Simulation Methods in Physics I

Worksheet 3: Molecular Dynamics 2 and Observables

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1 Molecular Dynamics at a Desired Temperature

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

$$\frac{1}{2}k_B T = \frac{E_{\mathrm{kin}}}{3N} \tag{1}$$

$$= \frac{1}{3N}\sum_{i=1}^{N}\frac{(f_{\mathrm{re}}\cdot \boldsymbol{v}^{(i)})^2}{2m} \tag{2}$$

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

$$f_{\mathrm{re}} = \sqrt{\frac{3Nk_B T}{2E_{\mathrm{kin}}}} \tag{4}$$