Simulating argon

Delft University of Technology

Ludwig Rasmijn
Sebastiaan Lokhorst
Shang-Jen Wang (4215974)

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Abstract

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Theory

Four questions have to be answered in order to simulate argon, these are:

1. What is the interaction between the argon atoms?
2. How do the argon atoms move around?
3. What are the boundary conditions?
4. What are the initial conditions?

These will be answered in the following sections.

2.1 Lennard-Jones potential

2.2 Velocity Verlet

In this section the question "How do the argon atoms move around?" will be answered.
Newton's equation of motion can be used to describe the motion of argon:

$$\boldsymbol{a}(t) \equiv \frac{d\boldsymbol{v}(t)}{dt} = \frac{d^2\boldsymbol{r}(t)}{dt^2} = \frac{\boldsymbol{F}(t)}{m}. \tag{2.1}$$

The Verlet algorithm was used to solve this ODE and in particular the velocity Verlet algorithm. There are two reasons for using this algorithm. Firstly it has a high order of accuracy $\mathcal{O}(h^3)$ and secondly it is very stable. The derivation for the velocity Verlet algorithm is as follows:
The Taylor expansions for the position:

$$\boldsymbol{r}(t+h) = \boldsymbol{r}(t) + h\frac{d\boldsymbol{r}(t)}{dt} + \frac{h^2}{2}\frac{d^2\boldsymbol{r}(t)}{dt^2} + \mathcal{O}(h^3). \tag{2.2}$$

Equation (**??**) can be expressed in terms of velocity and force:

$$\boldsymbol{r}(t+h) = \boldsymbol{r}(t) + h\boldsymbol{v}(t) + h^2\frac{\boldsymbol{F}(t)}{2m} + \mathcal{O}(h^3). \tag{2.3}$$

The Taylor expansion for velocity can be expressed as:

$$\boldsymbol{v}(t+h) = \boldsymbol{v}(t) + h\frac{d\boldsymbol{v}(t)}{dt} + \frac{h^2}{2}\frac{d^2\boldsymbol{v}(t)}{dt^2} + \mathcal{O}(h^3). \tag{2.4}$$

A second way to express the velocity in a Taylor expansion is:

$$\boldsymbol{v}(t) = \boldsymbol{v}(t+h) - h\frac{d\boldsymbol{v}(t+h)}{dt} + \frac{h^2}{2}\frac{d^2\boldsymbol{v}(t+h)}{dt^2} + \mathcal{O}(h^3). \tag{2.5}$$

Subtracting Equation (**??**) from Equation (**??**) can be expressed as:

$$2\boldsymbol{v}(t+h) - 2\boldsymbol{v}(t) = h\frac{d\boldsymbol{v}(t+h) + d\boldsymbol{v}(t)}{dt} + \frac{h^2}{2}\frac{d^2\boldsymbol{v}(t) - d^2\boldsymbol{v}(t+h)}{dt^2} + \mathcal{O}(h^3). \tag{2.6}$$

If the Taylor expansion is taken for $\boldsymbol{v}(t+h) = \boldsymbol{v}(t) + \mathcal{O}(h)$ then the term $\frac{d^2\boldsymbol{v}(t) - d^2\boldsymbol{v}(t+h)}{dt^2}$ from Equation (**??**) reduces to $\mathcal{O}(h)$ and Equation (**??**) can be expressed as:

$$\boldsymbol{v}(t+h) = \boldsymbol{v}(t) + \frac{h}{2}\frac{d\boldsymbol{v}(t+h) + d\boldsymbol{v}(t)}{dt} + \mathcal{O}(h^3). \tag{2.7}$$

So Equation(**??**) can then be expressed in terms of force:

$$\boldsymbol{v}(t+h) = \boldsymbol{v}(t) + \frac{h}{2m}(\boldsymbol{F}(t+h) + \boldsymbol{F}(t)) + \mathcal{O}(h^3). \tag{2.8}$$

2.3 Boundary conditions

2.4 Initial conditions