Atomic modeling of argon

Project 5, FYS-3150

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Abstract

The aim of this project is to numerically find the critical temperature for the two dimentional Ising model by using the metropolis algorithm. We will first test the implementation of the algorithm carefully, first by comparing with theoretical values calculated for a small system. Then we will see if the algorithm behaves as expected according to our physical intuition for a larger system.

When we have found a estimate for the critical temperature we will compare it to Lars Onsagers analytical result.

All source codes can be found at: `https://github.com/inakbk/molecular-dynamics-fys3150`.

Contents

1 Introduction

Molecular dynamics (MD) is a computer simulation method used to study atoms and molecule structure and movement. In a MD simulation the atoms or molecules are allowed to interact trough a force given by a potential for a given time. This makes it possible to study the systems development over time.

MD is a a type of N-body simulation since the simulation often consists of a large number of atoms or molecules. It is therefore possible to use MD to study stastistical properties of a large system consisting of N such atoms or molecules. For systems that obey the ergodic hypothesis the evolution of a single molecular dynamics simulation may be used to determine macroscopic thermodynamic properties of the system. This is because the time averages of an ergodic system correspond to microcanonical ensemble averages[1].

Often the main motivation to use Molecular dynamics is that it is not possible to determine properties of the system analytically because of the large number of particles. The main limitation for the numerical simulation is the computer recources available, but also cumulative errors in the numerical integration. The first is solved by applying periodic boundary conditions while the latter is solved by proper selection of algorithms and parameters. In this paper we will have a look at two numerical integration methods; the Euler-Cromer method and the Velocity Verlet integrator.

In this paper we will study the properties of a large system consisting of Argon atoms. And compare with experimental data(?). We will have a constant number of particles, a constant volume and a more or less constant engergy (depending on the integrator). We are more interested in the statistical properties of the system than in the individual motion of each of the particles. We want to sample microstates from the microcanonical ensemble (NVE). (?se over avsnittet over?)

The applications of MD is many ranging from chemical physics, materials science and the modelling of biomolecules. What areas of physics can it be used in? Chemistry and biology?(fra oppg) see 'Areas of application and limitations' at `https://en.wikipedia.org/wiki/Molecular_dynamics` and google

2 Theory

3 Numerical methods

3.1 Periodic boundaryconditions (PBCs)

To avoid problems with boundary effects we will apply periodic boundary conditions. This has a great analogy to 'old' video games such as Snake 2. If the snake head passes through one side of box, it re-appears on the opposite side with the same velocity. In the system of atoms this would mean that if an atom should leave the simulation box at one side it will enter on the oposite side with the same values for the physical parameters as it had before it left. This also implies that an attom at the edge of the box will interact with an atom at the opposite side of the box so that every atom have the same number of 'neighbours'.

MD simulations that use periodic boundary conditions have a large number of unit cells (define?)

[1] `https://en.wikipedia.org/wiki/Molecular_dynamics` 3.dec 11:25

The size of the simulation box must also be large enough to prevent unphysical behaviour. If the box is too small one unit cell (a few atoms) might interact with itself. In the Snake analogy this would mean that the "head" interacts with or bites its own "tail" trough the wall which is allowed in the game, but not very physical. Thus the box size have to be large enough relative to the size of a unit cell, length of the simulation and the desired accuracy[2].

The minimum image convention (due to calculation of forces) When an atom leave the simulation box it must re-enter the box on the opposite side. This leads to two possible strategic choices: (A) 'fold back' particles into the simulation box when they leave it, or (B) let them go on into the other side of the box?

....ahh, this is relevant for computing forces/potentials! An atom which has passed through one face of the simulation box should re-enter through the opposite face-or its image should do it. Evidently, a strategic decision must be made: Do we (A) âĂIJfold backâĂİ particles into the simulation box when they leave it, or do we (B) let them go on (but compute interactions with the nearest images)? The decision has no effect on the course of the simulation, but if the user in interested in mean displacements, diffusion lenghts, etc., the second option is preferable.

3.2 intergration methods

Euler-Cromer method and the Velocity-Verlet method (discussed in the lecture notes.)

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[2] https://en.wikipedia.org/wiki/Periodic_boundary_conditions#Practical_implementation:_continuity_and_the_minimum_image_convention