Esercizio dinamica molecolare

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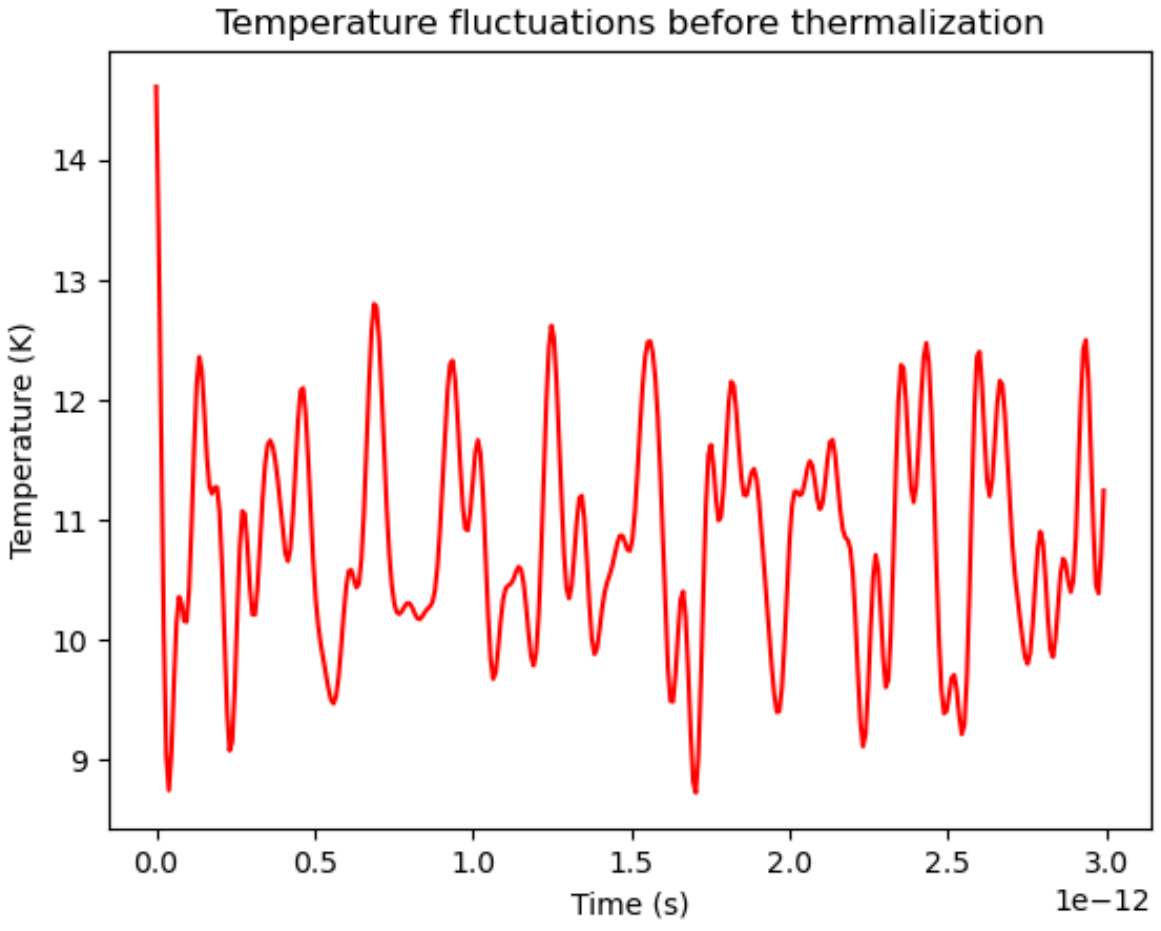
Sharp cutoff approach

- $r_c = 4.5\,\mathring{A}$,
- $T_{term} = 3 \times 10^{-12}\,s$,
- $T_{tot} = 10 \times 10^{-12}\,s$,
- $\Delta t = 8 \times 10^{-15}\,s$,
- sharp cutoff at r_c.

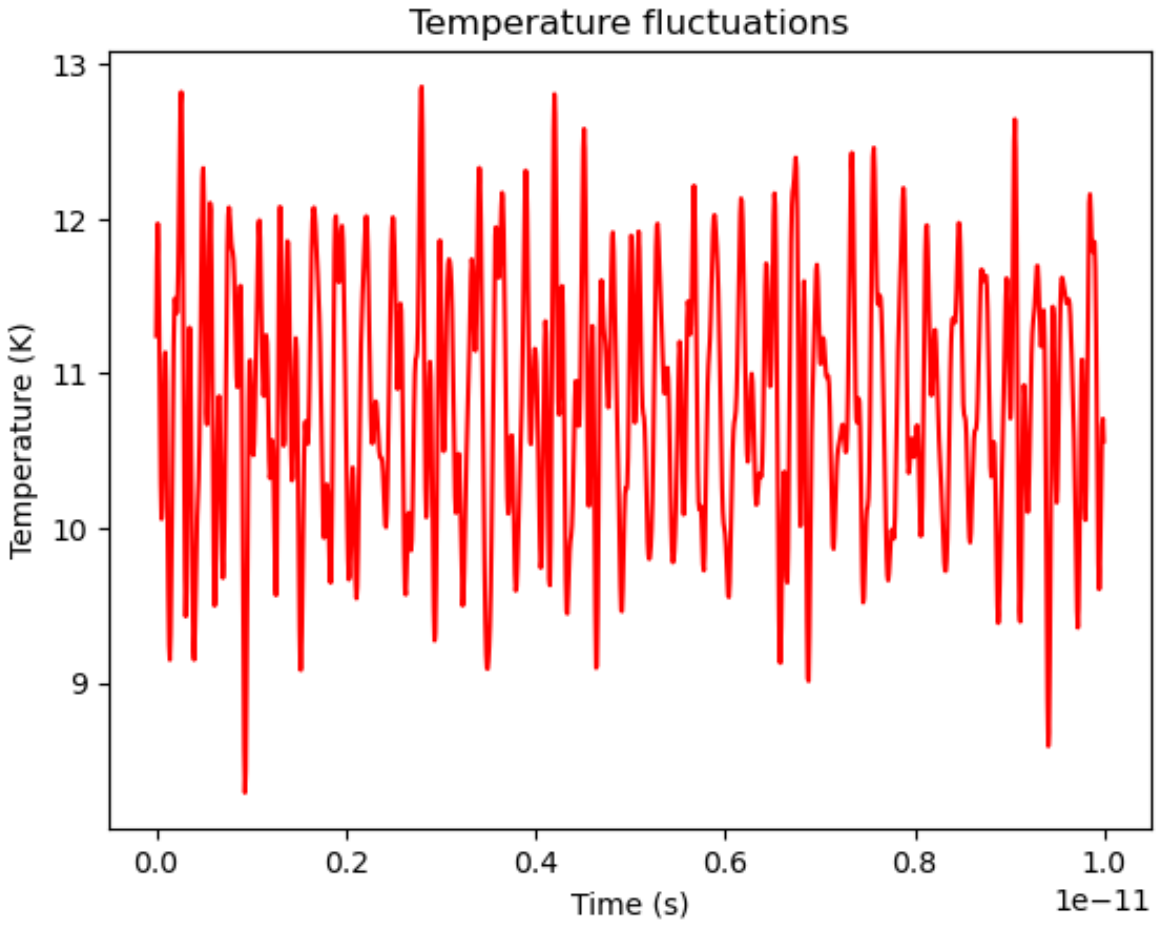
Sharp cutoff approach, initial temperature

