

Computational Physics

Lecture 5

Organisation of the course - Program

Feb 10 – Introduction to MD, interactions, EoMs, boundary conditions

Feb 17 – Choice of units, energy of the system

Feb 24 – Verlet integration algorithm, minimum image convention

Mar 01 – Setting up initial conditions

Mar 08 – Observing the simulation: correlations & pressure

Mar 15 – Individual discussions

First project deadline: Thursday March 21 (midnight)

First project reports

- Deadline 21/03 - midnight.
- Submit **report + code** for the group on *Brightspace*.
- See score sheet on *Brightspace*.
- See also the coding guidelines.

The code has to be able to run the simulations you show.

Organisation of the course

Any questions?

Project 1: Observing the simulation

Last weeks' summary

- Considered the equations of motion for a **system of particles interacting via the Lennard-Jones** potential assuming **Newtonian physics**.
- Looked at a way to efficiently deal with **periodic boundary conditions**.
- Use a set of **discretized equations** to move particles forward in time and develop a **method to conserve global quantities**.
- Introduced **dimensionless units** to capture the **essence of the physics at play**. Used this to argue **good values for the time-step length**.
- Discussed a way of **setting the initial positions and velocities** for a given choice of user-specified density and temperature.

Project goal: Simulate and analyse different phases

We wanted to simulate *solid*, *liquid* and *gaseous* Argon.

We have worked out **how to set up the system for a specified density-temperature pair.**

Goal: Pick pairs of (ρ, T) corresponding to the three phases of matter.

We can see what it “looks like” but better to construct some quantities.

Pair correlation

One way of measuring the level of organisation of the particles.

We compute **all the distances between every pair of particles**.

Pair correlation

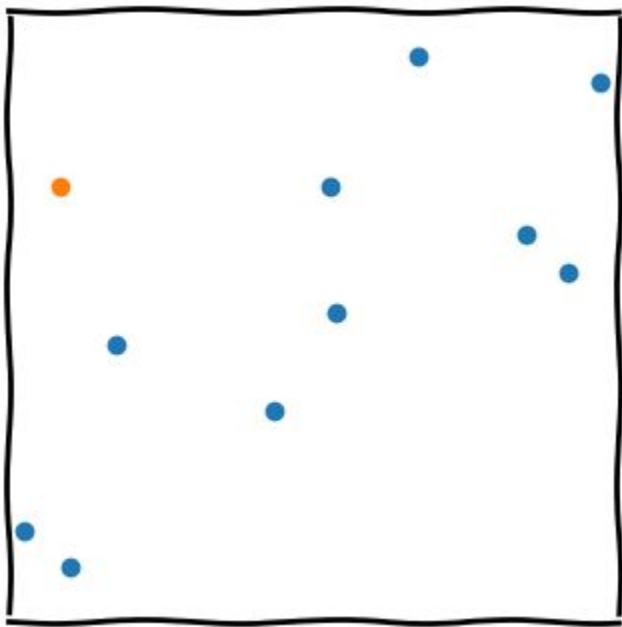
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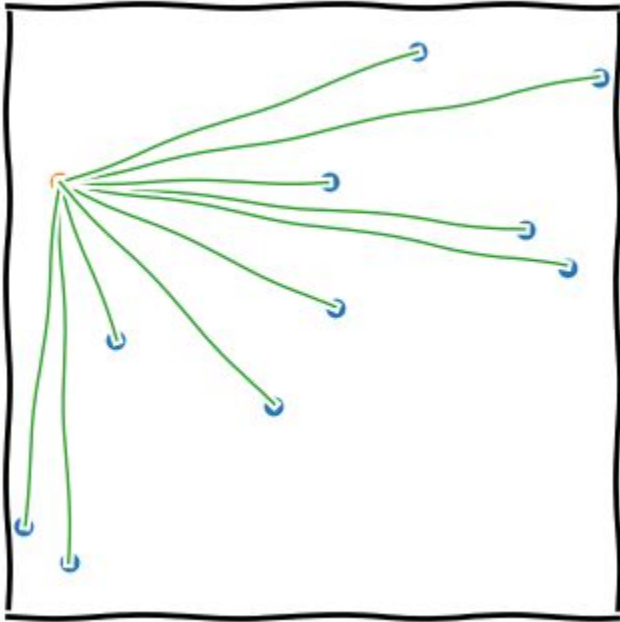
We then make a **histogram** of all the distance by counting how many are in the range $[r, r + \Delta r]$ (for every distance r).

We will call this histogram $n(r)$.

