Please describe (in no more than 300 words) your field of interest and its relationship to the following characterization of computational science "Computational science involves the innovative and essential use of high-performance computation, and/or the development of computational technologies, to advance knowledge or capabilities in a scientific or engineering discipline".

Current research into the solution of the molecular Schrödinger equation, one of the grand challenges of computational science, is limited because of the storage of the parameters describing the N-particle wavefunction and the huge number of iterations required for its solution. For correlated calculations, necessary for accurate physical predictions, chemists are currently limited to molecules with fewer than twenty electrons, even with large supercomputers [1]. This problem can be simplified by elimination the N-electron wavefunction in favor of the two-particle reduced-density-matrix (2-RDM) [2], which scales only as the fourth power in the number of electrons. The variational solution of quantum systems using the 2-RDM is extremely difficult due to the N-representability problem [3], which characterizes the difficulty of finding the appropriate set of 2-RDMs over which to minimize the energy. Recently, semidefinite programming has been used to accurately calculate properties of small molecules without using wavefunctions [4]. A new paradigm in semidefinite programming [5] has allowed the solution of the approximate Schrödinger equation using desktop computers for systems which previously required huge supercomputers by reduced the scaling with respect to system size from the 12^{th} power to the 6^{th} power.

I am currently working to implement the fast semidefinite programming algorithm developed in our group in parallel using supercomputers so that I can address quantum mechanical phenomena in chemistry and physics not accessible by other methods, such as DFT and perturbative techniques. Because the reduced-density-matrix approach is not limited to molecular calculations, and because semidefinite programming is used not only by physical scientists, but also economists and industrial engineers, the parallel implementation of our code will make a broad contribuation to many aspects of computational science.

In additional to computational research, I am extending my previous work on open-shell calculations [6] to atmospheric chemistry and combustion problems and applying new, more

accurate theories [7] to molecular problems. The long-term prospect of my research is a highly accurate and widely applicable quantum chemistry method which does not involve matrix diagonalization, thus avoid one of the greatest computational bottlenecks currently limiting this typ eof research.

[1] Zhengting Gan, Yuri Alexeev, Mark S. Gordon, and Ricky A. Kendall*, J. Chem. Phys.* **119**, 47 (2003).
[2] D. A. Mazziotti and Robert M. Erdahl, *Phys. Rev. A* **63**, 042113 (2001).
[3] A. J. Coleman and V. I. Yukalov, *Reduced Density Matrices: Coulson's Challenge* (Springer Verlag, New York, 2000).
[4] D. A. Mazziotti, *Phys. Rev. A* **65**, 062511 (2002).
[5] S. Burer and R. D. C. Monteiro, *Math. Program.* **95**, 329 (2003); D. A. Mazziotti, *Phys. Rev. Lett.* **93**, 213001 (2004); D. A. Mazziotti, *J. Chem. Phys.* **121**, 10957 (2004).
[6] J. R. Hammond and D. A. Mazziotti, in preparation.
[7] J. R. Hammond and D. A. Mazziotti, accepted by *Phys. Rev. A*.

Program of Study

Please describe (in no more than 300 words) how the courses listed in your planned program of study will contribute to the research in your field of interest.

My research involves computational solution of very large systems of equations describing quantum mechanical phenomena. My program of study contains courses involving both the physical and computational aspects of my research. My first year curriculum was devoted to understanding chemical phenomena using physics, specfically, group theory, quantum mechanics and statistical mechanics. The computational chemistry course offered in our department is an excellent background in to computational methods for quantum dynamics, electronic structure and molecular dynamics. In addition, I took a course on functional analysis for physicists to increase my mathematical proficiency.

This year, my coursework will provide me with the tools with which to implement my research using advanced computational techniques. Scientific Parallel Computing will contributed directly to my ability to use MPI to distribute computational tasks over large networks. Numerical Computation provides me with a better understanding of statical

methods for mathematical computation. Future coursework in Algorithms and Optimization will enhance the computational toolkit from which I can draw for future research. Courses in quantum computational and materials chemistry have or will extend my understanding of the far reaching computational and physical consequences of my research.

High-Performance Computation and Research

Please describe (in no more than 300 words) how high performance computing will impact your research. Assume for example you had unlimited access to a machine such as Seaborg at the National Energy Research Scientific Computing Center or Phoenix at Oakridge National Laboratory. What impact would such access have on your research?

The computational advances in my research group have allowed the computational solution of physical problems previously only accessible on EarthSim to be done on a Dell desktop because of the r^12 to r^6 reduction in computational scaling with respect to system size. If given unlimited resources on a supercomputer, I would be able to solve the approximate molecular Schrödinger equation for large systems to an accuracy that could only be dreamed of only a few years ago.

My current research into the simplication of the reduced-density-matrix formulation of molecular quantum mechanics using spin-adaptation allows a two-fold speedup with respect to previous implementations of this theory. My coursework in parallel scientific computation will give me the tools to distribute the computational work associated with solid-state physics and large biomolecules over large computing networks, allowing their solution in reasonable time periods. In the afforementioned course, I will interact with the staff of Argonne National Laboratory regarding their development of parallel computing technology. I hope that this will develop into a collaboration to combine their computational resources and parallel libraries to our efficient semidefinite programming code.