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



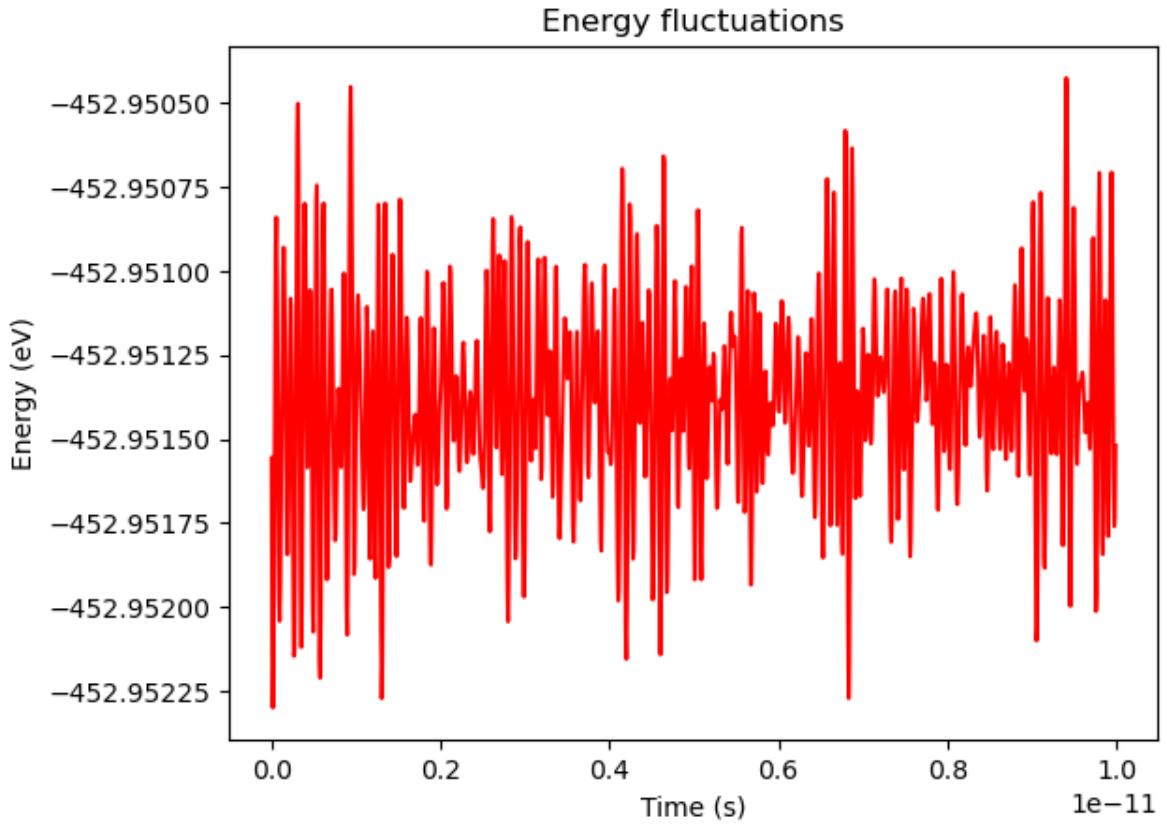
Sharp cutoff approach, initial temperature

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



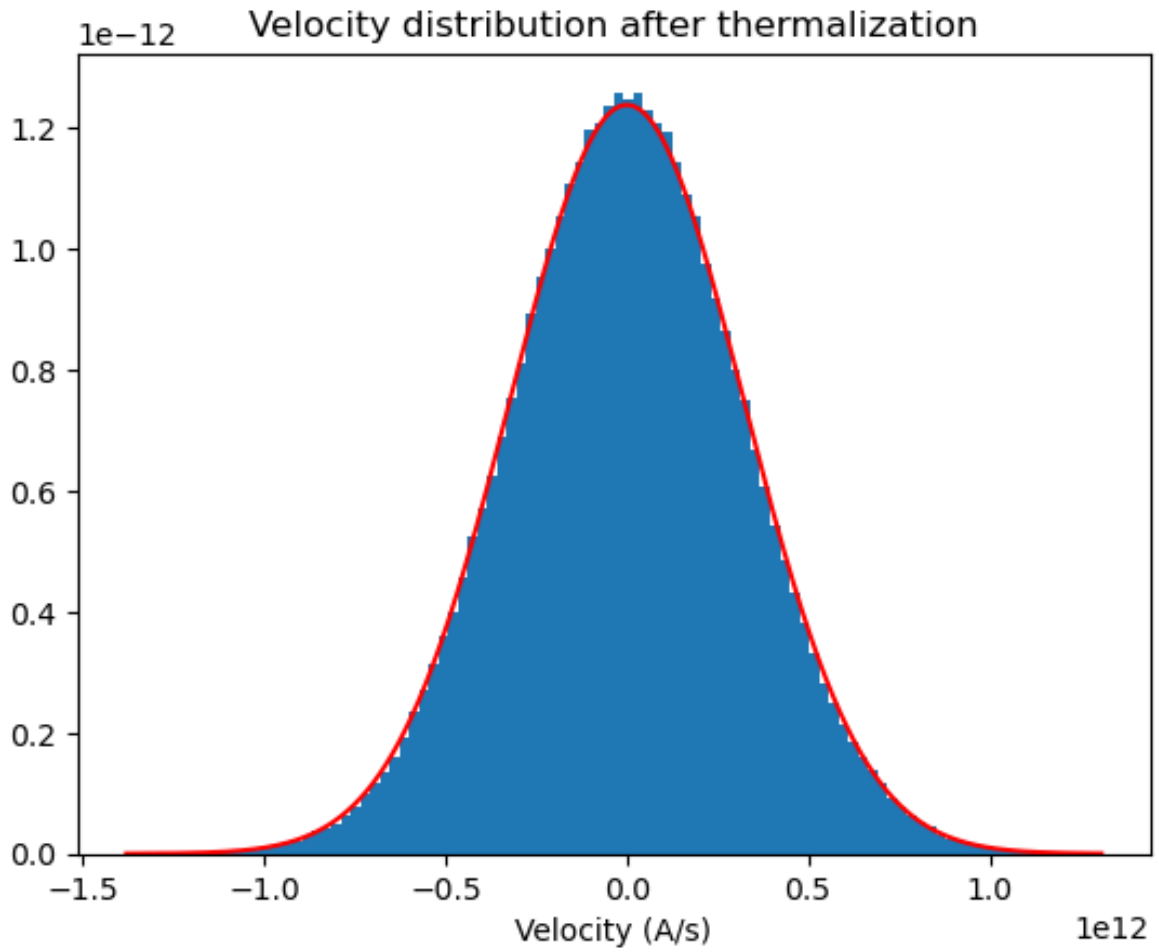
Sharp cutoff approach, energy conservation

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



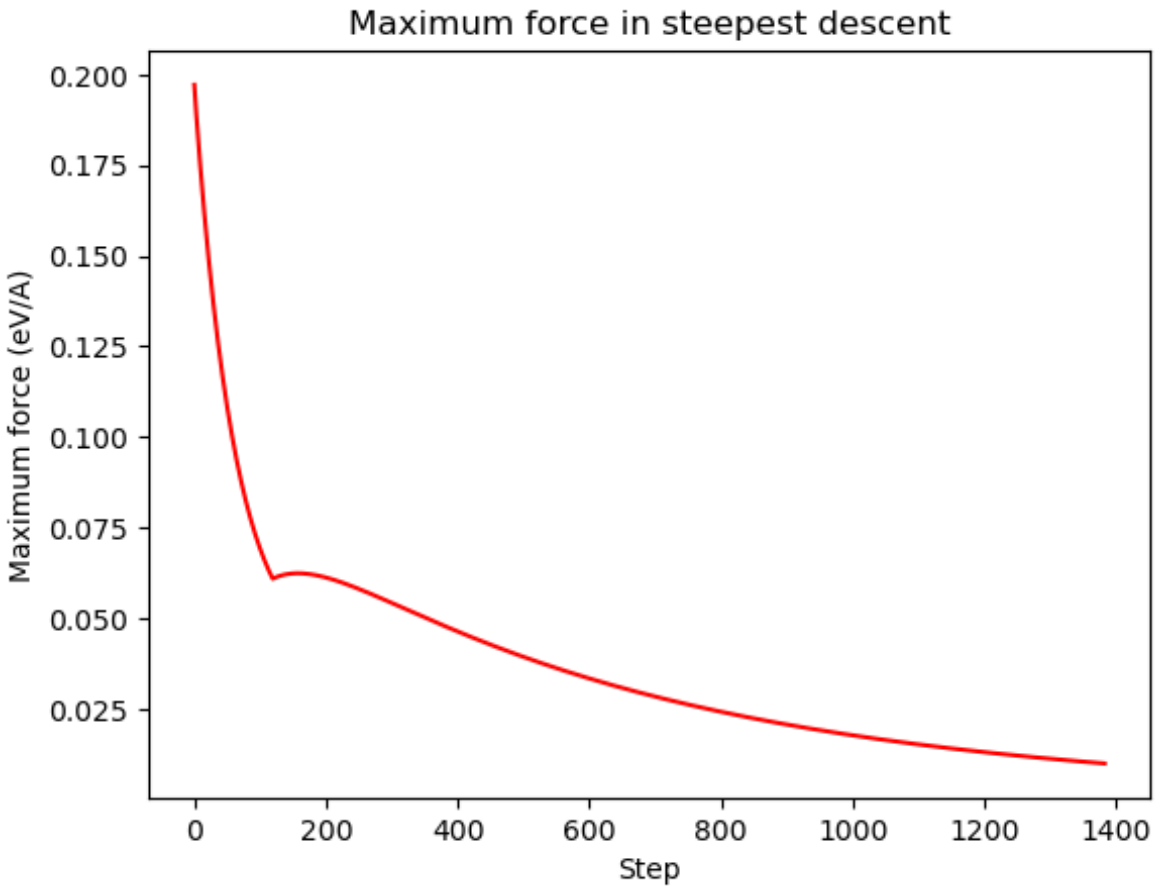
Sharp cutoff approach, velocity distribution

