TEMPLE UNIVERSITY
Department of Mathematics

Applied Mathematics and Scientific Computing Seminar

Room 617 Wachman Hall

Wednesday, 9 February 2011, Special Time 3:00 p.m.

Efficiently Generating a Million Preconditioners for Quantum Monte Carlo Simulations

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Abstract.

I will briefly introduce the Quantum Monte Carlo method for electronic structure computations and recent improvements to reduce the computational cost for larger systems. The main cost of Quantum Monte Carlo methods for electronic structure is in constructing a sequence of matrices, called Slater matrices, and computing the ratios of determinants for successive Slater matrices. This ratio determines the acceptance/rejection step in the Metropolis algorithm. Recent work has reduced the scaling of constructing Slater matrices for insulators to linear in the number of particles. However, computing determinant ratios remains cubic in the number of particles. With the long term aim of simulating much larger systems, we improve the scaling of computing the determinant ratios by using preconditioned iterative solvers. The crucial development is the efficient computation and adaptation of a long sequence of preconditioners for the Slater matrices. We discuss a combination of techniques to update preconditioners efficiently, recompute preconditioners occasionally, and reorder matrices when they are (too) far from diagonally dominant.

This is joint work with Kapil Ahuja (VT), David Ceperley (UIUC), Bryan Clark (Princeton), and Jeongnim Kim (UIUC)