

Esercizio dinamica molecolare

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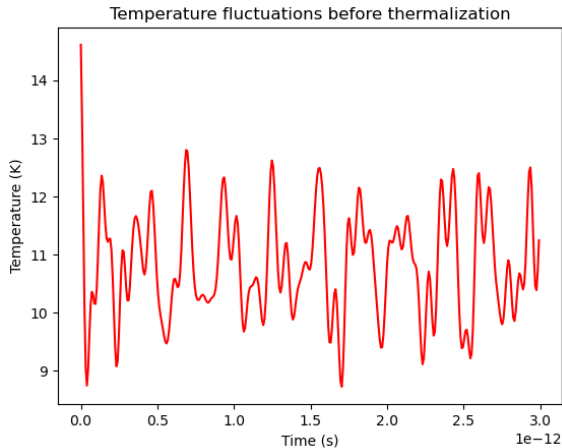
Aprile 2024

Sharp cutoff approach

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

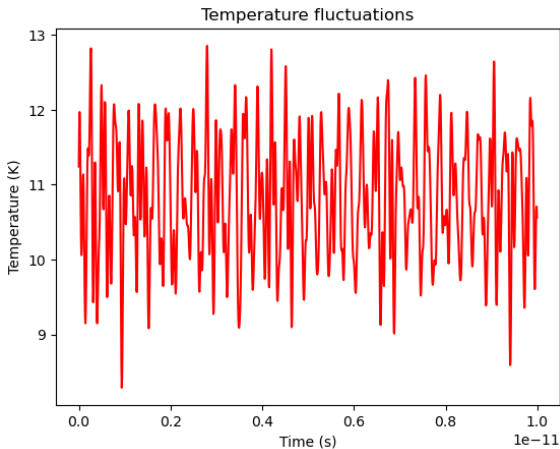
Sharp cutoff approach, initial temperature

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



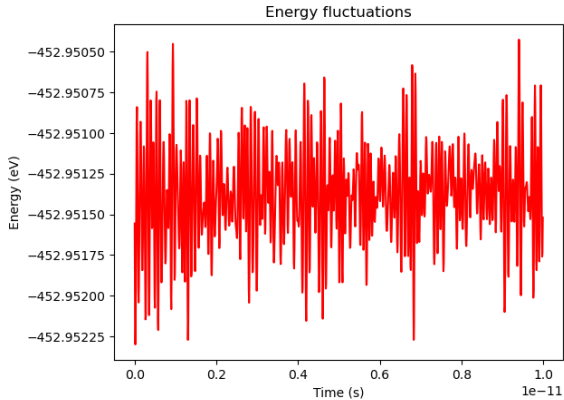
Sharp cutoff approach, initial temperature

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



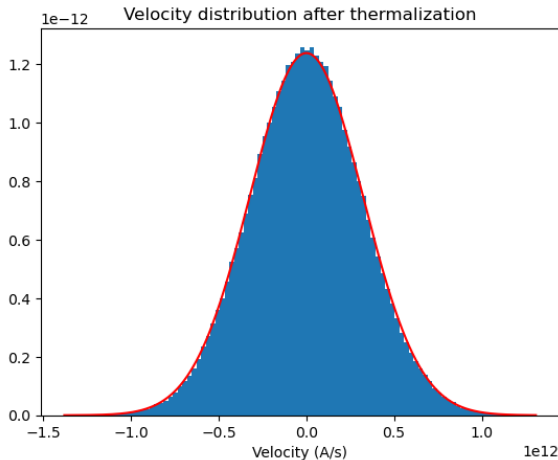
Sharp cutoff approach, energy conservation

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



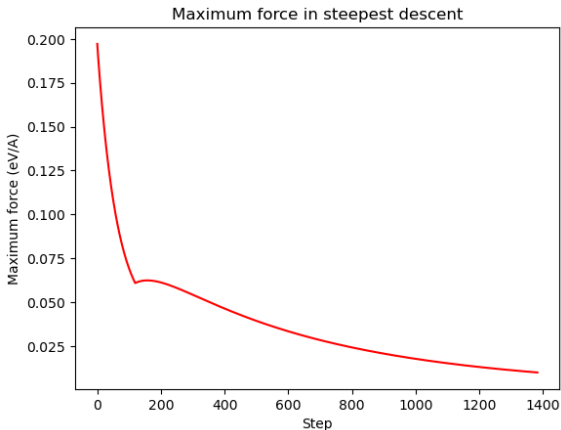
Sharp cutoff approach, velocity distribution