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



Sharp cutoff approach, steepest descent

$$F_{max} < 0.01\, eV/\mathring{A}$$



Sharp cutoff approach, steepest descent

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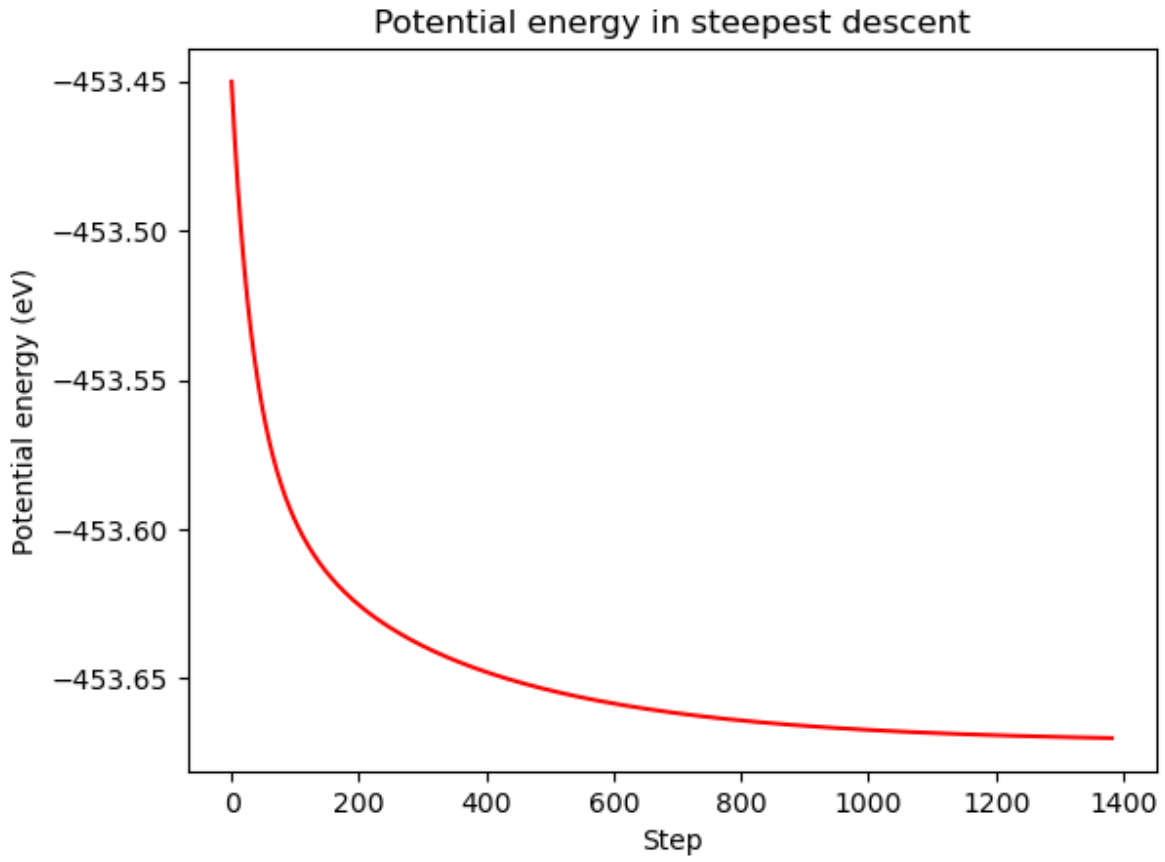
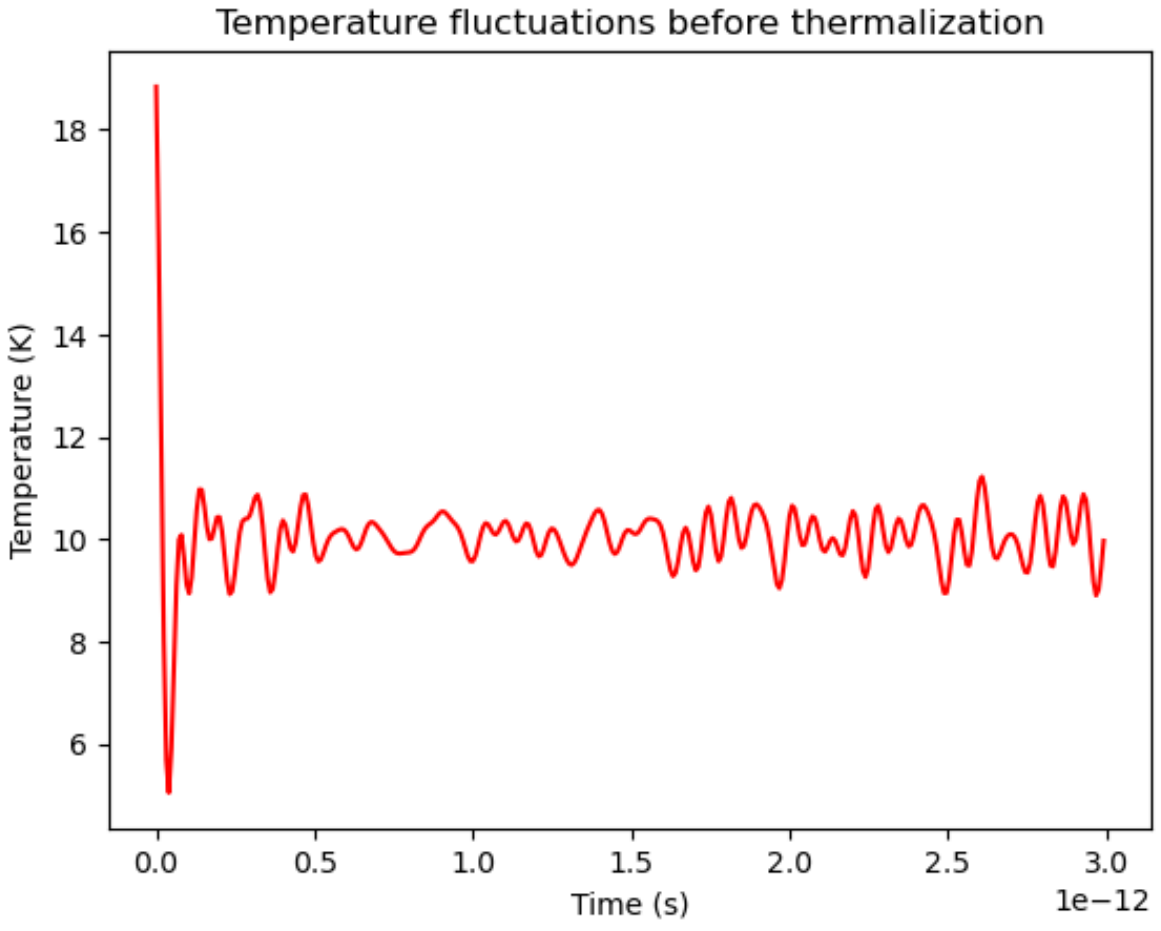


