Excercise 3

Consider the last frame of mystery.xyz as a starting configuration for your simulation.

Assignment 1. (2/5) Initiating temperature. Write a code *in programming language of your choice* to initiate temperature T=300K for your system. For this excercise you can trust the evenly-[0,1]-distributed random number generator in your system to work fine enough. After initiating the system (generating the velocities), the code should also calculate the instant temperature $T(0)$ and print it out. The code should also output $\mathbf{\Gamma}(0)$ in a file containing symbol, coordinates and velocities, on one line for each atom. We are obviously simulating bulk, so do not forget periodic boundary conditions where needed.

Assignment 2. (2/5) Neighbor list. Your standard MD code has a virus infection and cannot generate a Verlet neighborlist. Help your MD code to run by writing a program that generates this for your starting configuration. *You may use programming language of your choice.* Use small radius $r_m = 7.5$ Å and make the code to output the neighborlist (and nothing else) into a file that you also return to the assistant with your solution letter and the source codes. Needless to say, that you need to implement periodic boundary conditions. (Note: you can test your code by setting $r_m = 1.8$. Then only atoms in the same molecule should be neighbours.)

Assignment 3. (1/5) The neighborlist code you just made will probably cut some H_2O molecules leaving some atoms out. That is fine for assignment 2. Is that fine for a real simulation? If not, how would you modify your code? Written answer is enough for the points.

Return your solutions to Ville *moleculardynamicssimulations@gmail.com*, **latest by Friday excercise session 27.9.2013**. Please make a solution letter a single PDF and return also your codes (and output files) separately.