HOMEWORK ASSIGNMENT #4

due: Wednesday 3 pm, February 23

1. Lennard-Jones Potential

Use the molecular dynamics program of the Lennard-Jones potential "kvollmay/classes.dir/capstone.dir/MD.dir/lj_vs6.c to equilibrate the following configuration:
"kvollmay/classes.dir/capstone.dir/MD.dir/vvinit_N200_2
and to determine the equilibrated average temperature T, potential energy $U_{pot}$ and kinetic energy $U_{kin}$.

2. Soft Sphere Potential

We used in class the “cut off and shifted” Lennard-Jones potential:

$$
\bar{F}(r_{ij}) = \begin{cases} 
48 \left( \frac{1}{r_{ij}} - \frac{0.5}{r_{ij}^3} \right) r_{ij} & \text{for } r_{ij} < 2.5 \\
0 & \text{otherwise}
\end{cases}
$$

$$
U(r_{ij}) = \begin{cases} 
4 \left( \frac{1}{r_{ij}^2} - \frac{1}{r_{ij}} \right) - 4 \left( \frac{1}{(2.5)^2} - \frac{1}{(2.5)^3} \right) & \text{for } r_{ij} < 2.5 \\
0 & \text{otherwise}
\end{cases}
$$

The “cut off” ($r_{cut} = 2.5$) describes that the force and potential are 0 for $r_{ij} > 2.5$ and the “shift” means that we shift the potential.

Another commonly studied potential is the following cut off and shifted “soft sphere potential”:

$$
\bar{F}(r_{ij}) = \begin{cases} 
\frac{48}{r_{ij}^2} r_{ij} & \text{for } r_{ij} < 2.0 \\
0 & \text{otherwise}
\end{cases}
$$

(1)

$$
U(r_{ij}) = \begin{cases} 
\frac{4}{r_{ij}^2} - \frac{4}{(2.0)^2} & \text{for } r_{ij} < 2.0 \\
0 & \text{otherwise}
\end{cases}
$$

(2)

2a Make a sketch of $U(r_{ij})$ both for the Lennard-Jones potential and for the soft sphere potential.

2b Which kind of interaction does the soft sphere potential model?

2c Use the program lj_vs6.c (see problem 1) and modify it such that it simulates the soft sphere potential.

2d Compare the trajectories of the particles 1 and 2 and interpret your result.

3. Cellular Automata: Diffusion

We use now a model for the diffusion of for example some perfume, i.e. for the spreading of a gas in a room. We describe the room with a two dimensional lattice (i.e. as before for the game of life) where each cell has as value the concentration of the gas. Take for example a lattice of size 50x50 (program it as general as possible) and start with all cells equal to 0.0 but the cells of the last two rows equal to 1.0. This corresponds to the gas being at the beginning all at the bottom. The rules of the model are then that at each update a site’s value is replaced by the average of the eight neighbors (Moore’s neighborhood). Write the program and look at your results.