Sharp cutoff approach, steepest descent

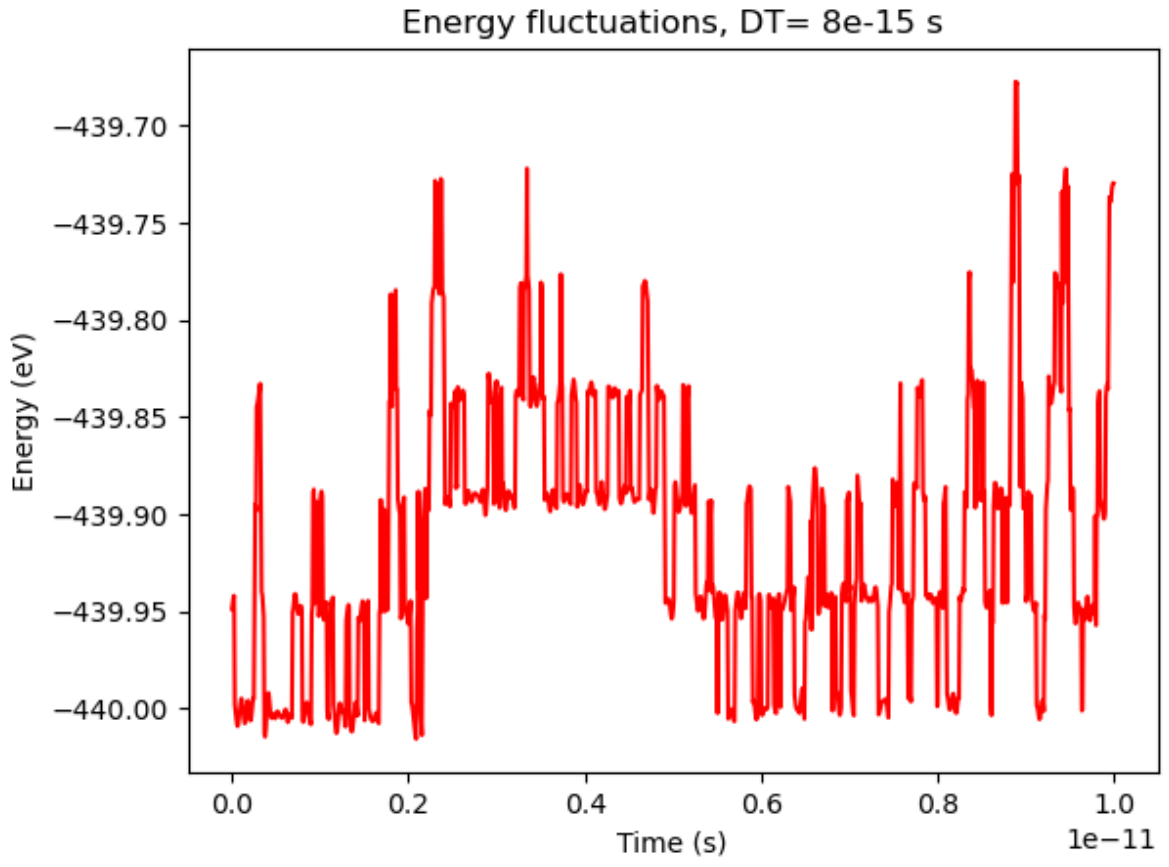
$$T_{init} = 20\,K \rightarrow \langle T \rangle = 10.06\,K$$



