Simulation Methods in Physics I

Worksheet 3: Molecular Dynamics 2 and Observables

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1 Restart the program where left it

2 Molecular Dynamics at a Desired Temperature

For the *velocity rescaling* thermostat we can derive the rescaling-factor f_{re} from equation (1).

$$\frac{3}{2}k_B T_0 = \frac{E_{\mathrm{kin},0}}{N} \tag{1}$$

$$= \frac{1}{N}\sum_{i=1}^{N}\frac{(f_{\mathrm{re}}\cdot \boldsymbol{v}^{(i)})^2}{2m} \tag{2}$$

$$= f_{\mathrm{re}}^2\frac{E_{\mathrm{kin}}}{N} \tag{3}$$

$$= f_{\mathrm{re}}^2\frac{3}{2}k_B T \tag{4}$$

$$f_{\mathrm{re}} = \sqrt{\frac{T_0}{T}} \tag{5}$$