Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

Continuum quantum Monte Carlo simulations of solids on GPUs[1]

KENNETH ESLER, JEONGNIM KIM, DAVID CEPERLEY, University of Illinois at Urbana-Champaign — Continuum quantum Monte Carlo (QMC) has proved to be an invaluable tool for predicting the properties of matter from fundamental principles. The multiple forms of parallelism afforded by QMC algorithms make it an ideal candidate for acceleration in the many-core paradigm on graphical processing units (GPUs). We present the results of porting the QMCPACK code to the NVIDIA CUDA platform. Using mixed precision on G200 GPUs and MPI for intercommunication, we observe typical full-application speedups of approximately 10x to 15x relative to quad-core Xeon CPUs alone, while reproducing the double-precision CPU results within statistical error. We discuss the algorithm modifications necessary to achieve good performance on this heterogeneous architecture and summarize the results of applying our code to structural and electronic phase transitions in bulk materials. Based on our experience, we make projections for the applicability of GPUs to other electronic structure methods.

[1]Supported by DOE contract no. DOE-DE-FG05-08OR23336

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Date submitted: 20 Nov 2009 Electronic form version 1.4