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



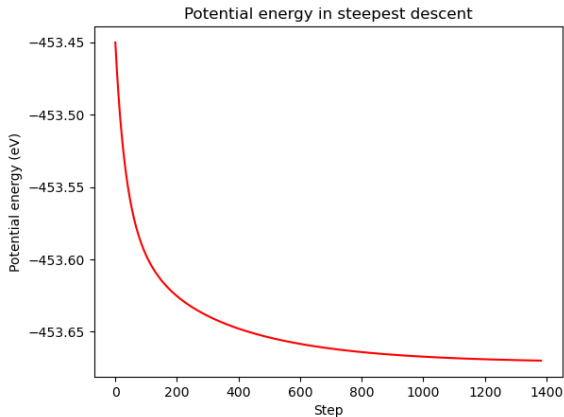
Sharp cutoff approach, steepest descent

$$F_{max} < 0.01 \text{ eV}/\text{\AA}$$



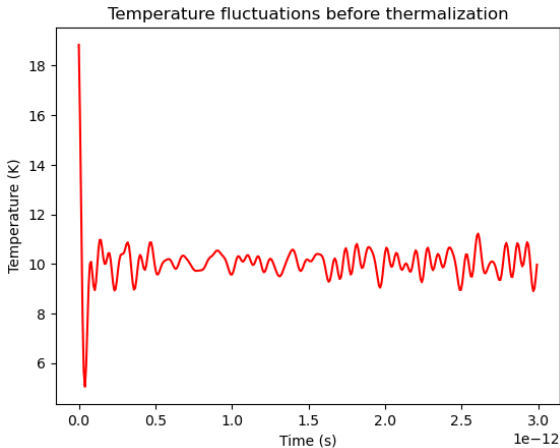
Sharp cutoff approach, steepest descent

$$F_{max} < 0.01 \text{ eV}/\text{\AA}$$



Sharp cutoff approach, steepest descent

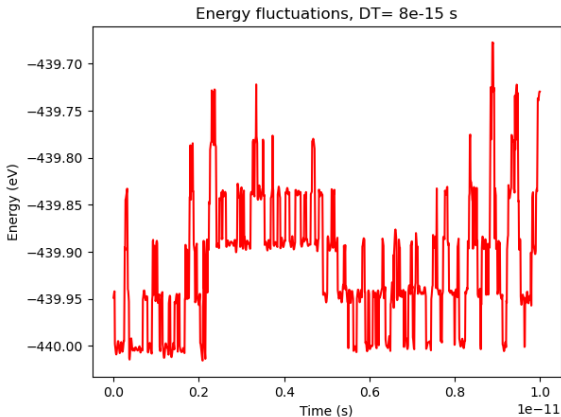
$$T_{init} = 20\text{ K} \rightarrow \langle T \rangle = 10.06\text{ K}$$



Sharp cutoff approach, energy at higher temperatures

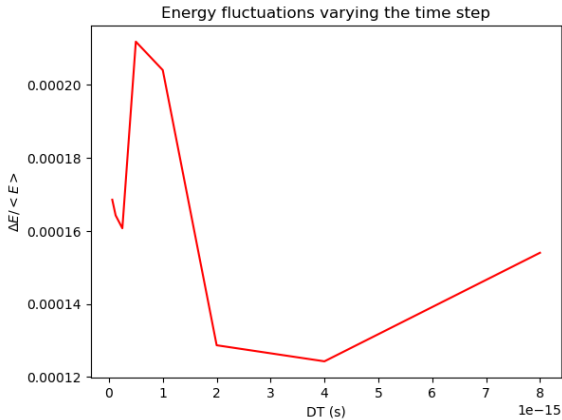
$$\langle T \rangle = 199.74 \text{ K}$$

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



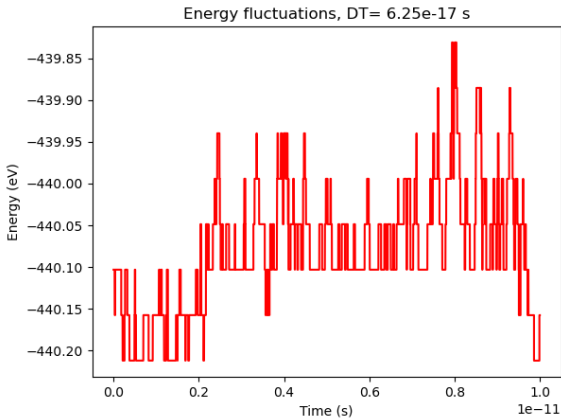
Sharp cutoff approach, energy

Lowering the time step does not solve the problem



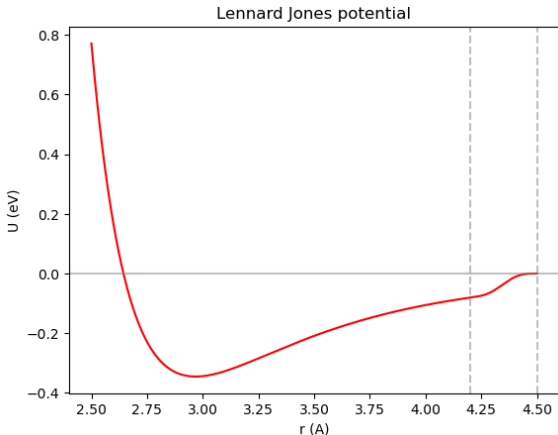
Sharp cutoff approach, energy at higher temperatures

