Programming projects:

In the two projects you are free to use any programming language but you are encouraged to use c or c++.
The basic requirements of the programming projects are stated below, for higher grades consult the assessment criteria. For each project, you should write you own programme from scratch and append it to the report containing a comprehensible description of the method and analysis of the simulation.
Each projects are presented in a written report with minimum 4 pages including graphs, but excluding the program source codes which should be well documented and appended.
These projects are individual and you should develop your own codes for

- **classical molecular dynamics simulations of a classical liquid.** You should calculate the total, kinetic and potential energies and their fluctuations, the heat capacity and the radial distribution function. All simulated quantities should be presented with a statistical analysis, and you are encouraged to calculate other properties and employ the radial distribution function with cut-off corrections to the total energy.

  1. Sketch a structure of the MD simulations program and discuss with course assistants.
  2. Aim to mimic the simulation from 1964 by Rahman in Phys. Rev. 136, A406, but use a smaller number of particles at least in the debugging process.
  3. Simulate liquid Argon in periodic boundary conditions (PBC), which has to be considered in any distance calculation, but allow the atoms to move freely out of the box.
  4. PBC is efficiently programmed using a nearest-integer-function.
  5. Initialise the system. For example with positions in a regular lattice, and randomised velocities.
  6. Calculate forces from the analytical derivative of the Lennard-Jones potential. Use the minimum image convention and include only interaction within a radial cut-off of half the box length.
  7. Use a short enough time-step to avoid an unstable solution of the equations of motion. Confirm equilibration and stability of simulation by monitoring E_{tot}, E_{pot} and E_{kin}, which should be stable within the natural fluctuations for a system of limited size. Viewing the coordinates graphical in the simulation box can be a convenient way to debug the program.
  8. Equilibrate the system at a certain temperature with temperature scaling for long enough time > 10 ps for the results not to depend on the starting conditions.
  9. Simulate long enough > 20 ps to get “reasonably smooth” curves in an ensemble of choice (most conveniently NVE)
  10. Dump coordinates and velocities of all atoms at regular intervals with a suitable time spacing.
  11. Analyse the trajectory and calculate the required properties.
  12. Sample any properties over the particles and time-frames.

13. Determine averages with error bars for the energy, heat capacity, radial distribution function (RDF).
14. Calculate the RDF by "bining" distances on a regular grid up to half the box length.
15. Play around. You are encouraged to try different methods and evaluate them against each other.

- **classical Monte Carlo simulations of a classical liquid.** You may instead choose an Ising model for the Monte Carlo project.

  1. Sketch a structure of the MC simulation program and discuss with course assistants.
  2. If you choose the classical liquid simply substitute the molecular dynamics integrator for the Monte Carlo algorithm and use the same program structure and analysis program as in the MD project, but remember that time is not defined in Monte Carlo. (If you keep it in mind when writing the molecular dynamics program above, it should be easily modified to perform a Monte Carlo simulation instead of a molecular dynamics simulation.) You should either make a comparison of results for static properties and efficiency between the MD and MC simulations.
  3. Or make a programme to simulate an Ising model (1D,2D, or 3D) at different temperatures. Perform sampling over initial conditions to determine energy, heat capacity, total magnetisation and pair correlation function. Derive the correlation length and compare to analytical expression for large separation.