From Self Consistency to SOAR: Solving Large Scale Nonlinear Eigenvalue Problems

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What is common among electronic structure calculation, design of MEMS devices, vibrational analysis of high speed railways, and simulation of the electromagnetic field of a particle accelerator? The answer: they all require solving large scale nonlinear eigenvalue problems. In fact, these are just a handful of examples in which solving nonlinear eigenvalue problems accurately and efficiently is becoming increasingly important.

Recognizing the importance of this class of problems, an invited minisymposium dedicated to nonlinear eigenvalue problems was held at the 2005 SIAM Annual Meeting. The purpose of the minisymposium was to bring together numerical analysts and application scientists to showcase some of the cutting edge results from both communities and to discuss the challenges they are still facing.

The minisymposium consisted of eight talks divided into two sessions. The first three talks focused on a type of nonlinear eigenvalue problem arising from electronic structure calculations. In this type of problem, the matrix Hamiltonian H depends, in a non-trivial way, on the set of eigenvectors X to be computed. The invariant subspace spanned by these eigenvectors also minimizes a total energy function that is highly nonlinear with respect to X on a manifold defined by a set of orthonormality constraints. In other applications, the nonlinearity of the matrix eigenvalue problem is restricted to the dependency of the matrix on the eigenvalues to be computed. These problems are often called *polynomial* or *rational* eigenvalue problems.

Currently, the most widely used method for tackling the electronic structure problem is the *Self Consistent Field* (SCF) iteration. The method solves a sequence of linear eigenvalue problems associated with the fixed Hamiltonian $H(X_i)$, where X_i is the approximation (to X) obtained in the previous iteration. At convergence, the difference between $H(X_i)$ and $H(X_{i-1})$ becomes negligible, i.e., the eigenvectors associated with the desired eigenvalues of $H(X_i)$ become *self-consistent*.

However, the convergence of SCF is not guaranteed. For many systems, the SCF iteration often fails to converge. Chao Yang, a staff scientist at Lawrence Berkeley National Laboratory (LBNL), presented an alternative approach he and collaborators Juan Meza and Ling-wang Wang (both at LBNL) recently developed. In their approach, the desired eigenvectors are obtained through a direct minimization of the total energy function. The algorithm they use projects the total energy function into a sequence of subspaces of small dimensions. By minimizing the total energy function within each of these subspaces, one can avoid solving a sequence of large linear eigenvalue problems. Furthermore, minimizing the total energy function directly also avoids some of the convergence problems encountered in SCF.

Robert Harrison, a computational chemist at the Oak Ridge National Laboratory and the University of Tennessee at Knoxville, who is also one of the original developers of the widely used chemistry package NWChem presented a novel approach to electronic structure calculation. He showed that by formulating the problem as an integral equation, one can avoid many difficult numerical issues associated with the differential operator. In particular, the smallest eigenvalues of the differential operator become the largest eigenvalues of the integral operator (which still depends nonlinearly on the eigenvectors to be computed). These eigenvalues tend to converge more rapidly. Furthermore, the smooth and rapid decay of the Green's function associated with the bound-state Helmholtz equation used in his formulation makes it possible to

represent the integral kernel by multi-wavelet basis. As a result, the convolution computation can be carried out efficiently using special multi-resolution techniques.

For certain type of nanoscale structures such as semiconductor pyramid quantum dots in which the carriers are confined in all three dimensions, the nonlinear eigenvalue problem that characterizes the wave equation associated with a single electron in the conducting band can be simplified to a rational eigenvalue problem in which the Hamiltonian depends merely on the eigenvalues to be computed. Heinrich Voss, a professor from the University of Hamburg, Germany, discussed the latest advances in solving this type of eigenvalue problem. In particular, he presented a nonlinear Arnoldi algorithm, the Jacobi-Davidson (JD) algorithm and a modified version of JD algorithm. He compared the performance of these different approaches, and pointed out that one should take advantage of the minimax characterization of the nonlinear eigenvalue problem when symmetry is present in the problem. His discussion on using the JD algorithm to solve general nonlinear eigenvalue problem was further elaborated by Professor Henk Van der Vorst from Utrecht University, the Netherlands who provided both theoretical background and numerical examples of using JD to solving polynomial eigenvalue problems.

