Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

A scalable sparse eigensolver for petascale applications MURAT KECELI, Chemical Sciences and Engineering Division, Argonne National Laboratory, Lemont, Illinois 60439, HONG ZHANG, PETER ZAPOL, Mathematics and Computational Science Division, Argonne National Laboratory, Lemont, Illinois 60439, DAVID DIXON, Department of Chemistry, The University of Alabama, Tuscaloosa, Alabama 35487, ALBERT WAGNER, Chemical Sciences and Engineering Division, Argonne National Laboratory, Lemont, Illinois 60439 — Exploiting locality of chemical interactions and therefore sparsity is necessary to push the limits of quantum simulations beyond petascale. However, sparse numerical algorithms are known to have poor strong scaling. Here, we show that shift-and-invert parallel spectral transformations (SIPs) method can scale up to two-hundred thousand cores for density functional based tight-binding (DFTB), or semi-empirical molecular orbital (SEMO) applications. We demonstrated the robustness and scalability of the SIPs method on various kinds of systems including metallic carbon nanotubes, diamond crystals and water clusters. We analyzed how sparsity patterns and eigenvalue spectrums of these different type of applications affect the computational performance of the SIPs. The SIPs method enables us to perform simulations with more than five hundred thousands of basis functions utilizing more than hundreds of thousands of cores. SIPs has a better scaling for memory and computational time in contrast to dense eigensolvers, and it does not require fast interconnects.

Murat Keceli
Chemical Sciences and Engineering Division,
Argonne National Laboratory, Lemont, Illinois 60439

Date submitted: 17 Nov 2014 Electronic form version 1.4