Übung: Monte Carlo, Molecular Dynamics

Sommersemester 2017 Übung zu Struktur und Simulation

This is a revision Übung which requires no computer.

Send a set of answers to struct.sim@outlook.com by 30 June 2017.

1. Questions

1. What is the relationship between force and acceleration, written in terms of vectors ?

2. What is the relationship between the force on a particle and the potential energy ?

3. I have three particles with in a line with charges $2q^+, q^-$ and q^+ as in

   The force acting on the middle particle is zero. I know the distance u. What is the distance v as a function of u ?

   Ask yourself if you need to use vectors or if simple scalars are enough to answer the question.

4. I have three particles at rest in a line with charges $2q^+, q^+$ and q^+ as in


   $u = \sqrt{2v}$. What is the force on the middle particle ?

   Imagine the outer two particles are fixed in space. Will the middle particle move ?

   Imagine the three particles are atoms in a protein, but the outer two are fixed. What would you expect to happen to the middle particle ?

5. The Lennard-Jones potential energy of two particles is often written as $U(r) = ar^{-6} + br^{-12}$ for some constants a and b.

   (a) What is the distance where the force is zero ? (in terms of a and b).

   (b) Is this the same as the distance where the energy is zero ?

6. In a sophisticated force field, one may use an exponential term for the repulsion between two atoms and say the energy U as a function of r is $U(r) = ae^{-br}$ for some constants a and b. What is the size (scalar) of the force acting on two particles ? Is the force ever zero ?

7. In a force field, there is a dihedral angle term of the form, $U(\vec{r}) = k(1 + \cos(2\phi - v_0))$ where v_0 is a constant angle. Use the chain rule to show the steps you would take to work out the force in terms of the

coordinates $\vec{r}_k$ of atom k.
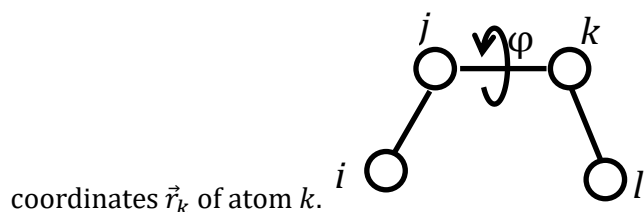
Given that $\frac{d\cos\theta}{d\theta} = -\sin\theta$ simplify the expression.

8. In a force field, I have a term for angles which looks like $U_{angle}(\vec{r}_i, \vec{r}_j, \vec{r}_k) = \frac{k}{2}\left(\cos\theta_{ijk} - \cos\theta_0\right)^2$. If atoms i,
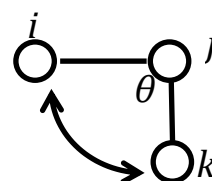
and k move away from each other is there a force acting on particle j ? Why ?

9. My molecular dynamics program can apply a cutoff for non-bonded interactions. Why is there a problem, in principle, with the forces at the cutoff boundary ?

10. You and I have different force fields for simulating water. We have slightly different charges on the hydrogen and oxygen atoms. In my force field, the partial charges on the H atoms are slightly more positive and the oxygens slightly more negative than in yours. When we simulate under identical conditions, we both find the same density. In terms of force field parameters, what could explain this ?