Esercizio dinamica molecolare

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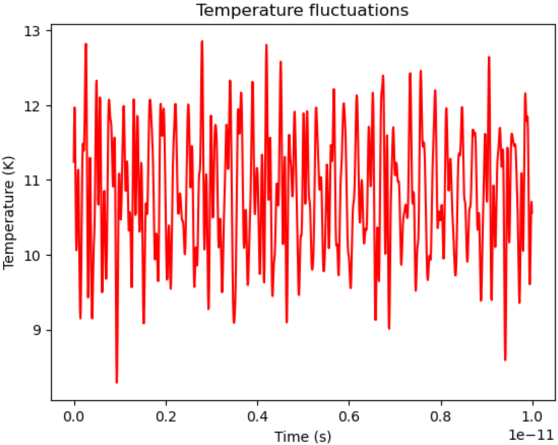
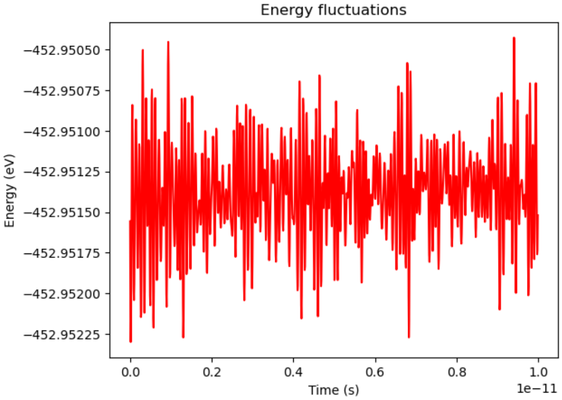
Sharp cutoff approach, temperature

$$T_{init} = 15\,K \rightarrow \langle T \rangle = 10.82\,K$$



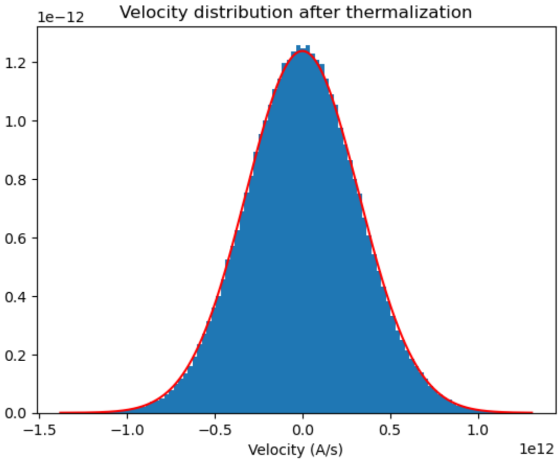
Sharp cutoff approach, energy

$$\frac{\delta E}{E} = 6.5 \times 10^{-7}$$



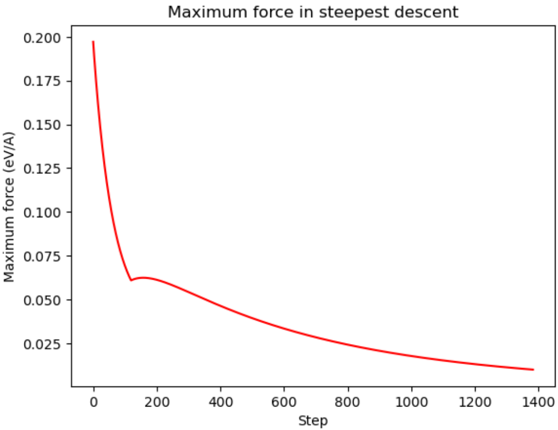
Sharp cutoff approach, velocity distribution

$$f(v_x) = \sqrt{\frac{M}{2\pi k_B T}} \exp\left(-\frac{M v_x^2}{2 k_B T}\right)$$