Pair correlation - Visually



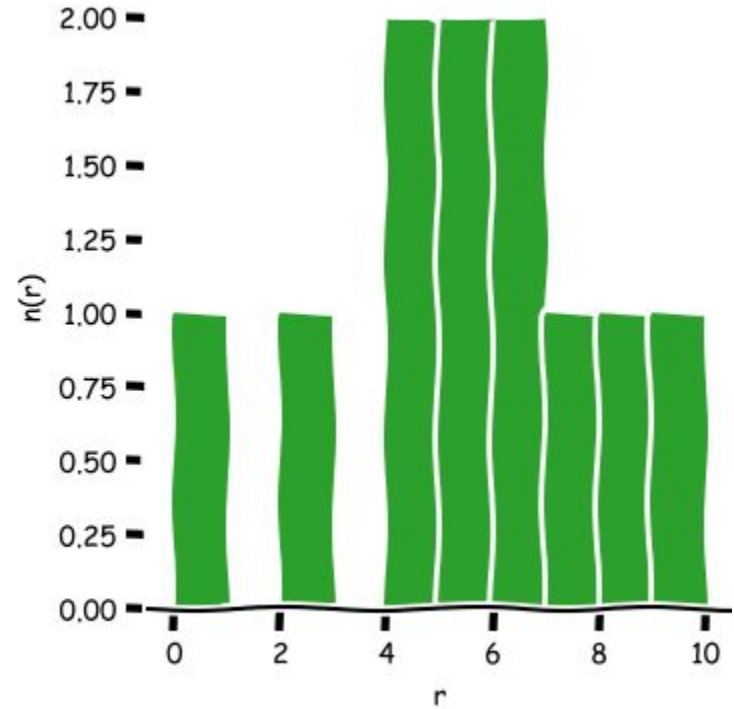
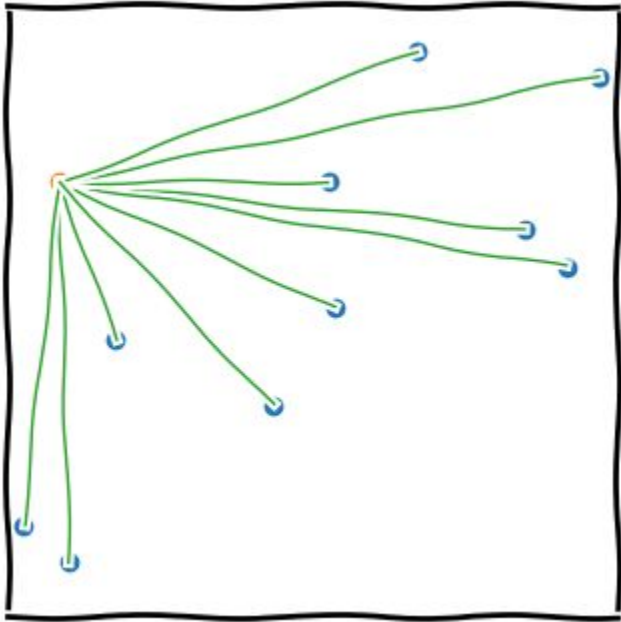
Pair correlation - Visually



*Note: I ignored the boundary condition
and minimal image convention here!*

You should include it!

Pair correlation - Visually



Then we consider another particle and add to the same histogram

Pair correlation

After having done that, we **repeat it for multiple times and multiple random realisations** of the initial positions and velocities for the same (ρ, T) pair.

We average these histograms to get $\langle n(r) \rangle$. “average over configurations”

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Thought experiment for you:

What should this look like for a crystal?

For a gas?

Pair correlation

“Traditionally”, some coefficients are added in front:

$$g(r) = \frac{2V}{N(N-1)} \frac{\langle n(r) \rangle}{4\pi r^2 \Delta r}$$

N = Number of particles

V = Volume

This leads to $g(r) = 1$ for a homogeneous distribution.

Pressure

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$$\frac{P}{k_B T \rho} = 1 - \frac{1}{3Nk_B T} \left\langle \frac{1}{2} \sum_i \sum_{j>i} r_{ij} \frac{\partial U(r_{ij})}{\partial r} \right\rangle$$

This can be derived from the virial theorem. (See Verlet 1961 for details)

The brackets are denoting **averaging over configurations** here again and the double sum is a “loop” over all the pairs of particles.

Question for you: What does this look like in dimensionless units?

Final Milestone

- Simulate Argon in **three different states of matter**, gas, liquid and solid for our base setup of $N = 108$ atoms in an **FCC start configuration**.
- For each setup, follow the **relaxation procedure** of the last lecture. After that, start the actual measurements.
- Measure the **pressure** of the system and plot the corresponding **pair correlation function**. (Check $g(r) = 1$ in the case of a gas!)
- Determine the pressure values together with an **estimate of the error** on the mean by performing several (e.g. 10) independent simulations.