Sharp cutoff approach, energy at higher temperatures

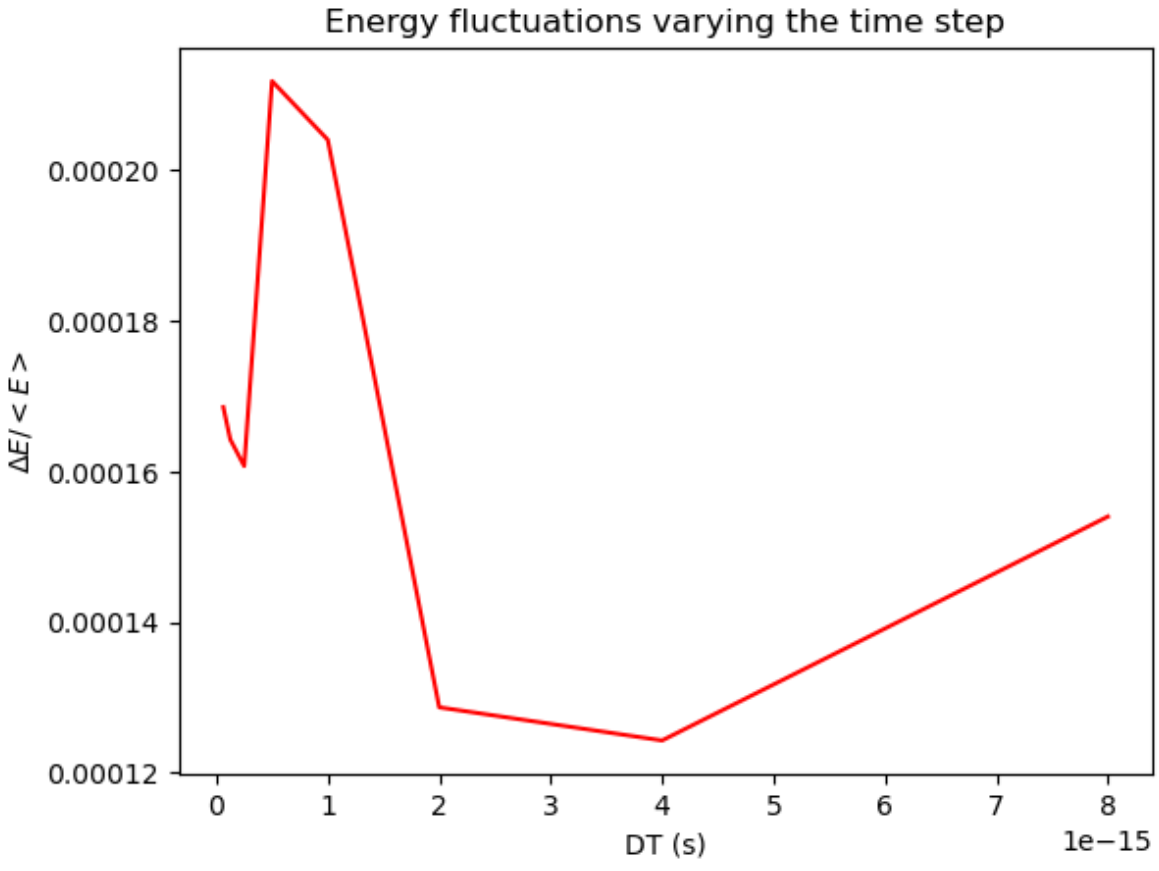
$$\langle T \rangle = 199.74\, K$$

$$\frac{\delta E}{E} = 1.54 \times 10^{-4}$$



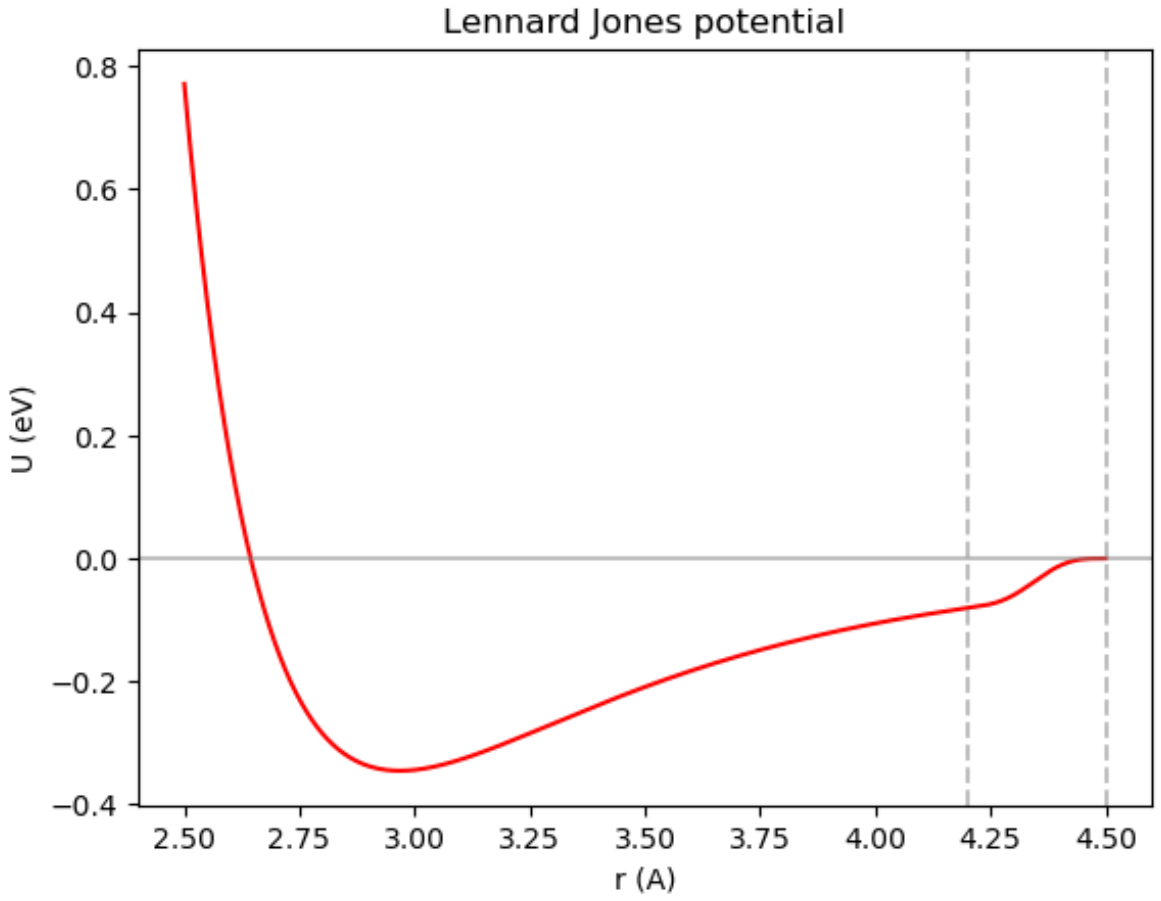
Sharp cutoff approach, energy

Lowering the time step does not solve the problem



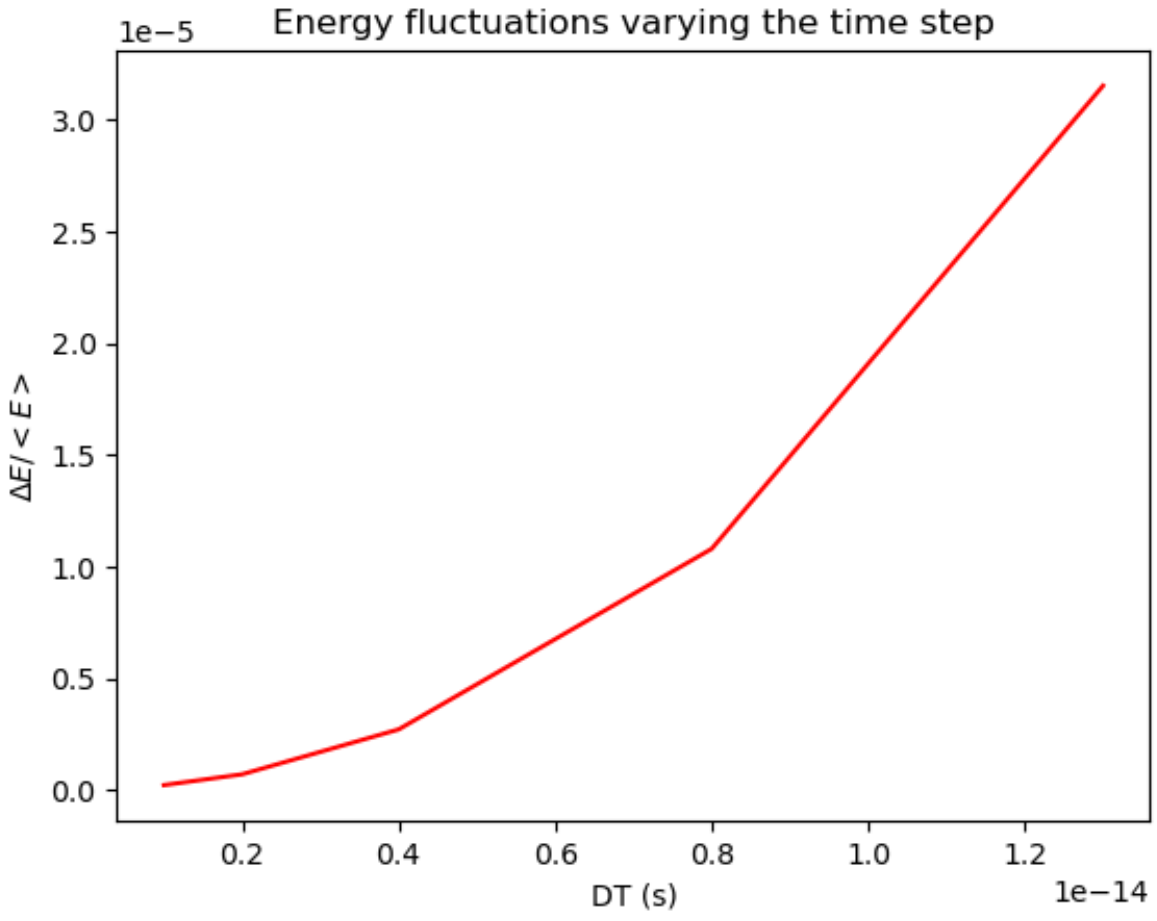
Polynomial junction approach

Insert 7th order polynomial junction between $r' = 4.2\,\mathring{A}$ and $r_c = 4.5\,\mathring{A}$.



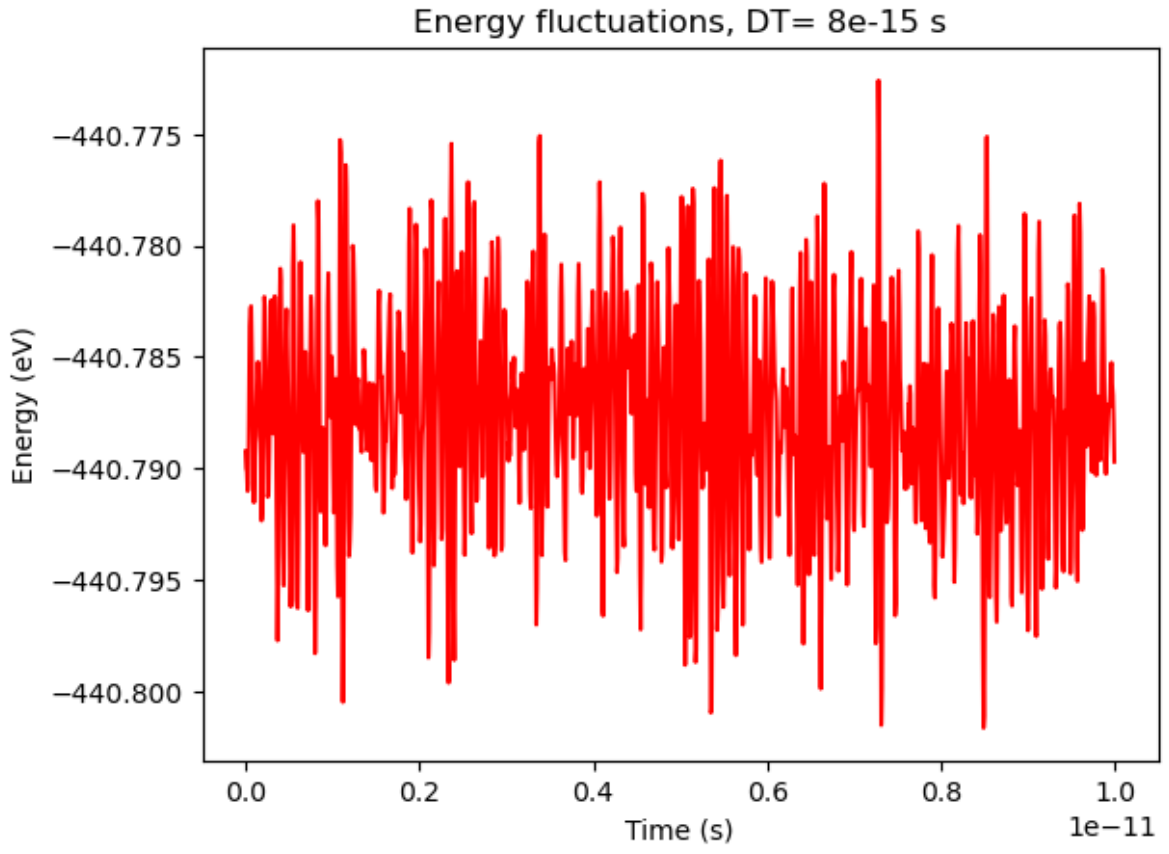
Polynomial junction approach, ideal timestep

Ideal timestep is $\Delta t = 8 \times 10^{-15}\, s$ as it gives $\frac{\delta E}{E} = 1.08 \times 10^{-5}$.

