Quantum Monte Carlo Simulations of Real Materials on GPU Clusters

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Quantum Monte Carlo (QMC) has proved to be an invaluable tool for predicting the properties of matter from fundamental principles, combining very high accuracy with extreme parallel scalability. In recent years, graphics processing units (GPUs) have provided a high-performance and low-cost new approach to scientific computing, and GPU-based supercomputers are now among the fastest in the world. The multiple forms of parallelism afforded by QMC algorithms make the method an ideal candidate for acceleration in the many-core paradigm. We present the results of porting the QMCPACK code to run on GPU clusters using the NVIDIA CUDA platform. Using mixed precision on GPUs and MPI for intercommunication, we observe typical full-application speedups of approximately 10x to 15x relative to quad-core CPUs alone, while reproducing the double-precision CPU results within statistical error.[1] We discuss the algorithm modifications necessary to achieve good performance on this heterogeneous architecture and present the results of applying our code to molecules and bulk materials.[2] We will also discuss steps we have taken towards the evaluation and elimination of pseudopotential error in the QMC simulations of solids.

[1] K. Esler, J. Kim, L. Shulenburger, D. Ceperley, "Fully accelerating quantum Monte Carlo simulations of real materials on GPU clusters", Computing in Science and Engineering (*preprint*) DOI: 10.1109/MCSE.2010.122 (2010).

[2] K.P. Esler, R.E. Cohen, B. Militzer, Jeongnim Kim, R.J. Needs, and M.D. Towler, "Fundamental High-Pressure Calibration from All-Electron Quantum Monte Carlo Calculations", Phys. Rev. Lett. **104**, 185702 (2010).