Intoduction to ESPResSo: Lennard-Jones fluid

Worksheet

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Throughout this tutorial, you will incrementally write an ESPResSo script to simulate a Lennard-Jones fluid. The worksheet deliberately does not give you all commands in detail. Instead, you should learn how to find the information using the available documentation.

1 Tcl

1. Extend the script such that it can generate $N = 1000$ random positions at a given density $\rho = 0.7$ in a simulation box with periodic boundary conditions.

2. *Optional:* Extend the script such that it can also generate $N = 1000$ positions on a FCC lattice in the box at the same density.

2 Compiling ESPResSo

1. Download and compile ESPResSo! Use either the latest release or get the development code.

2. Run `make check`.

3. *Optional:* Execute the above script using ESPResSo.

3 First steps in ESPResSo and Visualizing with VMD

1. Extend the script such that it generates particles at the generated positions and creates a VTF file containing the positions.

2. Visualize the system using VMD.

4 Lennard-Jones Simulation

1. Extend the script such that it sets up the LJ interaction and the basic simulation parameters:
   - LJ parameters $\sigma = 1$, $\epsilon = 1$
   - Time step $\Delta t = 0.1$
   - Langevin parameters $T \in \{0.3, 1.0, 2.0\}$, $\gamma = 0.5$

2. Let the system compute the forces on all particles (`integrate 0`) and compute the maximal force acting on any particle.

3. Extend the script such that it does a simulation of the Lennard-Jones fluid. What happens when you do this starting from the random configuration? What can you do to avoid this problem?

4. Simulate the fluid for some time and visualize it using VMD.

5. *Optional:* Extend the script such that it measures the radial distribtion function of the fluid after a given time.

6. *Optional:* Measure the equilbrium RDF for the different temperatures.

7. *Optional:* Extend the script such that it stores the simulation state and can load it again.