

Problem Set 6 – due Apr. 3

Download the basic MD program `lj.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.

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.

The program computes a quantity `tdist` based on the values of the arrays `dax`, `day` and `daz`. What is the significance of these arrays, and what is `tdist` good for?