David Bindel, a graduate student from University of California at Berkeley presented his latest approach to solving a complex symmetric *quadratic* eigenvalue problem arising from the simulation of resonance on microelectronic mechanical (MEMS) devices. High-frequency electromechanical resonators are important components in modern communication systems such as radio frequency (RF) ID tags and cell phones. Due to the latest advances in surface micromachining technology, it possible that, in the near future, we will have "Dick Tracy" phones that are smaller and require less power than today's cell phones. For these designs to work, it is necessary to minimize the amount of damping in the resonant components. While there are several tools that allow engineers to estimate the resonant frequencies of these devices, far fewer tools exist to estimate damping. Calculations of the damped resonances of such coupled-domain devices typically involve nonlinear eigenvalue problems with a variety of special structures.

In the second session, Christian Mehl from Technical University of Berlin described numerical techniques for solving a special type of polynomial eigenvalue problem arising from vibration analysis of rail tracks excited by high-speed trains. This problem—also highlighted in a plenary talk given by Volker Mehrmann, also from Technical University of Berlin—was described in the November 2004 issue of SIAM News (see "Accurate Eigenvalues for Fast Trains" by Ilse Ipsen). Yangfeng Su, a professor at Fudan University, China presented the latest results on structure-preserving methods for computing eigenvalues of skew-Hamiltonian and Hamiltonian (SHH) pencils. This type of eigenvalue problem arises from the passivity analysis of VLSI circuits and from complex gyroscopic quadratic eigenvalue problems. Liequan Lee, a computational scientist from the Stanford Linear Accelerator Center discussed the need for solving nonlinear eigenvalue problems arising from accelerator cavity design, a project currently funded by the U.S. Department of Energy's Scientific Discovery through Advanced Computing (SciDAC) program.

These three talks shared the common theme that many nonlinear eigenvalue problems possess special matrix structures and spectral properties. For example, the polynomial eigenvalue problem arising from the rail track vibrational analysis are known as *palindromic* eigenvalue problems due to the symmetric pattern of the polynomial. As a result, the desired eigenvalues are *symplectic*, i.e., if λ is an eigenvalue, so is λ^{-1}. Although some of these problems can be reduced or transformed into an equivalent linear eigenvalue problem, applying the standard

algorithm to these linear eigenvalue problems often destroys the special properties of the eigenvalue associated with the original nonlinear problem. Thus, it is highly desirable to develop numerical algorithms that can preserve the structures of the original problems and desired eigenvalues. Mehl discussed using a combination of a Jacobi-like algorithm and a technique originally developed by Alan Laub for computing Hamiltonian Schur form to solve palindromic eigenvalue problems. Su presented a structure-preserving method for solving eigenproblem of SHH pencils. Lee presented simulation results on using the Second Order Arnoldi (SOAR) method, developed by Zhaojun Bai and Su, to solve a quadratic eigenvalue problem (QEP) arising from the design of accelerator cavities with a single external waveguide coupling. The order of the QEP is roughly 3.2 million. With SOAR, the computation can be completed in two hours on a 256-node supercomputer with 400GB memory. This is several times faster than previous approaches. When the cavity is coupled with more than one external source, the corresponding eigenvalue problem becomes more complex. Lee presented simulation results obtained from using both the nonlinear Arnoldi iteration and a simple self consistent iteration, and pointed out that more research is required to understand the underlying structure of this type of nonlinear eigenvalue problem. These additional insights may be used to develop more effective solution strategies.

The SIAM minisymposium on nonlinear eigenvalue problem generated great interest and enthusiasm among both numerical analysts and application scientists at the meeting. It is evident from the minisymposium that the rapid growth in computing power and the advances in numerical algorithms have enabled application scientists and industrial practitioners to introduce additional complexity in their computational models to account for more complex and nonlinear phenomena. As computational tools for solving linear eigenvalue problems become mature, the research focus of the eigenvalue computation community is gradually shifting towards the development of methodologies for dealing with nonlinearity. Among the challenges faced by numerical analysts are the standard convergence issues as well as the need for developing algorithms that are capable of preserving structures of the eigenvalue problem.

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