Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Petascale orbital-free density functional theory enabled by small-box techniques MOHAN CHEN, MAE, Princeton University, Princeton, NJ, 08544, USA, XIANG-WEI JIANG, Institute of Semiconductors, Chinese Academy of Sciences, Beijing, China, HOULONG ZHUANG, MAE, Princeton University, NJ, 08544, USA, LIN-WANG WANG, Materials Science Division, LBNL, CA, 94720, USA, EMILY CARTER, MAE, Program in Applied and Computational Mathematics, and the Andlinger Center for Energy and the Environment, Princeton University, NJ, 08544, USA — Orbital-free density functional theory (OFDFT) is a quantum-mechanics-based method that utilizes electron density as its sole variable. The main computational cost in OFDFT is use of the ubiquitous fast Fourier transform (FFT), which is mainly used to evaluate the kinetic energy density functional (KEDF) and electron-electron Coulomb interaction terms. We design and implement a small-box FFT (SBFFT) algorithm to overcome the parallelization limitations of traditional FFT algorithms. In addition, a real-space truncation of the non-local Wang-Teter KEDF kernel is proposed. The scalability of SBFFT is demonstrated by efficiently simulating one full optimization step (electron density, forces, and stresses) of 1,024,000 lithium (Li) atoms on up to 131,072 cores. Other tests include calculations of physical properties of different phases of bulk Li, geometry optimizations of nanocrystalline Li, and molecular dynamics simulations of liquid Li samples. All of the tests yield excellent accuracy compared to the original OFDFT calculations, suggesting that the OFDFT-SBFFT algorithm opens the door to first-principles simulations of materials containing millions of atoms.

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Date submitted: 06 Nov 2015 Electronic form version 1.4