Week 2 January 11-15: Introduction to the course and start Variational Monte Carlo

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

Department of Physics and Center fo Computing in Science Education, University of Oslo, Oslo, Norway[1]

Department of Physics and Astronomy and Facility for Rare Ion Beams, Michigan State University, East Lansing, Michigan, USA[2]

Jan 14, 2021

Overview of week 2

Topics
- Introduction to the course and overview of topics to be covered
- Introduction to Variational Monte Carlo methods, Metropolis Algorithm, statistics and Markov Chain theory

Teaching Material, videos and written material
- Asynchronuous vidoes
- Lecture notes and reading assignments
- Additional (often recommended) background material

Textbook

There are no unique textbooks which cover the material to be discussed. For each week however, we will, in addition to our own lecture notes, send links to additional literature. This can be articles or chapters from other textbooks. A useful textbook is however

- Bernd A. Berg, *Markov Chain Monte Carlo Simulations and their Statistical Analysis*, World Scientific, 2004, chapters 1, 2

This book has its main focus on spin-models, but many of the concepts are general. Chapters 1 and 2 contain a good discussion of the statistical foundation.

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
- Learn to optimize with convex optimization methods functions that depend on many variables.
- Parallelization and code optimizations

Lectures and ComputerLab

- Lectures: Thursday (2.15pm-4pm). First time January 14. Last lecture May 6.
- Computerlab: Thursday (4.15pm-7pm), first time January 14, last lab session May 6.
- Weekly plans and all other information are on the webpage of the course
- **First project to be handed in March 26**.
- **Second and final project to be handed in May 31.**
- 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 397 in the Physics buidling) has no PCs, so please bring your own laptops. C/C++ is the default programming language, but programming languages like Fortran2008, Rust, Julia, and/or Python can also be used. All source codes discussed during the lectures can be found at the webpage of the course.

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, bootstrapping, jackknife and blocking methods.
- Eigenvalue solvers
- For project 2 there will be at least three variants:
  1. Variational Monte Carlo for fermions
  2. Hartree-Fock theory for fermions
  3. Coupled cluster theory for fermions (iterative methods)
  4. Neural networks and Machine Learning to solve the same problems as in project 1
  5. Eigenvalue problems with deep learning methods
  6. Possible project on quantum computing

Topics covered in this course

- Search for minima in multidimensional spaces (conjugate gradient method, steepest descent method, quasi-Newton-Raphson, Broyden-Jacobian). Convex optimization, gradient methods
- 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- and three-dimensional systems like quantum dots or atoms and molecules or systems from solid state physics
- **Simulation of trapped bosons using VMC (project 1, default)**
- **Machine learning and neural networks (project 2, default, same system as in project 1)**
- Extension of project 1 to fermionic systems (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.
- 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.

Quantum Monte Carlo Motivation

We start with the variational principle. Given a hamiltonian H and a trial wave function Ψ_T, the variational principle states that the expectation value of $\langle H \rangle$, defined through

$$E[H] = \langle H \rangle = \frac{\int d\boldsymbol{R} \Psi_T^*(\boldsymbol{R}) H(\boldsymbol{R}) \Psi_T(\boldsymbol{R})}{\int d\boldsymbol{R} \Psi_T^*(\boldsymbol{R}) \Psi_T(\boldsymbol{R})},$$

is an upper bound to the ground state energy E_0 of the hamiltonian H, that is

$$E_0 \leq \langle H \rangle.$$

In general, the integrals involved in the calculation of various expectation values are multi-dimensional ones. Traditional integration methods such as the Gauss-Legendre will not be adequate for say the computation of the energy of a many-body system.

Quantum Monte Carlo Motivation

The trial wave function can be expanded in the eigenstates of the hamiltonian since they form a complete set, viz.,

$$\Psi_T(\boldsymbol{R}) = \sum_i a_i \Psi_i(\boldsymbol{R}),$$

and assuming the set of eigenfunctions to be normalized one obtains

$$\frac{\sum_{nm} a_m^* a_n \int d\boldsymbol{R} \Psi_m^*(\boldsymbol{R}) H(\boldsymbol{R}) \Psi_n(\boldsymbol{R})}{\sum_{nm} a_m^* a_n \int d\boldsymbol{R} \Psi_m^*(\boldsymbol{R}) \Psi_n(\boldsymbol{R})} = \frac{\sum_n a_n^2 E_n}{\sum_n a_n^2} \geq E_0,$$

where we used that $H(\boldsymbol{R})\Psi_n(\boldsymbol{R}) = E_n \Psi_n(\boldsymbol{R})$. In general, the integrals involved in the calculation of various expectation values are multi-dimensional ones. The variational principle yields the lowest state of a given symmetry.

