MD softwares : LAMMPS

LAMMPS is a C++ code for classical molecular dynamics with a focus on material modeling. It is an acronym for Large-scale Atomic/Molecular Massively Parallel Simulator. It is also a free software optimized for OPENMP and OPENMPI libraries. The code is flexible in order to simulate various physical situations and can perform simulation with many different algorithms. The price to pay is to write an input script file which defines all parameters as well as the quantities to be monitored. All possibilities can be found in the manual of software at https://lammps.sandia.gov/doc/Manual.pdf. The last version of the manual (30/10/19) has been significantly reduced (1993 pages) compared to the 2018 version (2300 pages). Anyway, to start with LAMMPS is not always easy, and if you are a beginner you must follow the basic instructions and understand the meaning of the lines of a script file. The goal of this session is to illustrate the versatility of the software and the quality of the parallelization.

The binary file is called lmp (or lammps, it depends on your installation) and you can start a simulation by using the command

```
lm -in in.system
```

where in. system is a script file defining the system (particle types, ensemble, forces, boundary conditions,...), the different observables to be calculated and different correlation functions (static and dynamic).

1 Lennard-Jones system : performance analysis

The script file in.ljm2 is

```
# 3d Lennard-Jones
variable t index 5000
units lj
atom_style atomic

lattice fcc 0.8442
region box block 0 10.0 0 10.0 0 10.0
create_box 1 box
create_atoms 1 box
mass 1 1.0
velocity all create 4 87287 loop geom
pair_style lj/cut 2.5
pair_coeff 1 1 1.0 1.0 2.5
neighbor 0.3 bin
neigh_modify delay 0 every 40 check no
fix 1 all nve
thermo 200
thermo_style custom elapsed pe ke etotal press temp
run $t
```

The script file corresponds to a Molecular Dynamics in the NVE ensemble for a monodisperse Lennard-Jones model in three dimensions. The number of steps is equal to 5000. The ther-
modynamic quantities are the mean potential energy the mean kinetic energy the mean total energy per atom, the pressure and the temperature (for this last quantity, check the ratio between ke/temp)

By using the script file in.ljM2 compare the user time by running the program sequentially (by using one core) by using 4 cores with MPI, and last by using 4 cores with OPENMP. (In the last case, first type OMP_NUM_THREADS=4 and type lmp -in in.ljM2)

In order to start, one needs to verify that espressomd is available on your computer

1) First run the program sequentially by typing
   lmp -in in.ljM2
   A log file is created which contains a lot of information concerning the physical quantities obtained as well as the performances of the simulation.

2) Some parameters are set in the code and can be modified by adding a line in the script file
   The timestep can be modified by adding the line (before the last line of the script)
   timestep 0.001
   Rerun the simulation and analyze the evolution of the thermodynamic quantities.
   Increase the timestep to 0.01 and rerun. What do you observe?

3) Delete the timestep line and set the OMP variable as
   export OMP_NUM_THREADS=4
   Note and comment the performance changes. Unset this variable in the following unset OMP_NUM_THREADS

4) For using OPENMPI, it is necessary to run by using mpirun.
   By using the script file in.ljM2, type
   mpirun -n 4 lmp -in in.system
   Compare the user time by running the program sequentially (by using one core) and by using 4 cores with OPENMP by using 2 and 4 cores with MPI. How to run the program for the best efficiency.

2 Lennard-Jones system : NVT ensemble

5) Comment the line which set the NVE ensemble and add the line
   fix 1 all nvt temp 300.0 2000.0 200.0 What are the differences with the simulation in nve ensemble ?

3 Lennard-Jones system : Radial distribution function

6) Add two lines to the lammps script
   compute myRDF all rdf 100
   fix 2 all ave/time 1000 1 $t c_myRDF[*] file tmp.rdf mode vector
   Run the simulation again. At the end, a new file is created tmp.rdf. In order to display the radial function, you must extract the relevant quantities from the file tmp.rdf
   You can use this python file for plotting the figure by using the data in the file tmp.rdf.
import numpy as np
import matplotlib.pyplot as plt

fi=np.loadtxt("tmp.rdf",skiprows=106)
plt.plot(fi[:,1],fi[:,2],"r-")
plt.xlabel("r",fontsize=15)
plt.ylabel("g(r)",fontsize=15)
plt.xlim(0.5,2.5)
plt.tick_params(labelsize=15)
plt.tight_layout()
plt.show()

7) Modify the reduced density defined in the line lattice, run the simulation again. How does the radial distribution function evolve when the density decreases?

4 Lennard-Jones system : A simulation movie

8) In compiled lammps version provided by the distribution, the movie creation is not available, but it is possible to write a sequence of jpg files which can be combined by using the opencv library. The last step can done by using a python script named here movie.py

```python
import cv2

toto=range(0,10000,200)
files=[]

for tt in toto:
    files.append("image."+str(tt)+".jpg")

img_array = []
for fi in files:
    img = cv2.imread(fi)
    height, width, layers = img.shape
    size = (width,height)
    img_array.append(img)

out = cv2.VideoWriter('simu.avi',cv2.VideoWriter_fourcc(*'MJPG'), 15, size)

for i in range(len(img_array)):
    out.write(img_array[i])
out.release()
```

In order to create the jpg files, add the line in the lammps script

```
dump 2 all image 200 image.*.jpg type type center d 0.5 0.5 0.5
```

Rerun the simulation, run the python script and watch the movie by using vlc (or any video reader)
9) Add the parameter `zoom 1.2` in the previous line and create a new movie. What are the changes with the previous movie?

10) Increase the number of images during the simulation and modify the python file, accordingly. Rerun the simulation and the python script.

A How to install Lammps

11) Lammps is available in repository of many Linux distributions, but also for Windows and MacOs.

12) If you need the latest stable version, you can download on the web site https://lammps.sandia.gov/ This team developing this software is very active. The last stable version of Lammps dated 7 Aug 2019.