High-Performance Computing

Master of Science thesis project

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Quantum Monte Carlo using CPUs and GPUs

The aim of this thesis is to develop diffusion Monte Carlo (DMC) and a Variational Monte Carlo (VMC) programs written in OpenCL and/or CUDA, in order to test the potential of Graphical processing units (GPUs) in Monte Carlo studies of both bosonic and fermionic systems.

The thesis entails the development of VMC and DMC codes for bosons and fermions, tailored to run on large supercomputing cluster with thousands of cores. These codes will then be rewritten in OpenCL and/or CUDA and tested on different GPUs, in order to see if a considerable speedup can be gained. Such a speedup, if we at least an order of magnitude is gained compared with existing in C++/Fortran codes that run on present supercomputers, will have trememdous consenquences for ab initio studies of quantum mechanical systems. The prices of the GPUs are of the order of few thousands of NOK, compared with large supercomputers which can cost billions of NOK.

The physics cases will deal with Bose-Einstein condensation and studies of the structure of atoms like Neon or Argon or electrons confined to move in harmonic oscilaltor like traps. In this way, both bosonic and fermionic systems will be tested.

The aim is to use these methods and evaluate the ground state properties of a trapped, hard sphere Bose gas over a wide range of densities using VMC and DMC methods with several trial wave functions, as well as testing fermionic systems. These wave functions are used to study the sensitivity of condensate and non-condensate properties to the hard sphere radius and the number of particles. The traps we will use are both a spherical symmetric (S) harmonic and an elliptical (E) harmonic trap in three dimensions given by

$$V_{ext}(\mathbf{r}) = \begin{cases} \frac{1}{2}m\omega_{ho}^2 r^2 & (S) \\ \frac{1}{2}m[\omega_{ho}^2(x^2+y^2) + \omega_z^2 z^2] & (E) \end{cases} \tag{1}$$

with

$$H = \sum_i^N \left(\frac{-\hbar^2}{2m} \bigtriangledown_i^2 + V_{ext}(\mathbf{r}_i) \right) + \sum_{i<j}^N V_{int}(\mathbf{r}_i, \mathbf{r}_j), \tag{2}$$

as the two-body Hamiltonian of the system. Here ω_{ho}^2 defines the trap potential strength. In the case of the elliptical trap, $V_{ext}(x, y, z)$, $\omega_{ho} = \omega_\perp$ is the trap frequency in the perpendicular or xy plane and ω_z the frequency in the z direction. The mean square vibrational amplitude of a single boson at $T = 0K$ in the trap (1) is $< x^2 >= (\hbar/2m\omega_{ho})$ so that $a_{ho} \equiv (\hbar/m\omega_{ho})^{\frac{1}{2}}$ defines the characteristic length of the trap. The ratio of the frequencies is denoted $\lambda = \omega_z/\omega_\perp$ leading to a ratio of the trap lengths $(a_\perp/a_z) = (\omega_z/\omega_\perp)^{\frac{1}{2}} = \sqrt{\lambda}$.

We represent the inter-boson interaction by a pairwise, hard core potential

$$V_{int}(r) = \begin{cases} \infty & r \leq a \\ 0 & r > a \end{cases} \tag{3}$$

where a is the hard core diameter of the bosons. Clearly, $V_{int}(r)$ is zero if the bosons are separated by a distance r greater than a but infinite if they attempt to come within a distance $r \leq a$.

Similarly, for the fermionic systems we will study systems of electrons confined to move in two- and three-dimensional harmonic oscillator traps, so-called quantum dot systems.

Progress plan and milestones. The aims and progress plan of this thesis are as follows

- Develop a program that implements serially both variational and diffusion Monte Carlo methods for bosons and fermions.
- Implement interacting and non-interacting systems
- Implement various potentials
- Parallelise the program with MPI and OpenCL to use all the available cores
- Implement the blocking and the bootstrap methods for error calculation

The more explicit timeline is

1. Fall 2017: Develop a VMC and DMC code for boson in OpenCL and CUDA
2. Fall 2017: Develop a VMC and DMC code for fermions in OpenCL.
3. Spring 2018: Extensive benchmarks of codes and writeup of master thesis.

The thesis is expected to be finalized May/June 2018.