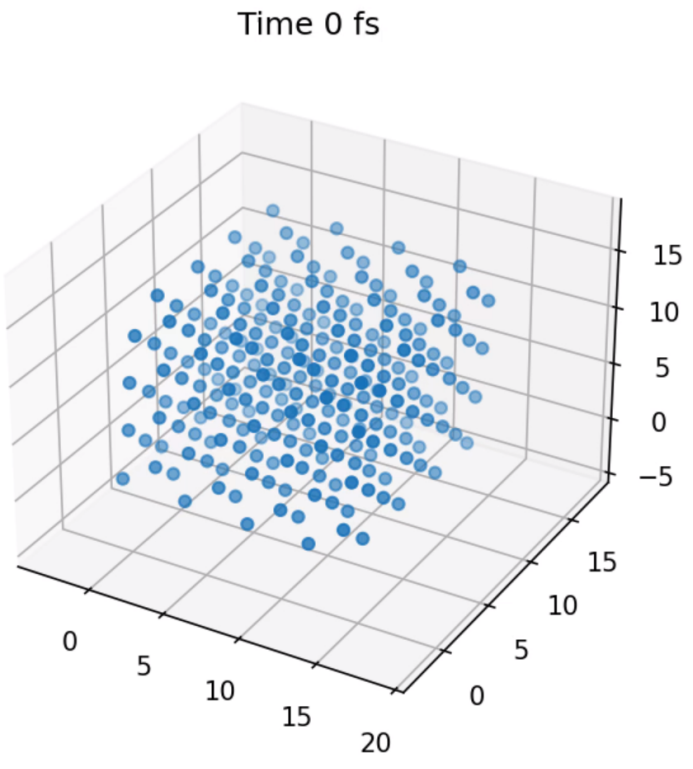


Polynomial junction approach, energy

$$\frac{\delta E}{E} = 1.08 \times 10^{-5}$$

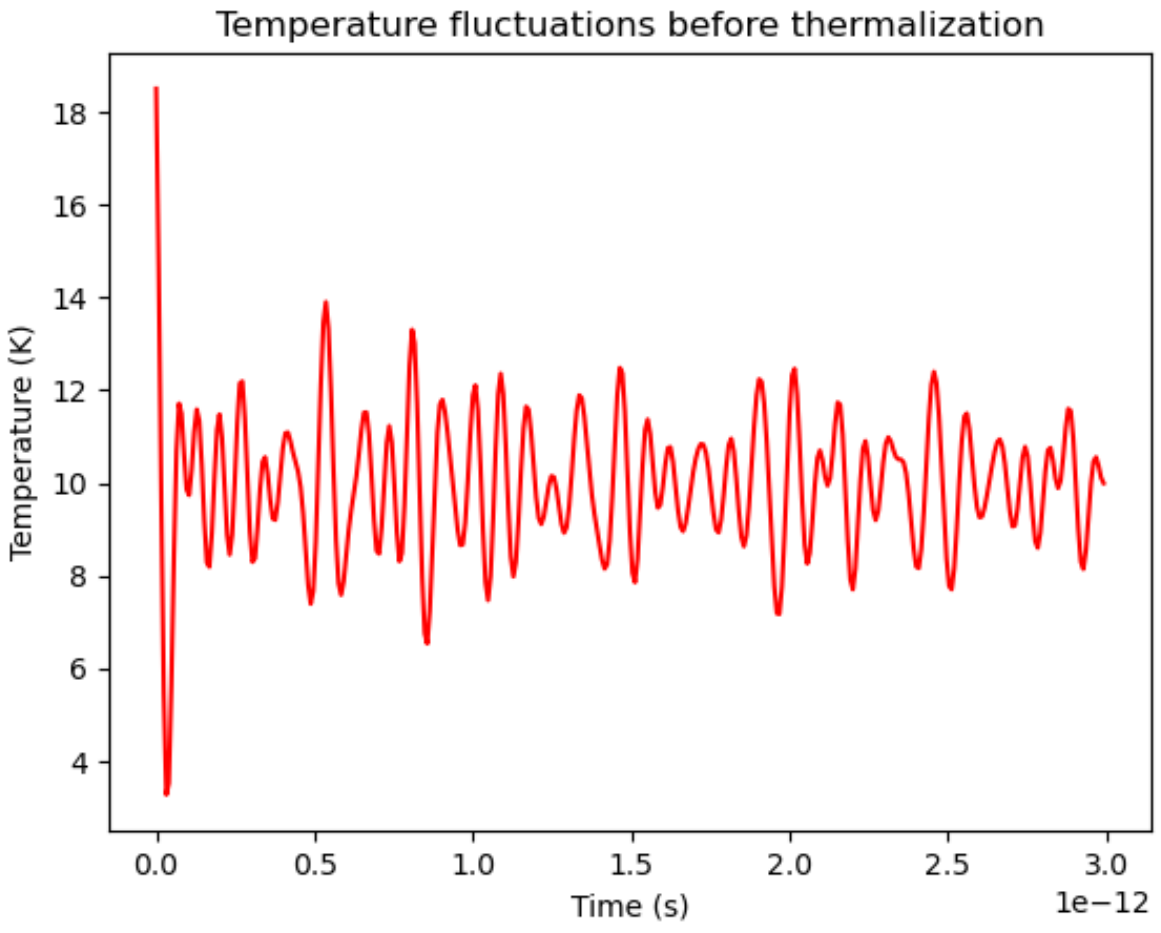


Polynomial junction approach, simulation



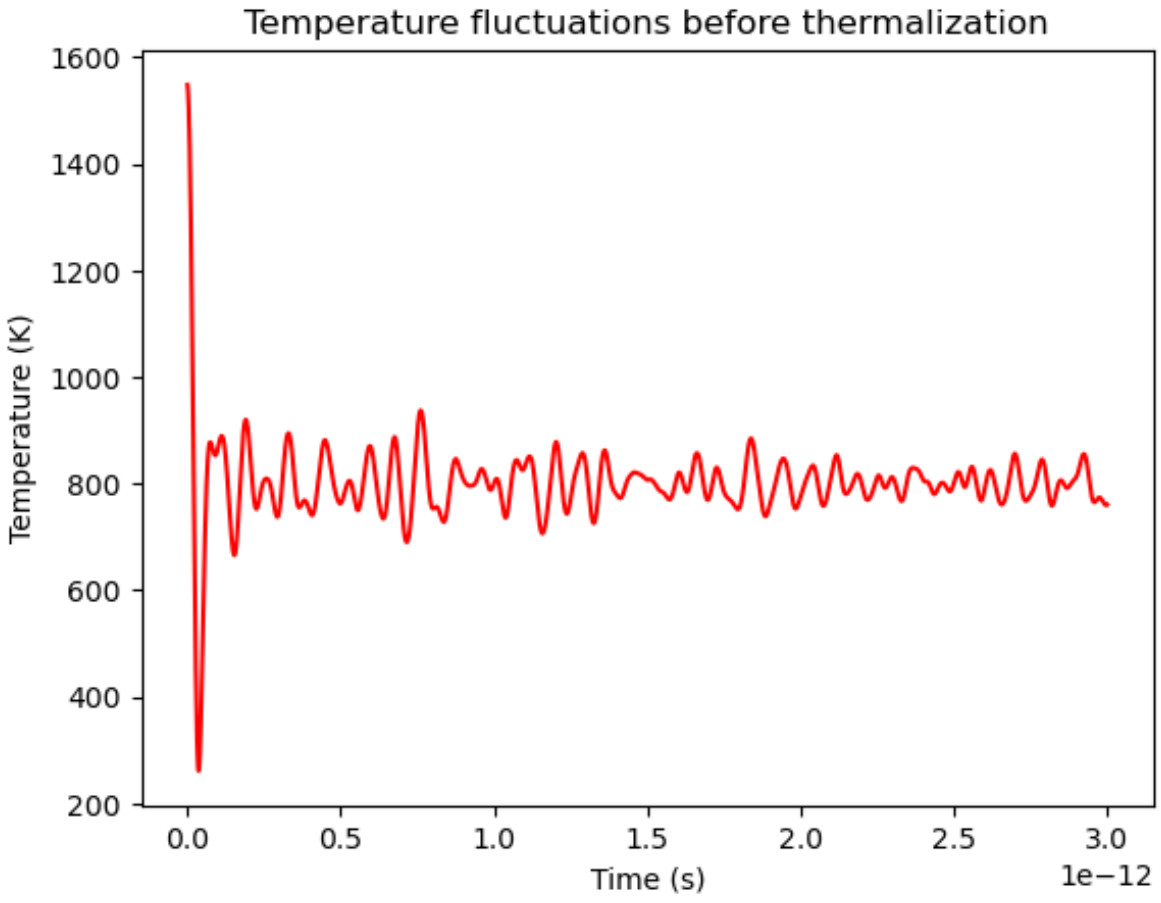
PBC, initial temperature

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

