**Restrained Electrostatic Potential**

The restrained electrostatic potential (RESP) approach is a highly regarded and widely used method of assigning partial charges to molecules for simulations

**Particle-Particle Particle-Mesh Method**

The PPPM method separates the interaction potential into the sum of a short-range function and a long-range function

**Nose-Hoover Thermostat & Barostat**

Barostatting means controlling the pressure in an MD simulation. [Thermostatting](https://docs.lammps.org/Howto_thermostat.html) means controlling the temperature of the particles. The fix npt commands include a Nose-Hoover thermostat and barostat in LAMMPS.

**Adsorption Isotherms**

Graphical user interface, text, application

Description automatically generated

**Self-Diffusion**

The key difference between self-diffusion and interdiffusion is that self-diffusion refers to the atomic migration in pure metals when all the atoms in the crystal structure that exchange positions are of the same type, whereas interdiffusion refers to the diffusion of atoms of one metal into another metal.

Self-diffusion describes the change in the position of the atoms in a crystal. Interdiffusion, on the other hand, can be described as the diffusional exchange of atoms across two materials that are in contact. Usually, the self-diffusion process is comparatively slower than the interdiffusion process, while interdiffusion is faster than many other diffusion processes that can take place in a crystal lattice.