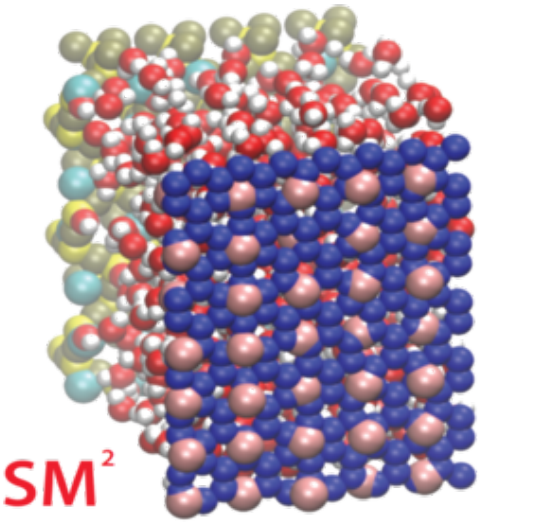
Non-equilibrium molecular dynamics workshop

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

- atoms_style ⇒ To define the attributes of the simulation pariticles.
- region ⇒ To define a geometeric region which can be later accessed in the LAMMPS script.
- group ⇒ To identify a set of particles as a single group.
- pair_style, pair_coeff ⇒ To define the interaction parameters for the particles.
- compute ⇒ To compute a quantity for a group of particles in the system.
- fix ⇒ To apply an operation to the system during the timestepping or minimization. Can also be used to output the quantities calculated using the *compute* command.
- dump, thermo_style ⇒ Output commands

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 LJ interaction parameters σ and ϵ are kept equal to 1.
- The LJ interaction cutoff, r_c is equal to 2.5σ.
- 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) of 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 Poiseuille System

- LAMMPS filename: poiseuille.lmp
- Here we simulate a system where a fluid is confined between two walls.
- All particles in the system are modelled as LJ particles.
- The values for LJ interaction parameters σ and ϵ between the fluid particles and between a fluid particle and a wall particle are kept equal to 1.
- The walls are kept as rigid i.e., there is no interaction between wall particles.
- The LJ interaction cutoff, $r_c = 2.5\sigma$
- Channel width: 20σ (L_z).
- Wall area: $10\sigma \times 10\sigma$ ($L_x \times L_y$).
- The system is equilibrated to a temperature, $T^* = 1.0$ by thermostating the fluid using a Nosé-Hoover thermostat.
- We apply an acceleration, $\vec{a} = 0.075\hat{i} + 0\hat{j} + 0\hat{k}$ (LJ units) to every fluid particle in the system to simulate a Poiseuille flow.
- The simulation outputs the velocity and density variation w.r.t the confined direction.

4 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) of the water system.
- The Self-diffusion coefficient (D) is calculated from the MSD of all oxygen atoms using the Einstein relation,

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

5 SLLOD System

- LAMMPS filename: sllod.lmp
- Here we simulate an atomic system containing LJ particles with density, $\rho^* = 0.8$.
- The values for LJ interaction parameters σ and ϵ are kept equal to 1.
- The LJ interaction cutoff, r_c is equal to 2.5σ.
- Initial system dimensions: $10\sigma \times 10\sigma \times 10\sigma$ ($L_x \times L_y \times L_z$).
- Initially the system is equilibrated to a reduced temperature $T^* = 1.0$, using a Nosé-Hoover thermostat in LAMMPS.
- After the initial equilibration an engineering strain rate, $\dot{\gamma}$ is applied to the system.
- Since application of a strain rate will change the simulation box dimensions, we use nvt/sllod thermostatting technique in LAMMPS to thermostat the system.
- The simulation outputs all the components of the pressure tensor of the system.
- The shear viscosity (η) is calculated from the off-diagonal(xy) element of the pressure tensor as,

$$\eta = -\frac{P_{xy}}{\dot{\gamma}}.$$

A Appendix

Here we briefly discuss on how to install and run LAMMPS, Visual Molecular Dynamics (VMD) and Packmol. LAMMPS require C language and MPI protocol to be pre-installed, hence make sure that both of them are already installed in your operating system (OS) before running the simulation. Data analysis and plotting will be done using Python language, hence it is recommended that you install Python and some of its libraries (Numpy, Scipy and Matplotlib) to run the Python scripts.

A.1 LAMMPS

A.1.1 Installing LAMMPS

Linux OS
$ sudo add-apt-repository ppa:gladky-anton/lammps
$ sudo add-apt-repository ppa:openkim/latest
$ sudo apt-get update
$ sudo apt-get install lammps-daily

Mac OS

Windows OS

A.1.2 Running LAMMPS

Enter the directory containing the LAMMPS input script and then type the following command in the terminal,
$ mpirun -np N lammps-daily $<$ *file_name.lmp*
$N \Rightarrow$ Enter the number of processors to be used for parallel computing.

A.2 VMD

A.2.1 Installing VMD

Download the latest version of VMD for the corresponding OS from here (You might need to create account with VMD inorder to download the package). After downloading the package unzip the package and open the terminal in the VMD directory and enter the following commands,
$ ./configure
$ cd src
$ sudo make install
$ vmd

A.2.2 Running VMD

To run a TCL script in VMD first enter the directory containing the VMD/TCL input script and then type the following command in the terminal,
$ vmd -dispdev text -e *file_name.tcl*

A.3 Packmol

A.3.1 Installing Packmol

Download Packmol from here. Unzip the package and then and open the terminal in the directory called packmol and enter the following commands,
$ make
$ sudo cp packmol /usr/local/bin/

A.3.2 Running Packmol

Enter the directory containing the Packmol input script and then type the following command in the terminal,
$ packmol $<$ *file_name.inp*