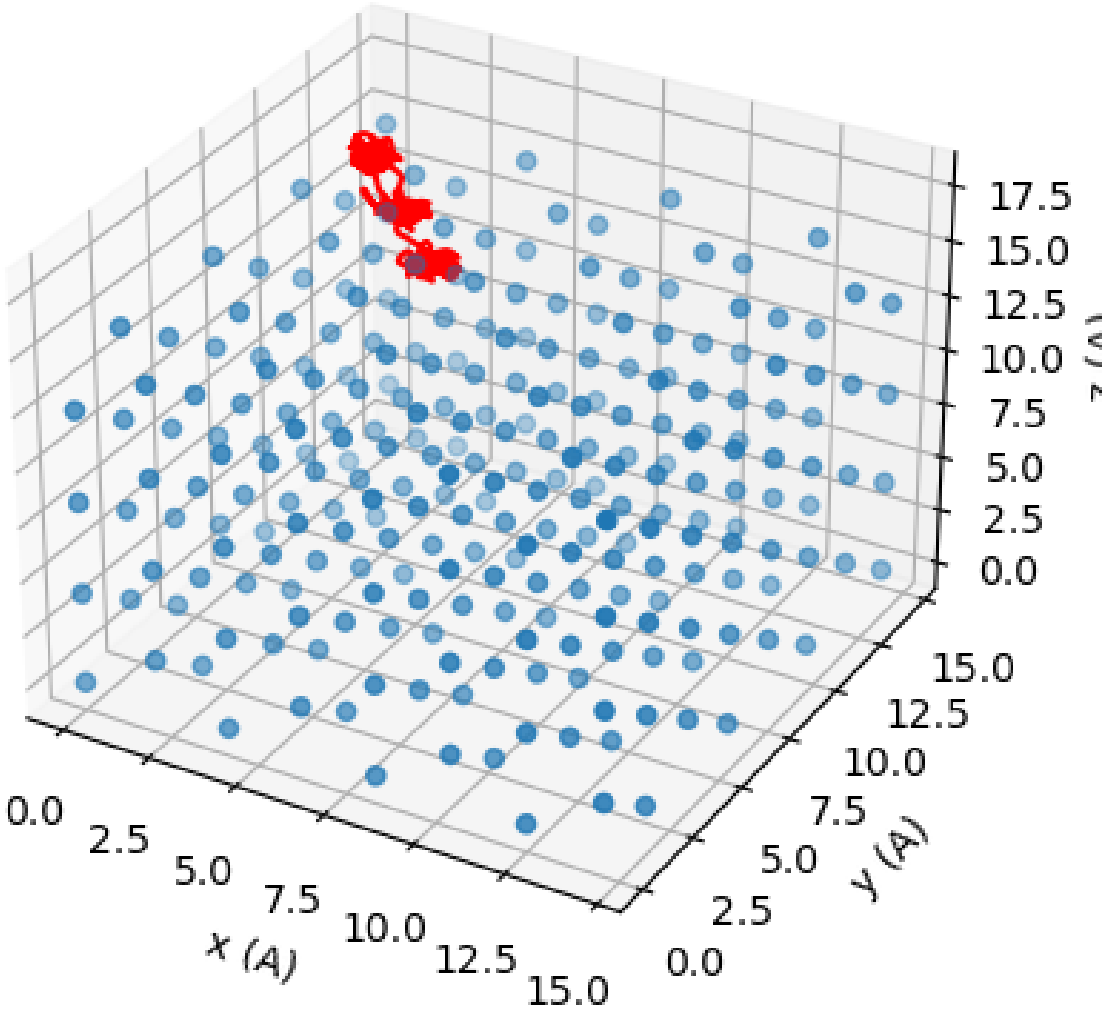


PBC, initial temperature

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

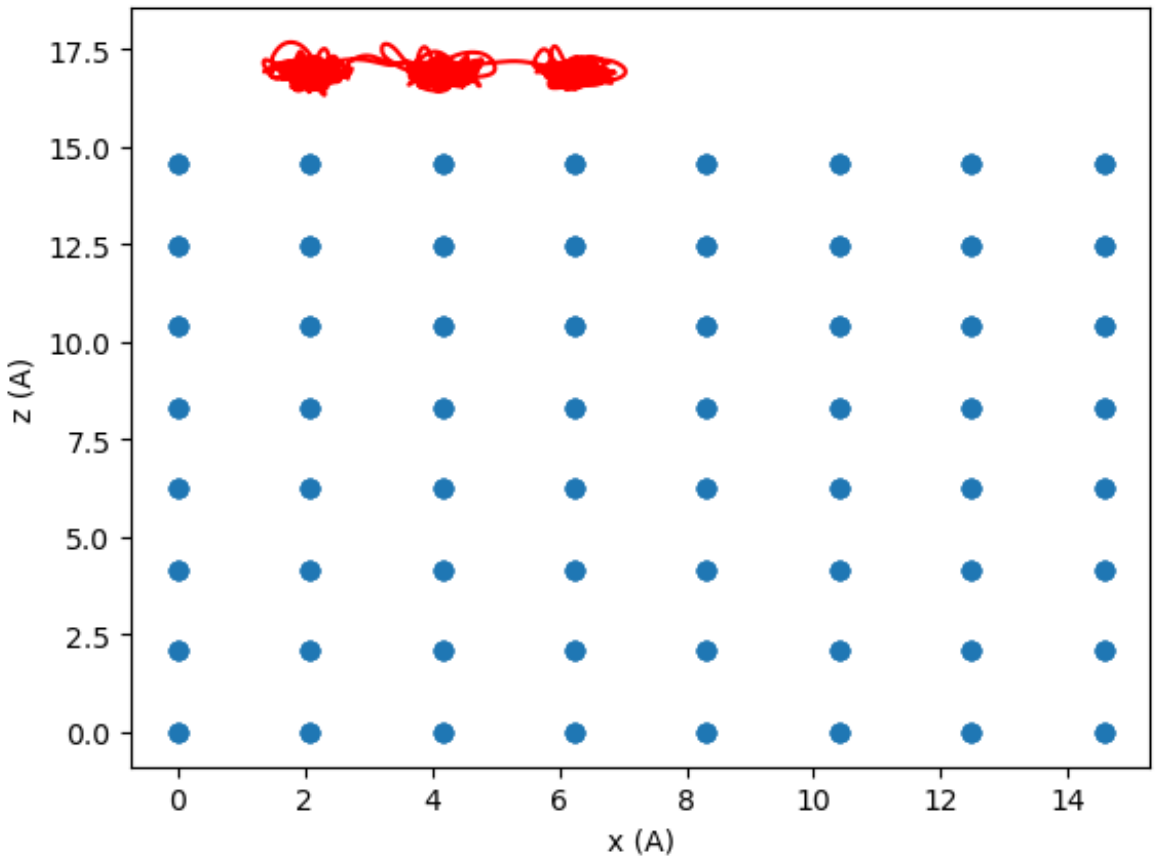


Extra atom trajectory, $T = 1000\,K$



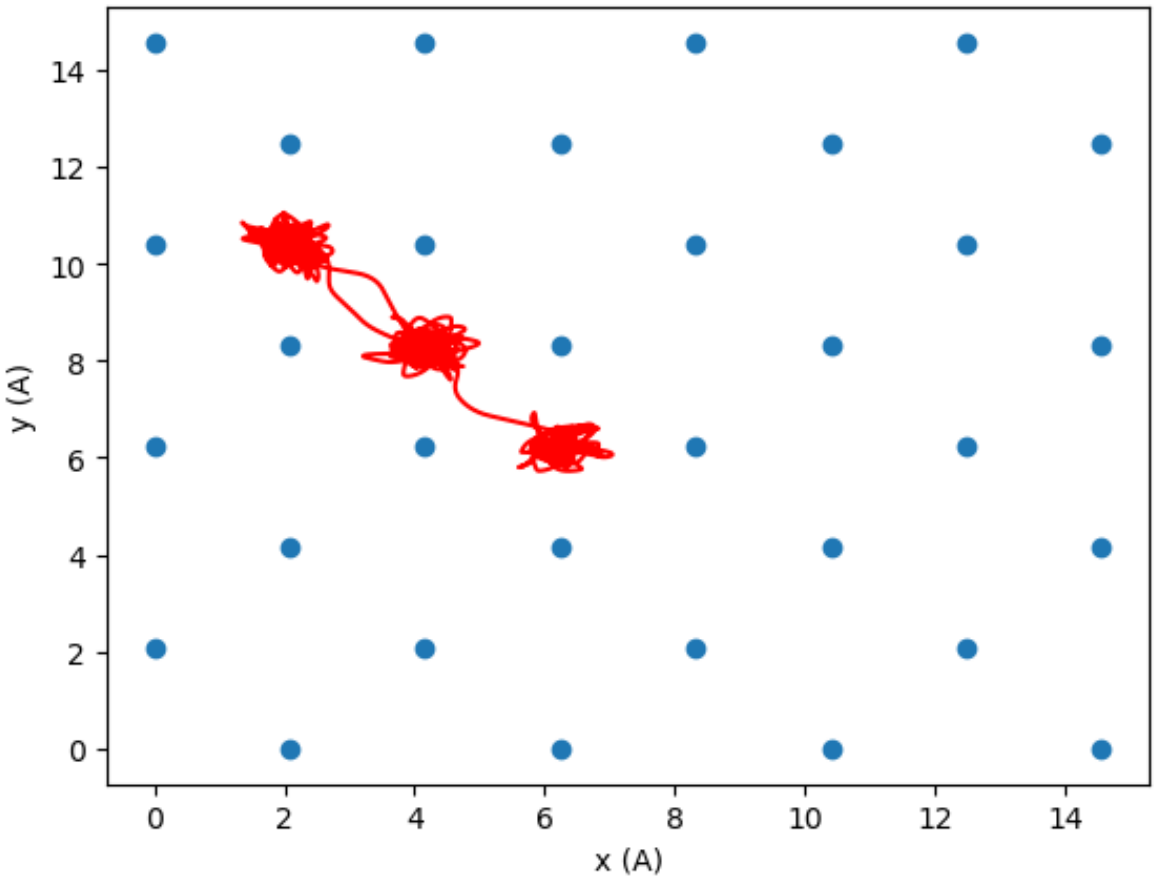
Extra atom trajectory, $T = 1000\,K$

Lateral view

