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ST 2012

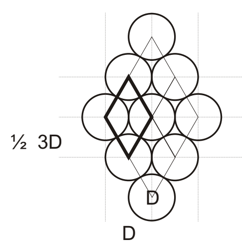
Scientific Computing II

Exercise A

June 25, 2012

Tutorial: 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:

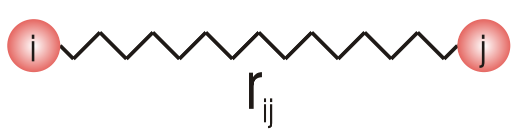


Determine a dense packing of spherical molecules in 3D and compute the resulting relative density given by the relation between the volume filled by molecules and the total volume of a surrounding box.

Tutorial: 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:

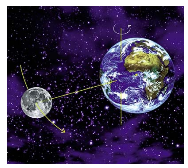


According to Hooke's Law

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

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.

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.

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.

Homework: Orders of Magitude

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 unlimeted cpu time on the fastest supercomputer with approximatelly 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?