Quantum Monte Carlo Motivation

In most cases, a wave function has only small values in large parts of configuration space, and a straightforward procedure which uses homogenously distributed random points in configuration space will most likely lead to poor results. This may suggest that some kind of importance sampling combined with e.g., the Metropolis algorithm may be a more efficient way of obtaining the ground state energy. The hope is then that those regions of configurations space where the wave function assumes appreciable values are sampled more efficiently.

Quantum Monte Carlo Motivation

The tedious part in a VMC calculation is the search for the variational minimum. A good knowledge of the system is required in order to carry out reasonable VMC calculations. This is not always the case, and often VMC calculations serve rather as the starting point for so-called diffusion Monte Carlo calculations (DMC). DMC is a way of solving exactly the many-body Schroedinger equation by means of a stochastic procedure. A good guess on the binding energy and its wave function is however necessary. A carefully performed VMC calculation can aid in this context.

Quantum Monte Carlo Motivation

- Construct first a trial wave function $\psi_T(\boldsymbol{R}, \boldsymbol{\alpha})$, for a many-body system consisting of N particles located at positions $\boldsymbol{R} = (\boldsymbol{R}_1, \ldots, \boldsymbol{R}_N)$. The trial wave function depends on α variational parameters $\boldsymbol{\alpha} = (\alpha_1, \ldots, \alpha_M)$.
- Then we evaluate the expectation value of the hamiltonian H

$$E[H] = \langle H \rangle = \frac{\int d\boldsymbol{R}\Psi_T^*(\boldsymbol{R}, \boldsymbol{\alpha})H(\boldsymbol{R})\Psi_T(\boldsymbol{R}, \boldsymbol{\alpha})}{\int d\boldsymbol{R}\Psi_T^*(\boldsymbol{R}, \boldsymbol{\alpha})\Psi_T(\boldsymbol{R}, \boldsymbol{\alpha})}.$$

- Thereafter we vary α according to some minimization algorithm and return to the first step.

Quantum Monte Carlo Motivation

Basic steps

Choose a trial wave function $\psi_T(\boldsymbol{R})$.

$$P(\boldsymbol{R}) = \frac{|\psi_T(\boldsymbol{R})|^2}{\int |\psi_T(\boldsymbol{R})|^2 \, d\boldsymbol{R}}.$$

This is our new probability distribution function (PDF). The approximation to the expectation value of the Hamiltonian is now

$$E[H(\boldsymbol{\alpha})] = \frac{\int d\boldsymbol{R}\Psi_T^*(\boldsymbol{R}, \boldsymbol{\alpha})H(\boldsymbol{R})\Psi_T(\boldsymbol{R}, \boldsymbol{\alpha})}{\int d\boldsymbol{R}\Psi_T^*(\boldsymbol{R}, \boldsymbol{\alpha})\Psi_T(\boldsymbol{R}, \boldsymbol{\alpha})}.$$

Quantum Monte Carlo Motivation

Define a new quantity

$$E_L(\boldsymbol{R}, \boldsymbol{\alpha}) = \frac{1}{\psi_T(\boldsymbol{R}, \boldsymbol{\alpha})}H\psi_T(\boldsymbol{R}, \boldsymbol{\alpha}),$$

called the local energy, which, together with our trial PDF yields

$$E[H(\boldsymbol{\alpha})] = \int P(\boldsymbol{R})E_L(\boldsymbol{R})d\boldsymbol{R} \approx \frac{1}{N}\sum_{i=1}^{N} E_L(\boldsymbol{R}_i, \boldsymbol{\alpha})$$

with N being the number of Monte Carlo samples.

Quantum Monte Carlo

The Algorithm for performing a variational Monte Carlo calculations runs thus as this

- Initialisation: Fix the number of Monte Carlo steps. Choose an initial $\boldsymbol{R}$ and variational parameters α and calculate $|\psi_T^\alpha(\boldsymbol{R})|^2$.
- Initialise the energy and the variance and start the Monte Carlo calculation.
  - Calculate a trial position $\boldsymbol{R}_p = \boldsymbol{R} + r * step$ where r is a random variable $r \in [0, 1]$.
  - Metropolis algorithm to accept or reject this move $w = P(\boldsymbol{R}_p)/P(\boldsymbol{R})$.
  - If the step is accepted, then we set $\boldsymbol{R} = \boldsymbol{R}_p$.
  - Update averages
- Finish and compute final averages.

Observe that the jumping in space is governed by the variable *step*. This is Called brute-force sampling. Need importance sampling to get more relevant sampling, see lectures below.

