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Notes on molecular dynamics simulations

Molecular dynamics simulations are used model atomic motions according to Newton's laws. As in any simulation, the first step is to find a convenient unit system so that the numbers the computer handles are a few orders of magnitude about 1. In this case, we choose:

- Unit of length: 1 Å$\equiv 1 \times 10^{-10}$ m.
- Unit of time: 1 ps $\equiv 1 \times 10^{-12}$ s
- Unit of mass: $u \equiv 1.66053886 \times 10^{-27}$ kg
- Unit of temperature: degrees Kelvin

Setting initial velocities:

For each direction of motion, statistical mechanics tells us that the average magnitude of the component of velocity is given by:

$$\frac{1}{2} m_i < v_{xi}^2 >= \frac{1}{2} k_B T. \tag{1}$$

Here $m_i = M_i u$ is the mass of the particle which can be expressed in terms of the atomic mass number M_i. Using the stand values for the Boltzmann constant $k_B = 1.3806505 \times 10^{-23}$ J/K, we find

$$\sqrt{< v_{xi}^2 >} = 9118.37304 \sqrt{\frac{T}{M_i}} \text{ Å/ps}. \tag{2}$$