Introduction to Computational Physics Lectures, FYS4411/9411

Morten Hjorth-Jensen Email morten.hjorth-jensen@fys.uio.no[1,2]

Department of Physics, University of Oslo[1]

Department of Physics and Astronomy and National Superconducting Cyclotron Laboratory, Michigan State University[2]

Jan 18, 2018

Aims

- Be able to apply central many-particle methods like the Variational Monte Carlo method to properties of many-fermion systems and many-boson systems.
- Understand how to simulate quantum mechanical systems with many interacting particles. The methods are relevant for atomic, molecular, solid state, materials science, nanotechnology, quantum chemistry and nuclear physics.
- Learn to manage and structure larger projects, with unit tests, object orientation and writing clean code
- Learn about a proper statistical analysis of large data sets
- Parallelization and code optimizations

Lectures and ComputerLab

- Lectures: Thursday (2.15pm-4pm), remotely. First time January 18.
- Computerlab: Thursday (4.15pm-7pm), first time January 18, last lab session May 10.
- Weekly plans and all other information are on the webpage
- Intensive week starts March 5 and ends March 8, week 10.
- **First project to be handed in March 16**.
- **Second and final project to be handed in June 1.**
- There is no final exam, only project work.

Course Format

- Two compulsory projects. Electronic reports only. You are free to choose your format. We use devilry to hand in the projects.
- Evaluation and grading: The two projects count 1/2 each of the final mark. No exam.
- The computer lab (room FV329) consists of 16 Linux PCs, but many prefer own laptops. C/C++ is the default programming language, but Fortran2008 and Python are also used. All source codes discussed during the lectures can be found at the webpage of the course. We recommend either C/C++, Fortran2008 or Python as programming languages.

Topics covered in this course

- Parallelization (MPI and OpenMP), high-performance computing topics. Choose between Python, Fortran2008 and/or C++ as programming languages.
- Algorithms for Monte Carlo Simulations (multidimensional integrals), Metropolis-Hastings and importance sampling algorithms. Improved Monte Carlo methods.
- Statistical analysis of data from Monte Carlo calculations, blocking method.
- Eigenvalue solvers
- For project 2 there will be three variants:
  1. Variational Monte Carlo for fermions
  2. Coupled cluster theory for fermions (iterative methods)
  3. Neural networks and Machine Learning to solve the same problems as in project 1

Topics covered in this course

- Search for minima in multidimensional spaces (conjugate gradient method, steepest descent method, quasi-Newton-Raphson, Broyden-Jacobian).
- Iterative methods for solutions of non-linear equations.
- Object orientation
- Data analysis and resampling techniques
- Variational Monte Carlo (VMC) for 'ab initio' studies of quantum mechanical many-body systems.
- Simulation of two-dimensional systems like quantum dots (project 2).
- Simulation of trapped bosons using VMC (project 1)
- Machine learning and neural networks (project 2)
- Coupled cluster theory (project 2)

Quantum Monte Carlo Motivation

Most quantum mechanical problems of interest in for example atomic, molecular, nuclear and solid state physics consist of a large number of interacting electrons and ions or nucleons.
The total number of particles N is usually sufficiently large that an exact solution cannot be found.
Typically, the expectation value for a chosen hamiltonian for a system of N particles is

$$\langle H \rangle = \frac{\int d\boldsymbol{R}_1 d\boldsymbol{R}_2 \dots d\boldsymbol{R}_N \Psi^*(\boldsymbol{R_1}, \boldsymbol{R}_2, \dots, \boldsymbol{R}_N) H(\boldsymbol{R_1}, \boldsymbol{R}_2, \dots, \boldsymbol{R}_N) \Psi(\boldsymbol{R_1}, \boldsymbol{R}_2}{\int d\boldsymbol{R}_1 d\boldsymbol{R}_2 \dots d\boldsymbol{R}_N \Psi^*(\boldsymbol{R_1}, \boldsymbol{R}_2, \dots, \boldsymbol{R}_N) \Psi(\boldsymbol{R_1}, \boldsymbol{R}_2, \dots, \boldsymbol{R}_N)}$$

an in general intractable problem.
This integral is actually the starting point in a Variational Monte Carlo calculation. **Gaussian quadrature: Forget it**! Given 10 particles and 10 mesh points for each degree of freedom and an ideal 1 Tflops machine (all operations take the same time), how long will it take to compute the above integral? The lifetime of the universe is of the order of 10^{17} s.

Quantum Monte Carlo Motivation

As an example from the nuclear many-body problem, we have Schroedinger's equation as a differential equation

$$\hat{H}\Psi(\boldsymbol{r}_1,..,\boldsymbol{r}_A,\alpha_1,..,\alpha_A) = E\Psi(\boldsymbol{r}_1,..,\boldsymbol{r}_A,\alpha_1,..,\alpha_A)$$

where

$$\boldsymbol{r}_1,..,\boldsymbol{r}_A,$$

are the coordinates and

$$\alpha_1,..,\alpha_A,$$

are sets of relevant quantum numbers such as spin and isospin for a system of A nucleons ($A = N + Z$, N being the number of neutrons and Z the number of protons).

Quantum Monte Carlo Motivation

There are

$$2^A \times \begin{pmatrix} A \\ Z \end{pmatrix}$$

coupled second-order differential equations in $3A$ dimensions.
For a nucleus like beryllium-10 this number is **215040**. This is a truely challenging many-body problem.
Methods like partial differential equations can at most be used for 2-3 particles.

Various many-body methods

- Monte-Carlo methods
- Renormalization group (RG) methods, in particular density matrix RG
- Large-scale diagonalization (Iterative methods, Lanczo's method, dimensionalities 10^{10} states)
- Coupled cluster theory, favoured method in quantum chemistry, molecular and atomic physics. Applications to ab initio calculations in nuclear physics as well for large nuclei.
- Perturbative many-body methods
- Green's function methods
- Density functional theory/Mean-field theory and Hartree-Fock theory

The physics of the system hints at which many-body methods to use.

Quantum Monte Carlo Motivation

Pros and Cons of Monte Carlo

- Is physically intuitive.
- Allows one to study systems with many degrees of freedom. Diffusion Monte Carlo (DMC) and Green's function Monte Carlo (GFMC) yield in principle the exact solution to Schroedinger's equation.
- Variational Monte Carlo (VMC) is easy to implement but needs a reliable trial wave function, can be difficult to obtain. This is where we will use Hartree-Fock theory to construct an optimal basis.
- DMC/GFMC for fermions (spin with half-integer values, electrons, baryons, neutrinos, quarks) has a sign problem. Nature prefers an anti-symmetric wave function. PDF in this case given distribution of random walkers ($p \geq 0$).
- The solution has a statistical error, which can be large.
- There is a limit for how large systems one can study, DMC needs a huge number of random walkers in order to achieve

Quantum Monte Carlo Motivation

Where and why do we use Monte Carlo Methods in Quantum Physics

- Quantum systems with many particles at finite temperature: Path Integral Monte Carlo with applications to dense matter and quantum liquids (phase transitions from normal fluid to superfluid). Strong correlations.
- Bose-Einstein condensation of dilute gases, method transition from non-linear PDE to Diffusion Monte Carlo as density increases.
- Light atoms, molecules, solids and nuclei.
- Lattice Quantum-Chromo Dynamics. Impossible to solve without MC calculations.
- Simulations of systems in solid state physics, from semiconductors to spin systems. Many electrons active and possibly strong correlations.