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GPU-Accelerated Large-Scale Electronic Structure Theory on Titan with a First-Principles All-Electron Code[1] WILLIAM PAUL HUHN, BJÖRN LANGE, VICTOR YU, VOLKER BLUM, MEMS Department, Duke University, SEYONG LEE, Computer Science and Math Division, Oak Ridge National Laboratory, MINA YOON, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory — Density-functional theory has been well established as the dominant quantum-mechanical computational method in the materials community. Large accurate simulations become very challenging on small to mid-scale computers and require high-performance compute platforms to succeed. GPU acceleration is one promising approach. In this talk, we present a first implementation of all-electron density-functional theory in the FHI-aims code for massively parallel GPU-based platforms. Special attention is paid to the update of the density and to the integration of the Hamiltonian and overlap matrices, realized in a domain decomposition scheme on non-uniform grids. The initial implementation scales well across nodes on ORNL's Titan Cray XK7 supercomputer (8 to 64 nodes, 16 MPI ranks/node) and shows an overall speed up in runtime due to utilization of the K20X Tesla GPUs on each Titan node of 1.4x, with the charge density update showing a speed up of 2x. Further acceleration opportunities will be discussed.

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