

Algorithms of Scientific Computing II

Exercise 1

1) Orders of Magnitude

In this exercise, we want to gain some understanding, systems of which size can still be simulated in a reasonable time. As practical example we want to do a molecular simulation of 1 liter of beer for 1 second. Try to find a generous estimate for the lower bound of the computation time. We make the following assumptions:

- A time step of our simulation should be 10^{-15} s.
- A liter of beer has the same molar mass as water ($18\frac{g}{mol}$).
- We apply a perfectly linear algorithm, which needs only one calculation per molecule per time step.
- We have unlimited cpu time on the fastest supercomputer with approximately 1 petaflops.
- We are perfect programmers, so our implementation always reaches peak performance.

What can we conclude? Assuming, Moore's Law continues to be valid, when does it make sense to start the simulation?

ANSWER:

The molar mass of water is $18\frac{g}{mol}$, so one liter of water contains

$$\frac{1000g}{18\frac{g}{mol}} = 55.5mol \approx 50mol.$$

The Avogadro constant ($6 \cdot 10^{23} \frac{1}{mol}$) gives the number of molecules per mol. So one liter of water contains

$$6 \cdot 10^{23} \frac{1}{mol} \cdot 50mol = 3 \cdot 10^{25}.$$

As we have a great algorithm, that's also the number of calculations per time step. Our supercomputer can perform 10^{15} operations per second, so the time needed to calculate one time step is

$$\frac{10^{25}}{10^{15}} = 10^{10}.$$

As one year has 10^7 seconds, we need 1000 years to calculate one time step. This means, we need

$$1000 \text{ years} \cdot 10^{15} = 10^{18} \text{ years}.$$

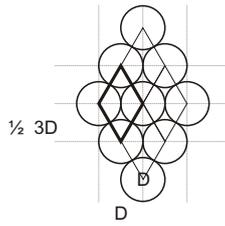
For comparison: the age of the universe is approximately 10^{10} years, so we had to wait only 100 Million times as long!

According to Moore's Law computational power doubles every 18 months, so in 3 years the calculation will take only $2.5 \cdot 10^{17}$ years. From the table, you can see, that in 90 years, the simulation would take only 1 year.

Starting year	calculation time in years
2011	10^{18}
2014	$2.5 \cdot 10^{17}$
2017	$6.25 \cdot 10^{16}$
...	...
2053	$9.31 \cdot 10^8$
...	...
2095	3.47
2098	0.87

2) Hard-Sphere Model in 3D

In 2D, the dense packing of the spheres standing for the molecules of an examined substance is given as shown here:



Determine a dense packing of spherical molecules in 3D and compute the resulting relative density given by the relation between the volume filled by molecules and the total volume of a surrounding box.

ANSWER:

As depicted, there exist three common ways to place atoms or molecules in a grid:

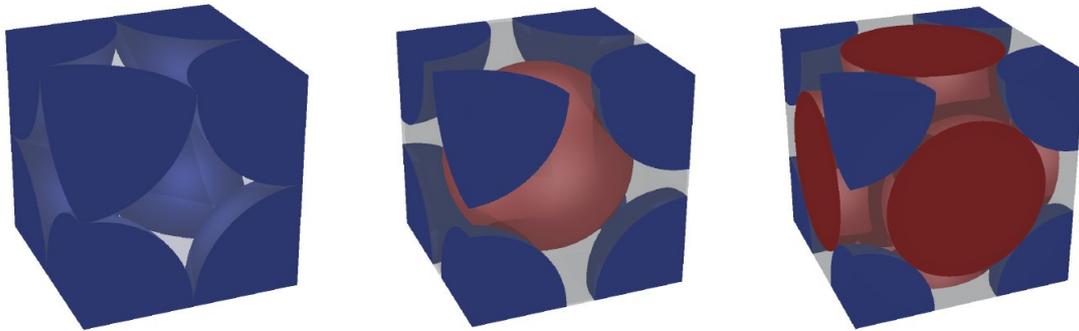


Abbildung 1: From left to right: corner-centered, cell-centered, surface-centered

Calculating the relative density for each of the orderings shows, that the surface-centered ordering represents the densest packing:

- corner-centered:
 - Volume of a cube: $V_{cube} = (2r)^3$
 - Volume covered by molecules: $V_{molecules} = \frac{4}{3}\pi r^3$
 - Relative density. $\rho = \frac{V_{molecules}}{V_{cube}} = \frac{\frac{4}{3}\pi r^3}{(2r)^3} = \frac{1}{6}\pi \approx 52\%$
- cell-centered:
 - Volume of a cube: $V_{cube} = \frac{64r^3}{3\sqrt{3}}$
 - Volume covered by molecules: $V_{molecules} = 2 \cdot \frac{4}{3}\pi r^3$

– Relative density. $\rho = \frac{V_{molecules}}{V_{cube}} = \frac{2 \cdot \frac{4}{3} \pi r^3}{\frac{64r^3}{3\sqrt{3}}} \approx 68\%$

- surface-centered:

– Volume of a cube: $V_{cube} = (2\sqrt{2}r)^3$

– Volume covered by molecules: $V_m = \frac{4}{3}\pi r^3 \cdot 4$

– Relative density. $\rho = \frac{V_{molecules}}{V_{cube}} = \frac{\frac{4}{3}\pi r^3 \cdot 4}{(2\sqrt{2}r)^3} = \frac{\frac{16}{3}\pi r^3}{16\sqrt{2}} \approx 74\%$

3) Potentials from Other Applications

Everybody knows potentials from other applications than molecular dynamics. In this tutorial, we consider the following two examples:

- Interaction of two bodies connected by a spring:



According to Hooke's Law

$$F(r) = -k(r - r_0)$$

holds for the force F between the two bodies at the ends of a spring stretched from its original (unloaded) length r_0 to r .

- Gravity between earth and moon:

According to Newton's laws, the gravity force between two bodies is given as

$$F(r) = -\frac{m_1 m_2 g}{r^2}.$$

- a) The relation between the force F and the potential U in a two-body system is given by the formula

$$F(r) = -U'(r).$$

Derive the potential for each of the two examples. In the case of the spring, the result is called a harmonic potential, in case of earth and moon, it's the gravitational potential.

Sketch F and U as functions of r , shortly explain the connection (steepness versus force value) of the two functions.

ANSWER:

For the spring, we get the potential energy

$$U_{\text{harm}}(r) = - \int F(r) dr = - \int -k(r - r_0) dr = \frac{1}{2}k (r - r_0)^2.$$

For earth and moon, we get the potential energy

$$U_{\text{grav}}(r) = - \int F(r) dr = - \int -\frac{m_1 m_2 g}{r^2} dr = -g \frac{m_1 m_2}{r}.$$

caused by a mass attraction of two bodies (planets, e.g.)

- b) The energy to be done for a change of the distance between the two bodies of a system from r_1 to r_2 is given by the formula

$$E = \int_{r_1}^{r_2} F(r) dr.$$

Transform this formula into a form that gives the energy E in dependence on the potential U .

ANSWER:

$$E = \int_{r_1}^{r_2} F(r) dr = U(r_2) - U(r_1).$$

- c) What indicates a high attraction force between two bodies?
- a steep descent of the potential,
 - a steep ascent of the potential,
 - a high positive value of the potential,
 - a high negative value of the potential,
 - a slow descent of the potential,
 - a slow ascent of the potential.

Remark: As can be seen from the examples above, negative forces are attraction forces and positive forces are repulsion forces.

Answer: b) If there's a steep ascent, there is a strong negative force according to $F = -\nabla U \Rightarrow$ high attraction.