Quantum Monte Carlo on Graphics Processing Units

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Abstract
Graphical Processing Units (GPUs) or “graphics cards” have been coming of age for general purpose calculations now that they are become programmable. GPUs have far more raw processing power than CPUs and thus, if one can translate a calculation into the expressions of graphics and the SIMD paradigm, one can expect large performance boosts. This of course depends upon the degree of algorithmic compatibility. The use of this specialized hardware is facilitated by the multibillion dollar gaming market, which pushes graphics hardware for higher performance on processors. Furthermore, the processing ability of these specialized processors can increase faster than the Moore's Law for CPUs. Current estimates are that GPUs will double their processing power every 6 to 12 months.

The Quantum Monte Carlo (QMC) algorithm used here is in the field of quantum chemistry, and can accurately solve the Schrödinger equation for molecules, albeit at substantial cost. QMC scales computationally with respect to molecule size better than any other first-principles approach, but its O(N^3) matrix multiplication is still a significant barrier. Focus in this research project has been on porting matrix multiplication (~3.3x as fast), basisfunction calculations (~22x), and Jastrow function calculations (~10x) onto the GPU for an overall speed up factor of approximately 10 for a C_{10}H_{10} molecule. Additional effort has been placed into minimizing the floating point relative error, providing results approximately an order of magnitude more precise, though at cost to the speed up.