Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

Data Parallel Real Symmetric Eigensolver for Approximate Eigen-Solutions in SCF[1] YIHUA BAI, Department of Mathematics and Computer Science, Indiana State University, GUOPING ZHANG, Department of Physics, Indiana State University — Solving large real symmetric eigenvalue problems is a demanding and time consuming task in electronic structure calculations. For example, when using the Su-Schrieffer-Heeger(SSH) model to study the fundamental properties of trans-polyacetylene (trans- PA), as well as many other materials, the size of Hamiltonian matrix increases with the chain length of the material and can become very large. A data parallel divide-and-conquered eigensolver has been developed for eigen-decomposition of real symmetric matrices with strong locality properties like those generated from trans- PA, that is, matrix elements with larger magnitudes are closer to the diagonal. This eigensolver computes the approximate eigen-solutions of real symmetric matrices to user prescribed accuracy tolerance. Performance tests show that this new implementation scales up well and is extremely efficient for the computation of electronic spectrum of trans-PA compared to traditional dense eigensolvers. In some cases, the savings is order of magnitude, with the potential of saving significant amount of computation time in iterative methods like SCF.

[1]Supported by the U. S. Army Research Office under Contract No. W911NF041038 and DOE grant No. DE-FG02-06ER46304.

Yihua Bai
Department of Mathematics and Computer Science, Indiana State University

Date submitted: 10 Nov 2006 Electronic form version 1.4