Department of Mathematical Sciences Colloquium

Tenure-track faculty position candidate in Computational Mathematics

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Accelerating Self-Consistent-Field Calculations Using Chebyshev-Filtered Subspace Iteration

Density-functional theory (DFT) has enjoyed great success in condensed matter physics, material science, and quantum chemistry.

There has been intense interest in applying DFT for electronic structure calculations to increasingly larger systems. However, applying DFT to very large systems can be overwhelmingly expensive, because of the high computational demands of solving a large eigenvalue problem within each self-consistent-field (SCF) iteration.

In this talk, we present a recently developed Chebyshev-filtered subspace iteration method. This method replaces the explicit eigenvalue-eigenvector calculations by directly approximating the basis of the desired eigensubspace using adaptive Chebyshev polynomials. In this approach, only the first SCF iteration requires solving an eigenvalue problem, for the purpose of providing a suitable initial subspace. No iterative eigensolvers are required for the remaining SCF iterations. Avoiding these expensive eigenvalue problems leads to significant speedup in SCF calculations. More than a ten-fold speedup over existing eigensolver-based methods is routinely obtained. More significantly, the new method enables us to perform a class of highly challenging DFT calculations that were not feasible before.

**Tuesday, February 21, 2006, at 1:30 pm in BUSN 312
The University of Texas at El Paso**

Please note the unusual room, day, and time for the Colloquium.

Refreshments will be served in front of the colloquium room 15 minutes before the start of the colloquium.

For further information, please contact Dr. Pavel Šolín, Bell Hall 220. Phone: (915) 747-6770, email: `solin@utep.edu`.