Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Spectral Gauss quadrature method with subspace interpolation for Kohn-Sham Density functional theory XIN WANG, US Army Rsch Lab - Aberdeen — Algorithms with linear-scaling ($\mathcal{O}(\mathcal{N})$) computational complexity for Kohn-Sham density functional theory (K-S DFT) is crucial for studying molecular systems beyond thousands of atoms. Of the $\mathcal{O}(\mathcal{N})$ methods that use a polynomial-based approximation of the density matrix, the linear-scaling spectral Gauss quadrature (LSSGQ) method (Suryanarayana *et al.*, JMPS, 2013) has been shown to exhibit the fastest convergence. The LSSGQ method requires a Lanczos procedure at every node in a real-space mesh, leading to a large computational pre-factor. We propose a new interpolation scheme specific to the LSSGQ method that lift the need to perform a Lanczos procedure at every node in the real-mesh. This interpolation will be referred to as subspace interpolation. The key idea behind subspace interpolation is that there is a large overlap in the Krylov-subspaces produced by the Lanczos procedures of nodes that are close in real-space. The subspace interpolation scheme takes advantage of the block-Lanczos procedure to group the Krylov-subspaces from a few representative nodes to approximate the density matrix over a large collection of nodes. Subspace interpolation outperforms cubic-spline interpolation by several orders of magnitude.

Xin Wang
US Army Rsch Lab - Aberdeen

Date submitted: 22 Dec 2015 Electronic form version 1.4