**Introduction to LAMMPS input structure**

* The input script is executed line by line form beginning end.
* It generally consists of the following parts:
  + Initialization settings
  + System definitions
  + Simulation setting
  + Simulation execution
* Initialization setting: the units, box dimensions, boundary types, style of atoms, etc.

clear

units metal

dimensions 3

boundary s s p

atomic\_style atomic

* System definition: region of simulation box, masses of atoms, types of atoms, etc.

region R block 0 10 0 10 0 10 units box

create\_box 2 R

mass 1 1000.0

mass 2 1.0

lattice sq 2.0 orient x 1 0 0 orient y 0 1 0 z 0 0 1

create\_atoms 1 region R

create atoms 2 single 5 5 5 units box

* Simulation settings: pair potentials are defined, output file to write atom coordinates, etc

pair\_style lj/cut 4.0

pair\_coeff 1 1 0.020 2.0

pair\_coeff 1 2 0.005 0.5

pair\_coeff 2 2 0.001 2.0

dump 1 all custom 100 out.lammpstrj id type x y z

* Simulation execution: a langevin thermostat and time integration of all atoms, number of iterations

fix 1 all langevin 100 1 435235

fix 2 all nve

run 10000