Chemical Engineering I5800 **Molecular Simulation** **fall 2024**

Problem Set 8 – due Nov. 13

Download the basic MD program lj_vv.f from Blackboard, compile it (in double precision!) and run it. Be sure that you understand everything in the program, and please ask questions if something is unclear.

1. Test the parameters in the Verlet list algorithm. In the code the skin thickness is set to 1.0 via the line "$rlist = (rc + 1.0) * *2$," and the resorting interval is set as "$ksort = 10$." Check whether this choice correctly includes all 2-body interactions.

2. Generate the pdf of x-velocities (called $x1(i), i = 1, np$ in the program) by summing over particles *and* time-averaging over the production part of the run. Compare the result to the theoretical expectation of a Gaussian with the appropriate mean and width.