method by Auslander and Tsao as a preprocess to scale the spectral into a normalized interval or region; it also leads to stand alone algorithms for decoupling an invariant subspace by automatically scaling and implicitly squaring the matrices involved in.

Acknowledgments

I thank Christian H. Bischof and Ron Shepard for organizing the workshop and inspiring the work introduced here. I also thank my colleagues on the PRISMproject (see <http://www.mcs.anl.gov/Projects/PRISM>) for sharing the ideas and experience on invariant subspace decomposition methods.

Eigenvalue Calculations in Collision Dynamics

George Schatz

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This talk will discuss two ways in which eigenvalue calculations are used in studying the collisions of atoms and molecules. We first consider the conventional use of eigenvalue calculations to determine vibration/rotation energies and wavefunctions for the fragments before and after collision. The Hamiltonian to be diagonalized is usually obtained by quadrature over basis functions, or by DVR. It is usually dense, with dimensions of a few thousand, and we typically want hundreds of eigenvalues and eigenfunctions. The second application is in the calculation of flux correlation functions. Miller has demonstrated that the rate constant may be obtained by summing the eigenvalues of a matrix that is roughly $(H - E + ie)^2$, where H is the Hamiltonian, E the energy, and e a small constant. The eigenvalues of this matrix are mostly large, but since it is the inverses of the eigenvalues that are summed, it is only the few small eigenvalues that are of interest. This leads to a numerically ill-behaved problem that has hindered practical use of this method.

**Invariant Subspace Decomposition Method and Lanczos Method
for Large Scale Nonsymmetric and Complex Symmetric Eigenvalue Problems**

Zhaojun Bai

James Demmel

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We will begin our presentation with a discussion of some large scale nonsymmetric and complex symmetric eigenvalue problems we have been working on recently. These eigenvalue problems come from quantum chemistry, physics, electrical engineering and other areas of computational science and engineering. They are challenging from the view points of mathematical theory, numerical algorithms, software development and availability of computer resources. We will discuss numerical techniques in invariant subspace decomposition method and Lanczos method for solving these large scale eigenvalue problems. Software availability and performance benchmarks in both serial and parallel computing environment will also be presented.

Computation of High-Energy Molecular Eigenstates

Robert E. Wyatt

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The study of high-energy molecules is the focus of considerable effort in physical chemistry. On the theoretical side, the goal is to compute the interior eigenpairs associated with the large Hamiltonian matrix. The dimension of \mathbf{H} can range from several thousand to several million. The present study will emphasize applications of the Lanczos algorithm driven by a spectral filter, $f(\mathbf{H})$. The filter is designed to pick out eigenvalues near a test input energy E . A successful filter is the system Green function, $(E\mathbf{1}-\mathbf{H})^{-1}$. Application of this strategy to a large molecular application will be described. In addition, results from a parallel version of this code will be described.

Applications of Three-Term Recursion Relation and Pseudodiagonalization in *ab initio* Quantum Chemistry

Peter Pulay

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Two topics will be reviewed. The first is the inclusion of the 3-term recursion relation familiar from the theory of conjugate gradients in the Davidson eigenvector method [1] for large matrices (dimension over 10^6) [2, 3, 4, 5]. The primary goal of this is to save storage space which is a bottleneck in full CI or large multi-reference CI calculations [6].

The second topic is the application of pseudodiagonalization, familiar from semiempirical theory [7] in large-scale SCF (and DFT) calculations. Three recent developments will soon eliminate the dreaded “integral bottleneck” from SCF-type theories. (1) the progress to large molecules, enabled by increased computer power, which leads to the milder asymptotic $O(N^2)$ scaling instead of $O(N^4)$; (2) parallelization of integral and Fock matrix calculation; (3) new methods of constructing Coulomb and Fock matrices. Thus the $O(N^3)$ matrix diagonalization becomes the rate-determining step for large calculations. Shepard [8] has recently formulated a method, based on Bacskay’s second order SCF theory, which avoids the diagonalization bottleneck. I will summarize our experience with pseudodiagonalization, based on first-order SCF theory. This method was implemented for the parallel calculation of NMR chemical shifts. [9]

