

Initialization...

Compute-energy-and-force

input: xx, yy, zz

output: $fx, fy, fz, \text{virial}, \text{pot-energy}$

istep=0

istep++

print-xyz

if istep % xyzfreq == 0

input: ~~xx, yy, zz~~ xx, yy, zz

output: trajxyz

calc-props

if istep % thermo-freq == 0
|| istep == n-timesteps

input: $vx, vy, vz, \text{virial}, \text{pot-energy}$
output: $KE, PE, TotE, Temp, Press$

print-props

input: $KE, PE, TotE, Temp, Press$
output: thermodynamic data
printed to screen

update-positions

input: fx, fy, fz

output: xx, yy, zz

pbc

input: xx, yy, zz

output: xx, yy, zz

compute-energy-and-force

input: xx, yy, zz

output: $fx, fy, fz, \text{virial}, \text{pot-energy}$

update-velocities

input: fx, fy, fz

output: vx, vy, vz

if istep > cl.n-timesteps

simulation complete

if istep <= cl.n-timesteps