

Introducing MD theory

- MD is based on simulation particle (atoms) velocities using Newton's laws of classical dynamics.
- The velocities and or accelerations are used to calculate kinematic quantities.
- MD simulation is relevant when the simulation is representative of the corresponding macrosystem.

Understanding the dynamics of point particles

- Net force acting on a particle is given by:

$$F_{net} = m \frac{d^2 r}{dt^2}$$

- Where r is the distance and t is time.
- The energy (potential) between two atoms (idealized as two static balls held together by a spring) is approximated by:

$$E = -\frac{1}{2} k(r - r_e)^2$$

- Other approximations exist like the Lennard-Jones potential.
- Where k is the spring constant, r is the distance between the atoms and r_e is the equilibrium distance.
- $dE = F \times dr$. So, the force between the two atoms is then given by:

$$F = \frac{dE}{dr}$$

- Therefor:

$$\begin{aligned} F_{net} &= \sum_{all\ pairs} F = - \sum_{all\ pairs} \frac{dE}{dr} \\ \frac{d^2 r}{dt^2} &= \frac{1}{m} F_{net} \\ \frac{d^2 r}{dt^2} &= -\frac{1}{m} \sum_{all\ pairs} \frac{dE}{dr} \end{aligned}$$

Performing iterative updates using the Velocity Verlet algorithm

- From Newton's Laws of motion,

$$r(t + \Delta t) = r(t) + v(t)\Delta t + \frac{1}{2} \frac{F_{net}(t)}{m} \Delta t^2$$

- Where v is velocity or dr/dt .
- According to the Verlet Algorithm:

$$v(t + \Delta t) = v(t) + \frac{1}{2} \left[\frac{F_{net}(t)}{m} + \frac{F_{net}(t + \Delta t)}{m} \right] \Delta t$$

- Other update methods exist including the Euler algorithm.

Examining temperature and velocity distribution of particles

- According to Maxwell-Boltzmann velocity distribution:

$$f(v_i) = \sqrt{\frac{m}{2\pi k_B T}} \exp\left(-\frac{mv_i^2}{2k_B T}\right)$$

- Where k_B is Boltzmann's constant and T is Temperature
- For a particle in 3 dimensions

$$f(v_x, v_y, v_z) = f(v_x) \times f(v_y) \times f(v_z)$$
$$f(v_x, v_y, v_z) = \left(\frac{m}{2\pi k_B T}\right)^{\frac{3}{2}} \exp\left(-\frac{m(v_x^2 + v_y^2 + v_z^2)}{2k_B T}\right)$$

- In spherical coordinates:

$$f(v) = \sqrt{\frac{2}{\pi}} \left(\frac{m}{k_B T}\right)^{\frac{3}{2}} v^2 \exp\left[-\frac{mv^2}{2k_B T}\right]$$

Implementing MD simulation practices

- Simulation systems often consist of a small cell (simulation box) that is representative of a larger system. It can then be assumed that the larger system is made up of replicas of these cells.
- Period boundary conditions are normally employed in MD simulations. Where, when an atom exits the simulation box, its image enters from the opposite side of the wall. The coordinates are then wrapped (readjusted) or unwrapped (unadjusted).
- In LAMMPS, trajectory output files may include an image flag to keep track of wrapped and unwrapped coordinates. When an atom exits the simulation box in the positive direction, the image flag will increase by one and decrease by one if it exits in the negative direction.
- Thus *unwrapped coordinate = image flag × box side length*
- An atom only interacts with neighbors in a cutoff radius from the atom in question.
- In LAMMPS, if an atom crosses the area covered by the radius during iteration, a dangerous build warning is raised and the area readjusted.