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
```