References

- [1] E. R. Davidson, *J. Comput. Phys.*, **17**, 87 (1975).
- [2] S. Saebo and P. Pulay, *J. Chem. Phys.*, **86**, 914 (1987).
- [3] J. H. van Lenthe and P. Pulay, *J. Comp. Chem.* **11**, 1164 (1990).
- [4] C. W. Murray, S. C. Racine and E. R. Davidson, *J. Comp. Phys.* **103**, 382 (1992).
- [5] J. M. Bofill and J. M. Anglada, *Chem. Phys.* **183**, 19 (1994).
- [6] R. Shepard, *J. Comp. Chem.* **11**, 45 (1989).
- [7] J. Stewart, P. Császár, and P. Pulay, *J. Comp. Chem.* **3**, 227 (1982).
- [8] R. Shepard, *Theor. Chim. Acta* **84**, 343 (1993).
- [9] K. Wolinski, R. Haacke, J. F. Hinton, and P. Pulay, to be published.

**Towards Usable and Lean Parallel
Linear Algebra Libraries**

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In this talk, we introduce a new parallel library effort, as part of the PLAPACK and PRISM projects, that attempts to address discrepancies between the needs of applications and parallel libraries. A number of contributions are made, including a new approach to matrix distribution, new insights into layering parallel linear algebra libraries, and the application of “object based” programming techniques which have recently become popular for (parallel) scientific libraries. We present an overview of a prototype library, the SL_{library}, which incorporates these ideas. Preliminary performance data shows this more application-centric approach to libraries does not necessarily adversely impact performance, compared to more traditional approaches.

Highly Excited Vibrational States of Polyatomic Molecules

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Variational treatments of highly excited vibrational states are reviewed. Using the water molecule as an example of three anharmonically coupled harmonic oscillators, normal mode product basis functions are introduced to obtain a matrix representation of the Hamiltonian. The shortcomings and advantages of this representation are discussed. Other coordinate choices and basis sets, in particular the discrete variable representation, are reviewed. The vibrational states for a planar molecule of acetylene are calculated using the discrete variable representation for the bending degrees of freedom. Perturbative treatments of molecular vibrations are also considered. The vibrations of acetylene and carbon dioxide molecules were used to illustrate the strengths and weaknesses of this method.

Diagonalization Techniques in Electron Propagator Theory

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Propagator methods in quantum chemistry determine transition energies and probabilities without wavefunctions or total energies for individual states. Propagator poles and residues may be obtained from a generalized eigenvalue problem where techniques developed for large configuration interaction calculations can sometimes be adapted. Solution of the Dyson equation is equivalent to a partitioning of the eigenvalue problem occurring in electron propagator theory. Quasiparticle approximations may be recovered by a simple restriction of the ionization operator space. Pole search techniques for the Dyson equation that depend on the evaluation of derivatives of the self-energy matrix are shown to be highly efficient for outer valence ionization energies and electron affinities. In the random phase approximation of the polarization propagator, where excitation energies and transition moments are calculated, two approaches have been taken. In the first, a generalized eigenvalue problem with a non-positive metric matrix is considered. In the second, an ordinary eigenvalue problem with a nonsymmetric matrix is solved. Algorithms corresponding to these distinct approaches are compared.

Experiments with Multilevel Diagonalization

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I will describe the results of some experiments using full multilevel diagonalization methods with application to matrices generated from both numerical wavefunctions and selected-CI Hamiltonians.

DVRs and FBRs: Sparse vs. Full Representations

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In quantum dynamics of molecular systems, the solutions of PDEs (the Schrodinger equation) in up to six dimensions are desired in some finite region of coordinate space. Basis set expansions (FBRs) produce full matrix representations of the eigenvalue problems. For direct product representations, these can be converted to sparse discrete variable representations (DVRs) which can be solved more easily. I will discuss briefly the relation between FBRs, DVRs, collocation, and their applicability to various multidimensional problems.