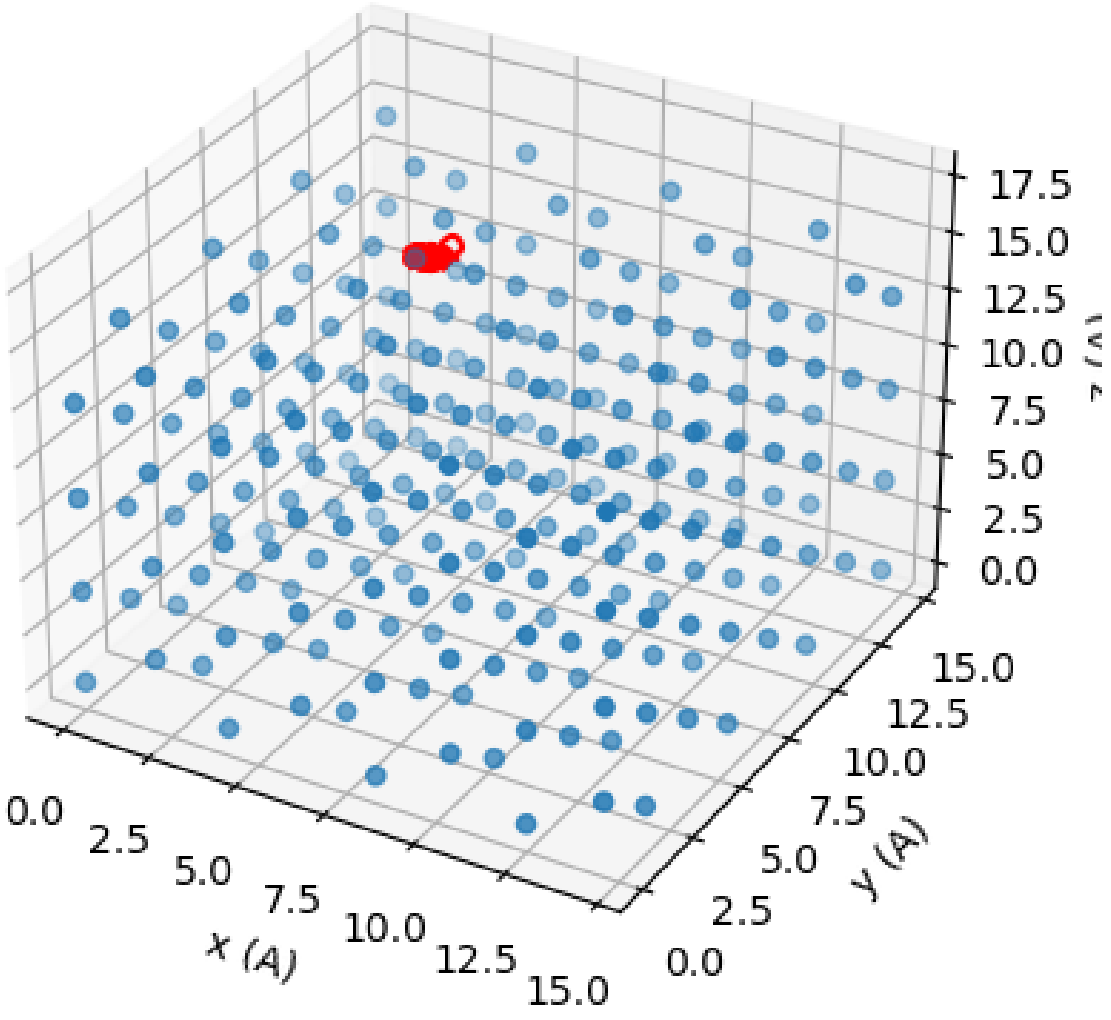


Extra atom trajectory, $T = 1000\,K$

View from above with only first layer

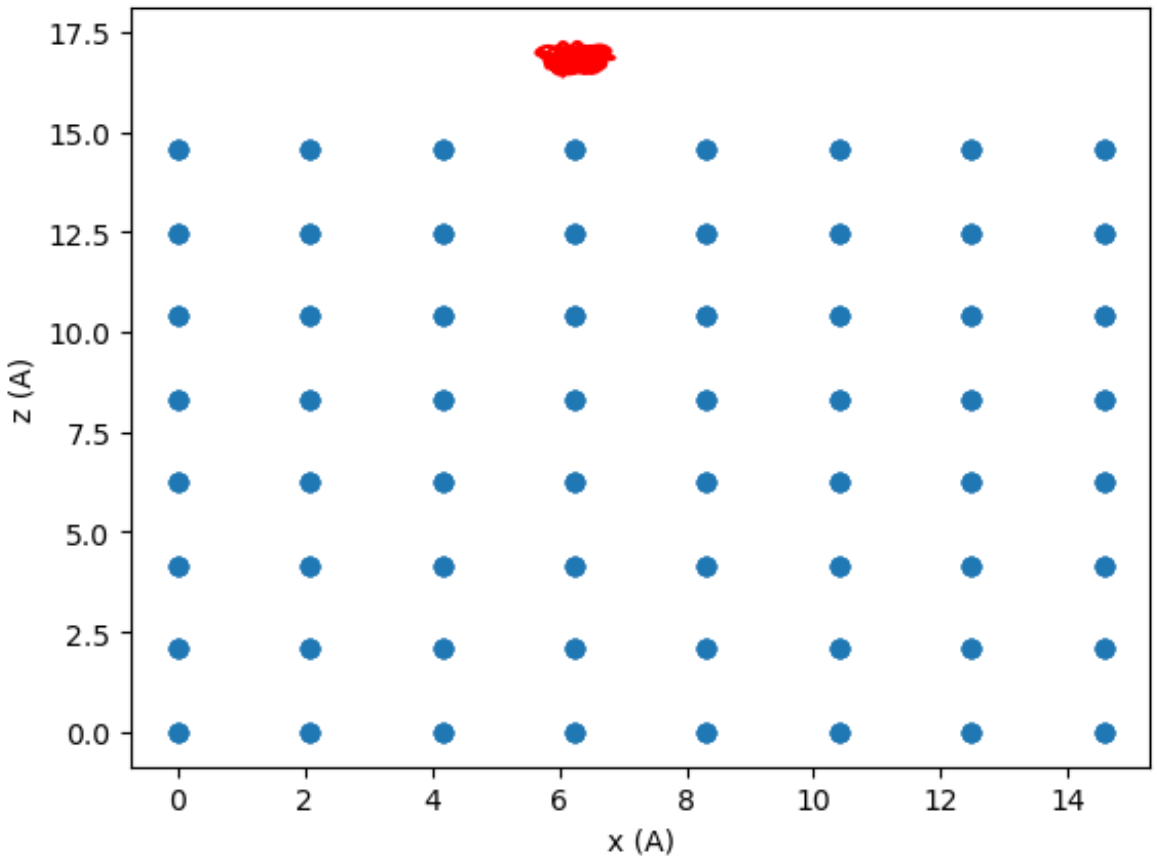


Extra atom trajectory, $T = 600\,K$



Extra atom trajectory, $T = 600\,K$

Lateral view



Extra atom trajectory, $T = 600\,K$

View from above with only first layer