Final Milestone

Choice of initial conditions (in our dimensionless units) to try:

- **Gas:** $\rho = 0.3$ $T = 3.0$
- **Liquid:** $\rho = 0.8$ $T = 1.0$
- **Solid:** $\rho = 1.2$ $T = 0.5$

Question for you: Do these correspond to the correct phases?

Final milestones

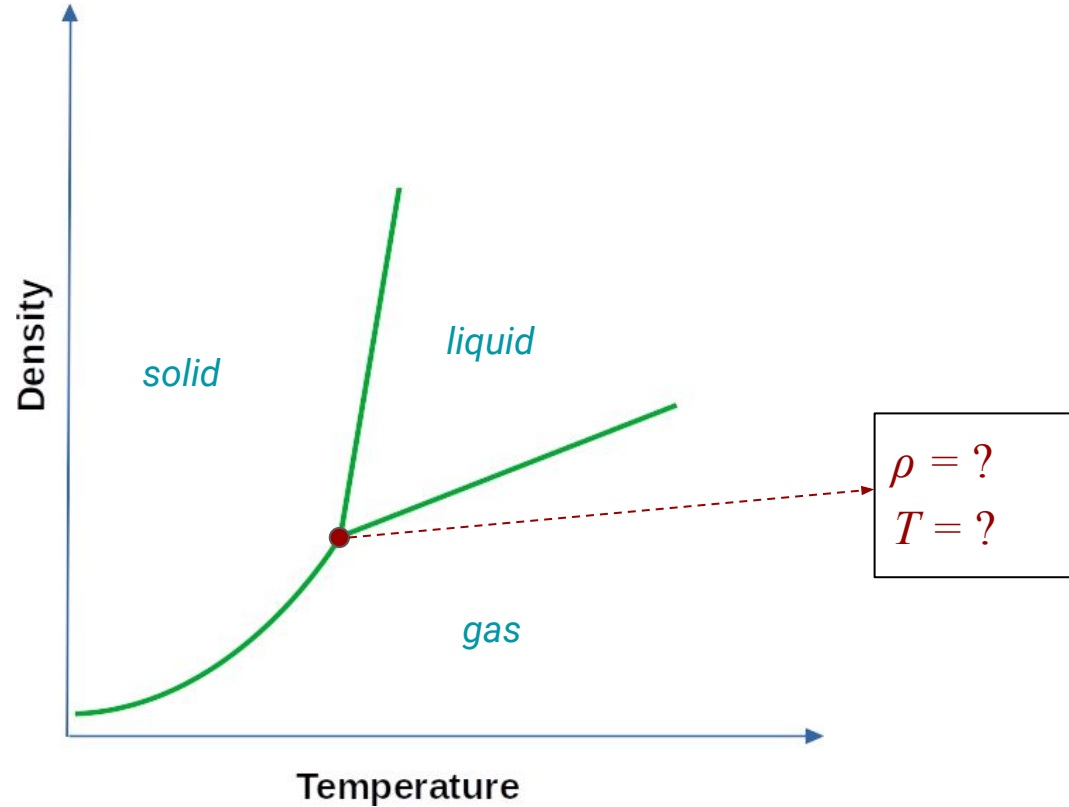
Any questions?

