

Session 4 : Molecular Dynamics - correction

1. If we derive u_{lj} , we get

$$f_{lj} = -\vec{\nabla} u_{lj} = \frac{48\vec{r}}{r^2} \left[\left(\frac{\sigma}{r} \right)^{12} - 0.5 \left(\frac{\sigma}{r} \right)^6 \right] \quad (1)$$

The force is repulsive for $r < 2^{1/6}\sigma$ and attractive for $r > 2^{1/6}\sigma$.

2. For short-range interactions, to avoid the computation of forces with all the copies of the system (periodic boundary conditions), we could only account for interactions between particles closer to a cut-off distance r_c . Is this truncation negligible on the generic behavior of the system. In the evaluation of the total potential energy, the truncation results a systematic error

$$Err = \frac{N\rho}{2} \int_{r_c}^{\infty} dr u(r) 4\pi r^2 \quad (2)$$

Clearly , the truncation is valid only if the tail correction Err is small. In particular, $u(r)$ must decay more rapidly than $1/r^3$.

If we use only truncated potential, there is a non-negligible impulsive contribution to the pressure due to the discontinuous change of the potential at r_c . Then we shift the potential to make it continuous.

3. Time: $\sigma\sqrt{m/\epsilon}$, temperature: ϵ/k_B , density: σ^{-3} , pressure: σ^3/ϵ .
4. see the course of Prof. Everaers.
5. see the corrected code.
6. see the corrected code.
7. see the corrected code.
We impose that the velocity of the center of mass is zero to avoid a global translation of the system.
Initial positions are put on a lattice to avoid appreciable overlap of the atomic and molecular cores.
8. The total energy has to be constant in time. However, if dt is too big, the Taylor expansions of the equations of motion are no more valid and the Verlet algorithms do not conserve energy anymore.
9. By definition, the average kinetic energy at equilibrium is proportional to the temperature:
 $\langle E_{kin} \rangle = 3N/2k_B T$