Quantum Monte Carlo: hydrogen atom

The radial Schroedinger equation for the hydrogen atom can be written as

$$-\frac{\hbar^2}{2m}\frac{\partial^2 u(r)}{\partial r^2} - \left(\frac{ke^2}{r} - \frac{\hbar^2 l(l+1)}{2mr^2}\right)u(r) = Eu(r),$$

or with dimensionless variables

$$-\frac{1}{2}\frac{\partial^2 u(\rho)}{\partial \rho^2} - \frac{u(\rho)}{\rho} + \frac{l(l+1)}{2\rho^2}u(\rho) - \lambda u(\rho) = 0,$$

with the hamiltonian

$$H = -\frac{1}{2}\frac{\partial^2}{\partial \rho^2} - \frac{1}{\rho} + \frac{l(l+1)}{2\rho^2}.$$

Use variational parameter α in the trial wave function

$$u_T^\alpha(\rho) = \alpha\rho e^{-\alpha\rho}.$$

Quantum Monte Carlo: hydrogen atom

Inserting this wave function into the expression for the local energy E_L gives

$$E_L(\rho) = -\frac{1}{\rho} - \frac{\alpha}{2}\left(\alpha - \frac{2}{\rho}\right).$$

A simple variational Monte Carlo calculation results in

α	$\langle H \rangle$	σ^2	$\sigma/\sqrt{N}$
7.00000E-01	-4.57759E-01	4.51201E-02	6.71715E-04
8.00000E-01	-4.81461E-01	3.05736E-02	5.52934E-04
9.00000E-01	-4.95899E-01	8.20497E-03	2.86443E-04
1.00000E-00	-5.00000E-01	0.00000E+00	0.00000E+00
1.10000E+00	-4.93738E-01	1.16989E-02	3.42036E-04
1.20000E+00	-4.75563E-01	8.85899E-02	9.41222E-04
1.30000E+00	-4.54341E-01	1.45171E-01	1.20487E-03

We note that at $\alpha = 1$ we obtain the exact result, and the variance is zero, as it should. The reason is that we then have the exact wave function, and the action of the hamiltonian on the wave function

$$H\psi = \text{constant} \times \psi,$$

yields just a constant. The integral which defines various expectation values involving moments of the hamiltonian becomes then

$$\langle H^n \rangle = \frac{\int d\boldsymbol{R}\Psi_T^*(\boldsymbol{R})H^n(\boldsymbol{R})\Psi_T(\boldsymbol{R})}{\int d\boldsymbol{R}\Psi_T^*(\boldsymbol{R})\Psi_T(\boldsymbol{R})} = \text{constant}\times\frac{\int d\boldsymbol{R}\Psi_T^*(\boldsymbol{R})\Psi_T(\boldsymbol{R})}{\int d\boldsymbol{R}\Psi_T^*(\boldsymbol{R})\Psi_T(\boldsymbol{R})} = c$$

This gives an important information: the exact wave function leads to zero variance! Variation is then performed by minimizing both the energy and the variance.

For bosons in a harmonic oscillator-like trap we will use is a spherical (S) or an elliptical (E) harmonic trap in one, two and finally three dimensions, with the latter given by

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

where (S) stands for symmetric and

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

as the two-body Hamiltonian of the system.

We will represent the inter-boson interaction by a pairwise, repulsive potential

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

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

Our trial wave function for the ground state with N atoms is given by

$$\Psi_T(\mathbf{R}) = \Psi_T(\mathbf{r}_1, \mathbf{r}_2, \ldots \mathbf{r}_N, \alpha, \beta) = \prod_i g(\alpha, \beta, \mathbf{r}_i)\prod_{i<j} f(a, |\mathbf{r}_i - \mathbf{r}_j|), \tag{4}$$

where α and β are variational parameters. The single-particle wave function is proportional to the harmonic oscillator function for the ground state

$$g(\alpha, \beta, \mathbf{r}_i) = \exp\left[-\alpha(x_i^2 + y_i^2 + \beta z_i^2)\right]. \tag{5}$$

For spherical traps we have $\beta = 1$ and for non-interacting bosons ($a = 0$) we have $\alpha = 1/2a_{ho}^2$. The correlation wave function is

$$f(a, |\mathbf{r}_i - \mathbf{r}_j|) = \begin{cases} 0 & |\mathbf{r}_i - \mathbf{r}_j| \leq a \\ (1 - \frac{a}{|\mathbf{r}_i - \mathbf{r}_j|}) & |\mathbf{r}_i - \mathbf{r}_j| > a. \end{cases} \tag{6}$$

Simple example, the hydrogen atom. The radial Schroedinger equation for the hydrogen atom can be written as (when we have gotten rid of the first derivative term in the kinetic energy and used $rR(r) = u(r)$)

$$-\frac{\hbar^2}{2m}\frac{d^2u(r)}{dr^2} - \left(\frac{ke^2}{r} - \frac{\hbar^2 l(l+1)}{2mr^2} \right) u(r) = Eu(r).$$

We will specialize to the case with $l = 0$ and end up with

$$-\frac{\hbar^2}{2m}\frac{d^2u(r)}{dr^2} - \left(\frac{ke^2}{r} \right) u(r) = Eu(r).$$

Then we introduce a dimensionless variable $\rho = r/a$ where a is a