Extensions

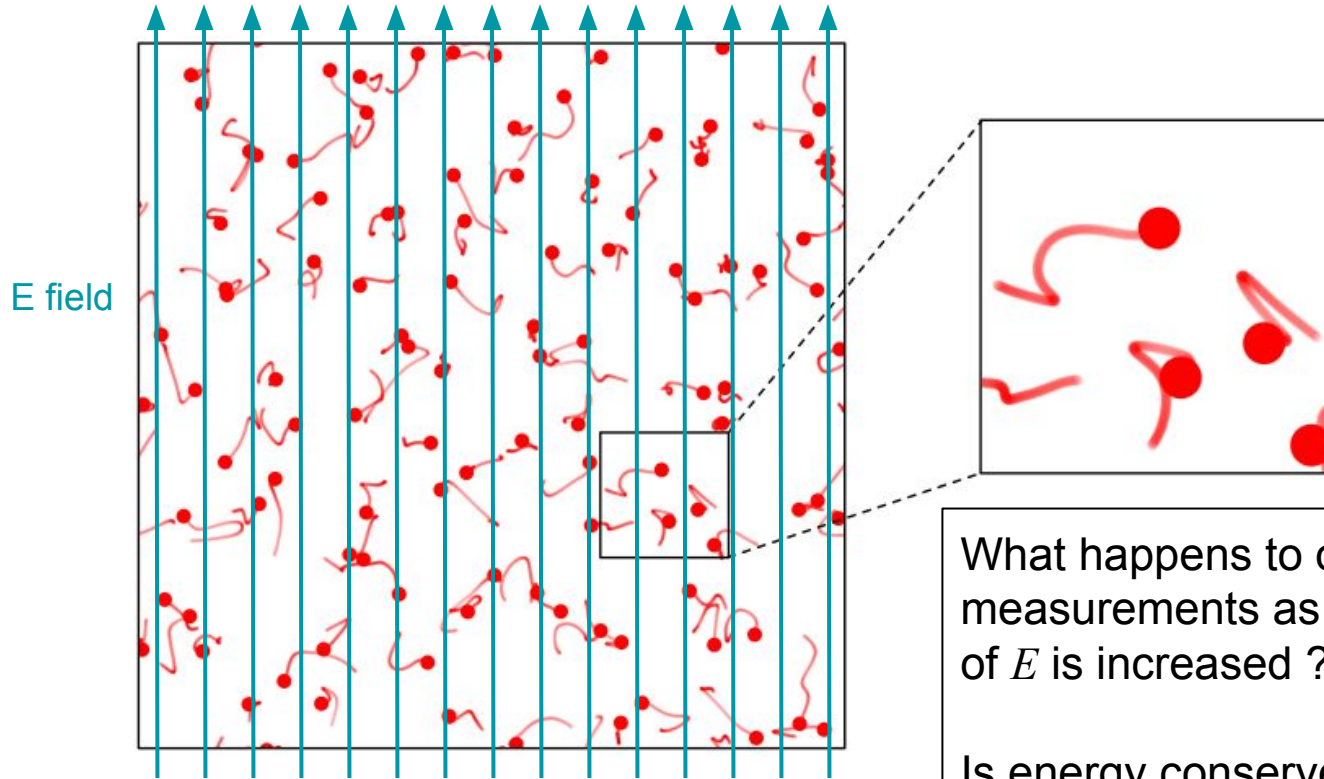
To get the **final 10% grade** on the project, tackle **one** of the following:

1. Identify the triple-point of the system. Describe the strategy you used. Does it match the real one?
2. Add an external electric potential (say along z), add a charge to the particles and discuss the effect this has when changing the field's magnitude.
3. Run a simulation with 3000 (or more) particles by implementing a better interaction finding algorithm.

Extension option 1 - Triple point



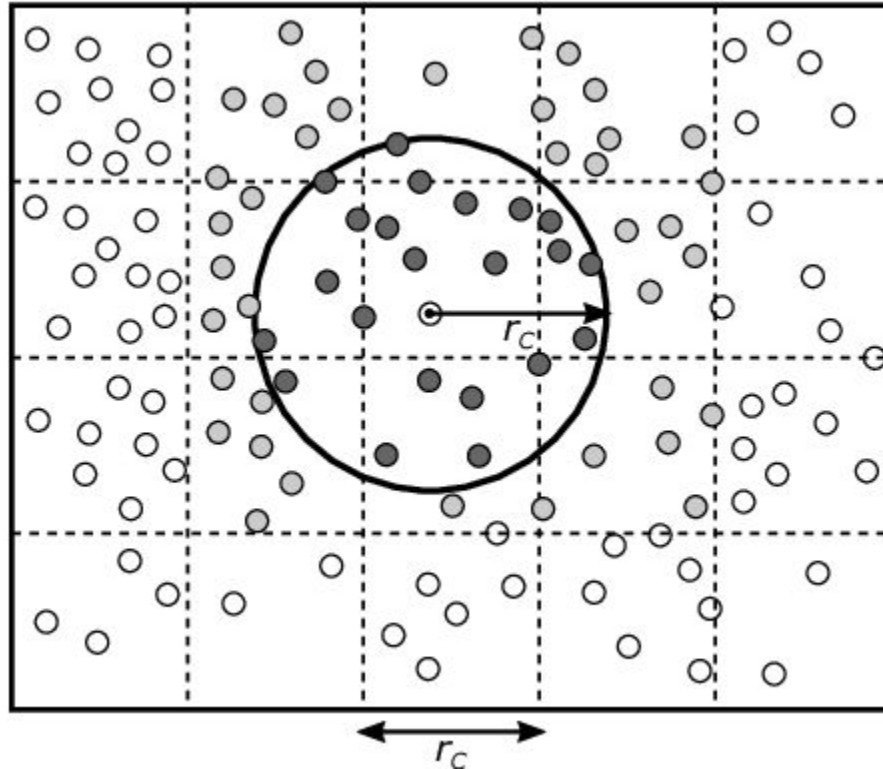
Extension option 2 - Electric field



What happens to our P and $g(r)$ measurements as the magnitude of E is increased ?

Is energy conserved ?

Extension option 3 - Bigger simulations



Use a more advanced algorithm to cut down on the number of interactions to compute and speed up the calculation.

Target: 3000+ particles