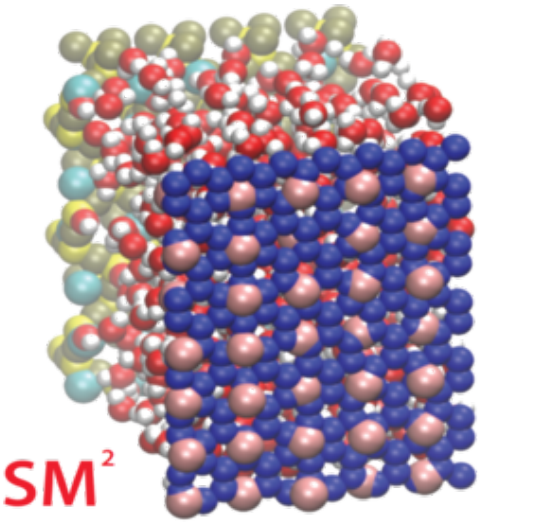
Non-equilibrium molecular dynamics workshop

LAMMPS Hands-on Session



Contents

1 Running an MD simulation

To run a molecular dynamics (MD) simulation using Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) we generally need two files. The first file is called a LAMMPS input script which consists of the commands required to run a MD simulation. The second file called the system file contains the description of the system, atom coordinates, bonds, system size, etc. and is read by the LAMMPS script at the start of a simulation. In some cases the system can be created in the LAMMPS script itself and in such cases we require only the LAMMPS input script to run the simulation. A general outline of a LAMMPS MD simulation is given below,

1. Setting up the system
(In this step either the system information is read by LAMMPS or the required system is created in the input script itself.)

$\Downarrow$

2. Providing interaction potentials
(In this step the atomic/molecular interaction information is provided to LAMMPS. For complex or real systems we should refer the literature to obtain the appropriate values for interaction parameters.)

$\Downarrow$

3. System minimization
(In this step LAMMPS adjust the atom coordinates to attain a minimum potential energy state for the system. Though not necessary it is advisable to perform this step since it can prevent the system from blowing up due to bad intial system configuration.)

$\Downarrow$

4. Setting up the system temperature
(In this step LAMMPS will bring the system to the required temperature. Different thermostatting schemes are available in LAMMPS to achieve the required temperature.)

$\Downarrow$

5. Running the system in the required ensemble and output
(In this step the system is allowed to evolve in the required statistical ensemble and output information is collected from LAMMPS for further analysis.)

1.1 Some frequently used LAMMPS commands

- pair_style, pair_coeff ⇒ To define the interaction parameters for the particles.
- set ⇒
- fix ⇒
- compute ⇒
- dump, thermo_style ⇒

2 Atomic System

- LAMMPS filename: atomic.lmp
- Here we simulate an atomic system containing Lennard-Jones (LJ) particles with reduced density, $\rho^* = 0.8$.
- The values for interaction parameters σ and ϵ were kept equal to 1.
- System dimensions: $10\sigma \times 10\sigma \times 10\sigma$ ($L_x \times L_y \times L_z$).
- System is equilibrated to a reduced temperature $T^* = 0.8$, using a Nosé-Hoover thermostat in LAMMPS.
- The simulation outputs the radial distribution function (RDF) for the present atomic system.
- The RDF values obtained from the simulation is compared with the RDF plot given in Page 70 of the book 'Computer Simulation of Liquids' by Allen and Tildesley.

3 Water System

- LAMMPS filename: water.lmp
- Here we simulate a water box containing 256 SPC/E water molecules with density 1 g cm^{-3}.
- The values for interaction parameters is taken from 'Mark, P., & Nilsson, L. (2001). Structure and dynamics of the TIP3P, SPC, and SPC/E water models at 298 K. The Journal of Physical Chemistry A, 105(43), 9954-9960.'
- Simulation box dimensions: $20 \times 20 \times 20$ Å^3 ($L_x \times L_y \times L_z$).
- System is initially equilibrated to a temperature of 298 K and 1 bar pressure, using a Nosé-Hoover barostat in LAMMPS.
- The simulation outputs RDF ($g_{H-H}(r)$, $g_{H-O}(r)$, and $g_{O-O}(r)$) and Mean square displacement (MSD) for the water system.
- The Self-diffusion coefficient (D) is calculated from the MSD of all oxygen atoms using the Einstein relation,

$$\text{MSD} = \lim_{t\to\infty} \langle |\vec{r}(t^* + t) - \vec{r}(t^*)| \rangle = 6Dt.$$