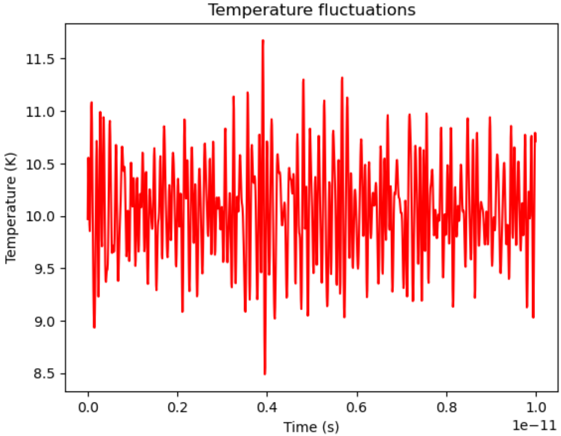
Sharp cutoff approach, steepest descent

$$F_{max} < 0.01\, eV/Å$$



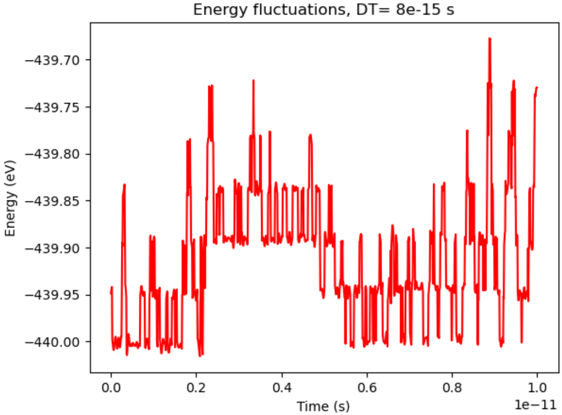
Sharp cutoff approach, steepest descent

$$T_{init} = 20\,K \rightarrow \langle T \rangle = 10.06\,K$$



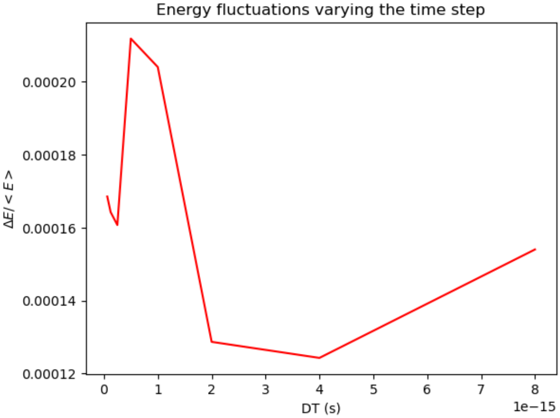
Sharp cutoff approach, energy

$$\langle T \rangle = 199.74\, K$$
$$\frac{\delta E}{E} = 1.54 \times 10^{-4}$$



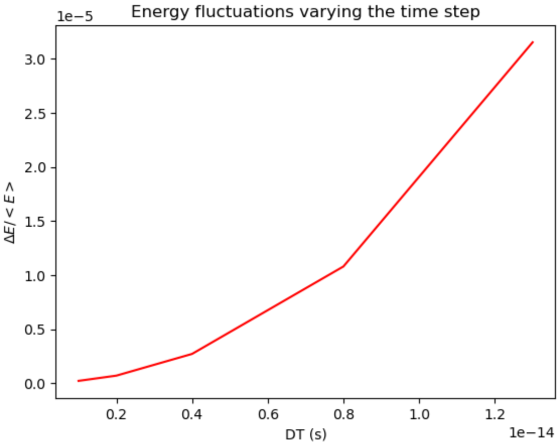
Sharp cutoff approach, energy

Lowering the time step does not solve the problem

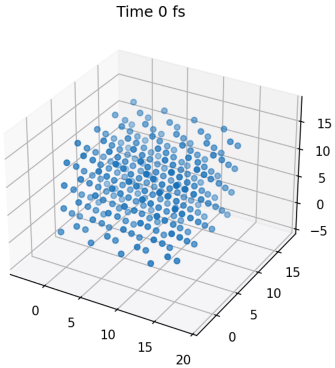


Polynomial junction approach, ideal timestep

The ideal timestep is $\Delta t = 8\,fs$ as it gives $\frac{\delta E}{E} = 1.08 \times 10^{-5}$.

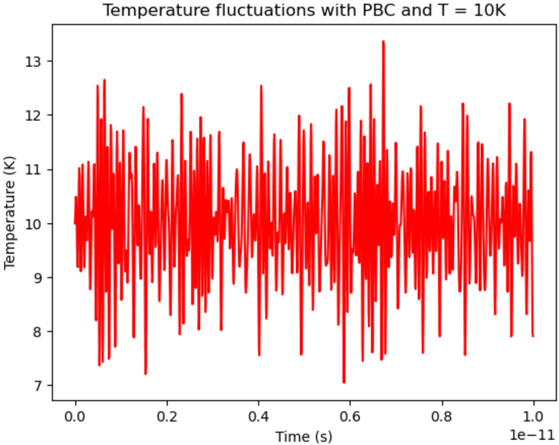


Polynomial junction approach, simulation



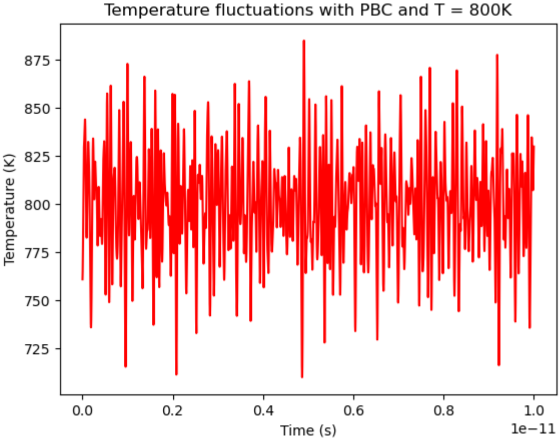
PBC, temperature

$$T_{init} = 20\,K \rightarrow \langle T \rangle = 10.001\,K$$



PBC, temperature

$$T_{init} = 1550\,K \rightarrow \langle T \rangle = 800.6\,K$$



PBC, extra atom

$$T_{init} = 1550\,K \rightarrow \langle T \rangle = 800.6\,K$$