Thermostats

The objective for a thermostat is to up- or downregulate the temperature of a given MD system. Reasons we might want to use a thermostat include

- Initialize a system at a specfici temperature
- Sample a cannonical ensamble (NVT) instead of a micro-cannonical ensamble (NVE)

A thermostat effectively simulates the connection of the system to a heat bath. For a thermostat to be labeled *effective* or *good* it is not only sufficient to get and or keep the system at a given temperature, but it should also

- Preserve real thermodynamics, i.e., it should sample the correct distribution for the cannonical ensamble—the Boltzmann distribution.
- Preserve real dynamics, this is a bit harder to define, as it depends on what kind of measurement or result we are interested in. As we will see in this project for example. A bad theromstat might very well keep the system at the right temperature, but due to the nature of the temperature-regulation, the diffusion of the system is disturbed from what it should be in a real physical system.

If a thermostat fails to do this, it might lead to artifacts that are non-physical, i.e., that don't show up in the real world. Or they might give us wrong statistics, meaning our result will not agree with statistics. A good example is the flying ice cube effect, which we will come back to.

There are many possible thermostats that are commonly used, some examples are

- Berendsen thermostat
- Andersen thermostat
- Nóse-Hoover