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Implementation of the Small Box Fast Fourier Transformation Method within Orbital-Free Density Functional Theory MOHAN CHEN, Princeton University, XIANG-WEI JIANG, State Key Laboratory of Superlattices and Microstructures, Institute of Semiconductors, Chinese Academy of Sciences, LIN-WANG WANG, Material Science Division, Lawrence Berkeley National Laboratory, EMILY CARTER, Princeton University — Orbital-Free density functional theory (OFDFT) is a first-principles quantum mechanics method that uses the electron density as its only variable. The main computational cost in OFDFT are Fast Fourier Transforms (FFTs), used to evaluate both the kinetic energy density functional and the Coulomb term. The Small Box Fast Fourier Transform (SBFFT) technique is a newly developed method for solving the Poisson equation using a large number of processors [1]. We further adopt this SBFFT for the non-local kinetic energy density functional (KEDF) term frequently used in OFDFT, for which multiple FFTs are required. An efficient truncation of a real space KEDF kernel is proposed in order to take the advantage of SBFFT. This new method yields similar results as the original OFDFT formulation, as tested on bulk crystals, defects, and surfaces. Finally, we report progress in implementing all the mentioned techniques in PROFESS (PRinceton Orbital-Free Electronic Structure Software) [2]. [1] Xiang-Wei Jiang, Shu-Shen Li and Lin-Wang Wang, Comp. Phys. Comm. (in press). [2] L. Hung, C. Huang, I.Shin, G. Ho, V. L. Ligneres, and E. A. Carter, Comput. Phys. Comm., 181, 2208 (2010).

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