

MD Simulation Notes

Armaan Ahmed

April 2023

A basic MD Simulation is based off of Newtonian physics:

$$ma = F$$

For a molecule i , need to sum over all the pairwise interactions. Then can numerically integrate or use:

$$\frac{x(t+dt) - x(t)}{dt} = v(t)$$

For solated system, there are too many particles. So, we use implicit solvent:

$$ma = F + F_{drag} + F_{noise}$$

The drag and noise encapsulate the effect of the solvent on the particle (ie drag force on the molecule). Essentially water is treated as just a continuum. Noise term accounts for the brownian motion, which is the “kick” given off by the water molecules. With implicit solvent, we need to use more parameteres, ie what is viscosity of water.

TwoChain_np.chain specifies the number of bonds, number of molecules, locations, velocities

“Atoms”:

Index,chain,atom_type,

“Velocities”:

“Bonds”:

Index,bond_type,bonded_atom_1,bonded_atom_2.

Can also define bond angle, but optional.

In “in_np.chain” file:

Units: scale Boundary considerations Atom_style: specifies the connections

read_data: topology of system

Bond_style: what type of connection (normally has harmonic potential)

Bond coeff: parameters of the bond.

special_bonds: get rid of pairwise interaction between bonded pairs.

Eg, lj 0.0 1.0 1.0

lj is a special parameter

pair_style: cutoff distance for the interactions.