OVITO

To explore molecular simulation, we start with LAMMPS for running simulations and we can visualize trajectories by using the software OVITO. To shorten simulation time, we recommand to use MPI for parallelization as described in the first session with LAMMPS. The two first examples correspond to equilbrium and non equilibrium simulations. We focus here on the use of ovito. The third exemple is a paradigmatic model of glassformers liquids for which we study some properties illustrating the slow relaxation at low temperature.

The dump files store the trajectories of the particles and can be large. Please clean your directory at the end of this session !

1 Equilibirum molecular dynamics

One considers a two dimensional lennard jones system. To visualize the relaxation of the system, particles defined in an initial slice are tagged with a blue color.

The script file **in.md** is

```
# 2d simulation

units  lj
atom_style atomic
dimension 2

lattice  sq2 0.8442
region  box prism 0 10 0 8 -0.5 0.5 0 0 0
create_box 2 box
create_atoms 1 box
mass  * 1.0

velocity all create 1.44 87287 loop geom

region  slice block 4 6 INF INF INF INF
set  region slice type 2

pair_style lj/cut 2.5
pair_coeff * * 1.0 1.0 1.0

neighbor 0.3 bin
neigh_modify delay 0 every 1

fix  1 all nvt temp 0.3 0.3 0.3 tchain 1

dump  1 all custom 100 dump.md id type x y z
```

```
thermo  1000

run  50000
```

The script file corresponds to a Molecular Dynamics in the NVT ensemble for a monodisperse Lennard-Jones model in deux dimensions. The number of steps is equal to 50000.

1. Run a simulation by using MPI.
2. A dump file d**ump.md** was created. This file contains the positions of all particles every 100 time steps. To obtain a visualization of the simulations, one uses ovito. In a terminal and in the directory the dump file was created, launch **ovito dump.md**. A grapihical window appears. On the bottom right part, click on the button **File contains time series**. The buttons for visualization are now active and launch the movie.
3. To modify the size of particles, click on the line Particles. It appears a window on the right and set the particle radius to 0.5. Restart the simulation movie
4. Change the temperature of the system by changing the parameters of the line **fix nvt** from 0.3 to 1. Run a new simulation and visualize by using ovito

2 Non equilibirum molecular dynamics

One considers a two dimensional lennard jones system. An external deformation of the simulation box is exerted and the system evolves to a non equilibrium state. A strain is exerted on the simulation box and the shape of the simulation box evolves with time.

The script file **in.nemd** is

```
# 2d NEMD simulation

units  lj
atom_style atomic
dimension 2

lattice  sq2 0.8442
region  box prism 0 10 0 8 -0.5 0.5 0 0 0
create_box 2 box
create_atoms 1 box
mass  * 1.0

velocity all create 1.44 87287 loop geom

region  slice block 4 6 INF INF INF INF
set  region slice type 2

pair_style lj/cut 2.5
```

```
pair_coeff * * 1.0 1.0 1.0

neighbor 0.3 bin
neigh_modify delay 0 every 1

fix  1 all nvt/sllod temp 0.3 0.3 0.3 tchain 1
fix  2 all deform 1 xy erate 0.01 remap v

dump  1 all custom 100 dump.nemd id type x y z


thermo  1000

run  50000
```

The script file corresponds to a Molecular Dynamics in the NVT ensemble for a monodisperse Lennard-Jones model in deux dimensions. The number of steps is equal to 50000.

1. Run a simulation by using MPI.
2. A dump file d**dump.nemd** was created. Launch the movie.
3. Change the temperature of the system by changing the parameters of the line fix nvt from 0.3 to 1. Run a new simulation and visualize by using ovito
4. Increase the size of the simulation by changing the command **region box prism 0 16 0 12 -0.5 0.5 0 0 0** . Change the parameters of the slice in order to have a slice remaining in the center of the simulation box.
5. Run and visualize the simulation again. Comment
6. For increasing the denisty of the simulation increase the value of the parameter lattice with the sequence $1, 1.2, 1.4$. Run and visualize the simulation. For the largest density, identify the microscopic mechanism of deformation.

3 Kob-Andersen model

The Kob-Andersen model is a model made of a mixture of two species of spheres interacting by a Lenard-Jones potential of different sizes. The ratio of particles of type A/B is 80 :20 as well as a set of parameters. This model is known for avoiding cristallization and/or demixing at low temperature. For temperatures below 0.5 (in reduced units), relaxation dynamics becomes slow and by decreasing the temperature one can observe dynamic arrest of the system.

We here consider the system at $T = 0.5$ and monitor the mean-square displacements of the two species.

The script file **inKALJnvemsdlog** is

```
#KALJ NVE, determine msd (logarithmic in time)
```

```
atom_style atomic
boundary p p p #periodic boundary cond. in each direction

read_data initconf_T05eq.data # read data file (incl.mass info)

pair_style lj/cut 2.5 # Define interaction potential.
pair_coeff 1 1 1.0 1.0 2.5 # type type eps sigma rcut
pair_coeff 1 2 1.5 0.80 2.0 #typeA typeB epsAB sigmaAB rcutAB=2.5*0.8=2.0
pair_coeff 2 2 0.5 0.88 2.2 #typeB typeB epsBB sigmaBB rcutBB=2.5*0.88=2.2

timestep 0.005 #Delta t

neighbor 0.3 bin
neigh_modify every 1 delay 0 check yes # Update neighbor

group A type 1
group B type 2
compute msdA A msd #default com=no and average=no so rvec(t=0) used
compute msdB B msd #default com=no and average=no so rvec(t=0) used
fix msdAfix A ave/time 1 1 1 c_msdA[4] file msdA.data
fix msdBfix B ave/time 1 1 1 c_msdB[4] file msdB.data
dump KAdump all custom 100 dump.KA id type x y z

variable tmsd equal logfreq3(1,200,100000)
variable tLJ equal step*dt
thermo_style custom v_tLJ c_msdA[4] c_msdB[4] pe etotal
thermo v_tmsd

# set numerical integrator
fix nve1 all nve # NVE; default is velocity verlet
run 100000
```

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 thermodynamic 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)

1. Run and visualiza the simulation with ovito
2. Two files were created which calculated the mean square displacements of the two specied of particles. Write a Python script able to load the two two files and to plot in a log-log scale. What do you observe ?
3. Comment the line dump and increase the simulation time by a factor 10 (Be careful, two parameters must be changed in the script). Rerun the simulation and plot the

mean square displacements. Can you estimate the scaling behavior of the curves at long time ?