Iterative Diagonalization and Wave Packet Dynamics

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Some connections between iterative diagonalization techniques and wave packet dynamics are noted. A particularly interesting connection, in my view, results when wave packet dynamics is written in the form of a (Chebyshev) three-term recursion. An old iterative method (“spectroscopic eigenvalue analysis”) due to Lanczos is then seen to be intimately related to the wave packet dynamics of a certain preconditioned Hamiltonian operator.

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Parallel Orthogonal Matrix Reduction Techniques

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In the context of the PRISM (Parallel Research into Invariant Subspace Methods) project, we are pursuing the development of algorithms and codes to compute the eigen-decomposition of symmetric matrix and the reduction of a symmetric matrix to banded and tridiagonal form. We give an overview of the PRISM approach and the computational approaches used to implement invariant subspace reduction, one of the kernels at the heart of this approach. As it turns out, the invariant subspace computation can be achieved very efficiently through a technique called Successive Bandreduction (SBR), which efficiently addresses general band reduction scenarios. We present results on parallel machines and present directions of future research.

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The Subspace Projected Approximate Matrix (SPAM) Modification of the Davidson Method

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A modification of the Davidson subspace expansion method, a Ritz approach, is proposed in which the expansion vectors are computed from a “cheap” approximating eigenvalue equation. This approximate eigenvalue equation is assembled using projection operators constructed from the subspace expansion vectors. The method may be implemented using an “inner/outer” iteration scheme, or it may be implemented by modifying the usual Davidson algorithm in such a way that exact and approximate matrix-vector product computations are interspersed. A multi-level algorithm is proposed in which several levels of approximate matrices are used. Examples are presented for the single-eigenvector computation step of rational-function direct-SCF wave function optimization in which the number of exact matrix-vector products is reduced by a factor of 3 compared to the usual Davidson approach.

ARPACK: General Purpose Software for the Large Scale Eigenvalue Problem

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An overview of the ARPACK software package along with some applications is presented. ARPACK is a collection of Fortran77 subroutines designed to solve large scale eigenvalue problems. The software is capable of solving large scale symmetric, nonsymmetric, and generalized eigenproblems from significant application areas. The software is designed to compute a few (k) eigenvalues with user specified features such as those of largest real part or largest magnitude. Storage requirements are on the order of $n*k$ locations. No auxiliary storage is required. A set of Schur basis vectors for the desired k -dimensional eigenspace is computed which is numerically orthogonal to working precision. Numerically accurate eigenvectors are available on request.

Matrix Eigenvalue Problems: Arnoldi Versus Nonsymmetric Lanczos Algorithms

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We consider two types of iterative procedures, Arnoldi and nonsymmetric Lanczos, which have been developed for large scale nonsymmetric eigenvalue computations $Ax = \lambda x$. We present theoretical and numerical comparisons between these methods. We prove that, in exact arithmetic, any type of convergence behavior which can be obtained using a nonsymmetric Lanczos procedure can also be obtained using an Arnoldi procedure but on a different matrix and with a different starting vector. Therefore, in this global sense, the convergence behavior of these two methods is the same.

Numerical experiments by other researchers, for example, L. Trefethen and F. Chatelin, have demonstrated that the convergence of iterative methods for solving either $Ax = b$ or $Ax = \lambda x$ can be adversely affected when A is highly nonnormal. It is therefore of interest to relate the behavior of either of these methods on any matrix to their behavior on normal matrices. We derive two results related to such comparisons.

In practical applications, however, we are interested in comparisons of these methods when they are applied to the same matrices, and in any changes in convergence behavior which may occur as we vary the nonnormality of the matrices. Therefore, we use an invariance property shared by both types of procedures to obtain a set of test matrices which allows us to make such comparisons. Through a set of numerical experiments using these test matrices, we consider the behavior of these types of procedures when they are applied to the same matrices.

Our limited experiments indicate that a Lanczos eigenvalue method may be less sensitive to changes in the nonnormality of the test matrices we use than an Arnoldi method is, and that approximations generated by an Arnoldi method may behave better than those generated by a Lanczos method when the test matrices are normal or near normal. The experiments also illustrate that the convergence behavior of either method is a complicated function of the choice of the starting vector, the nonnormality of the matrix, and the finite precision of the arithmetic.

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