Bad conservation even with $\Delta t = 6.25 \times 10^{-17} \text{ s}$



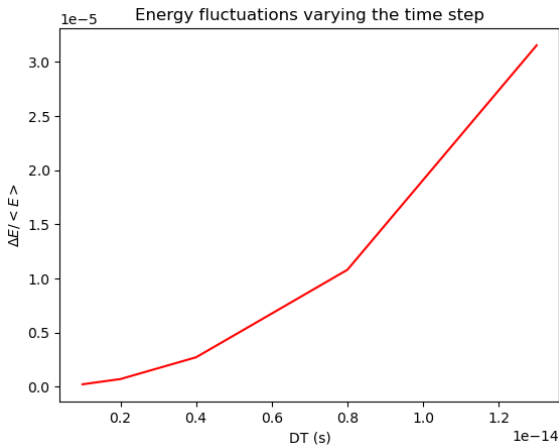
Polynomial junction approach

Insert 7th order polynomial junction between $r' = 4.2 \text{ \AA}$ and $r_c = 4.5 \text{ \AA}$.



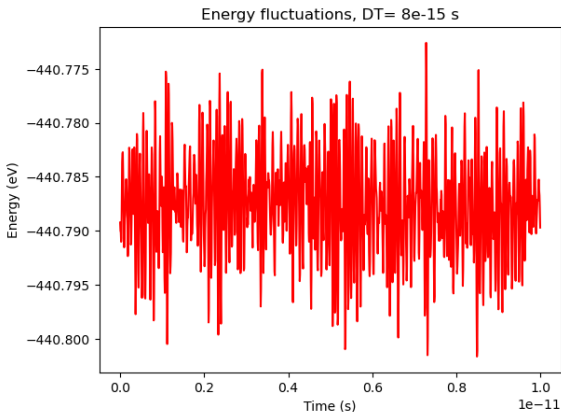
Polynomial junction approach, ideal timestep

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

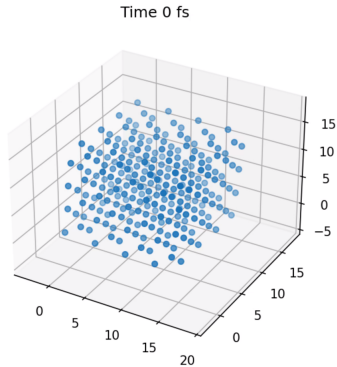


Polynomial junction approach, energy

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

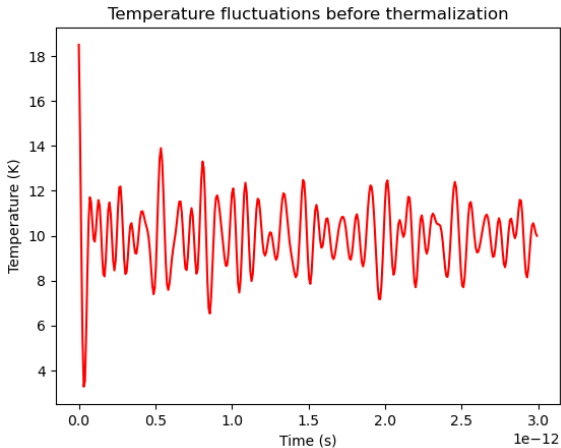


Polynomial junction approach, simulation



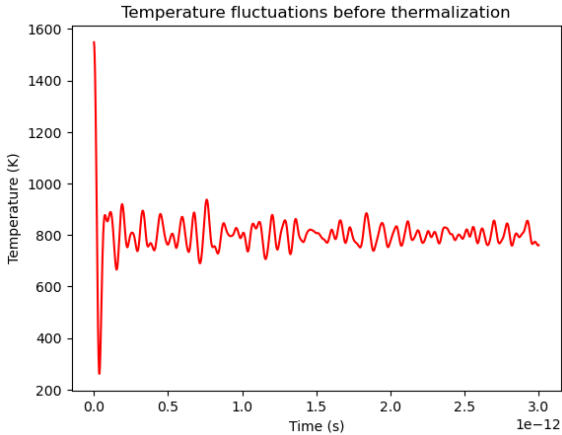
PBC, initial temperature

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

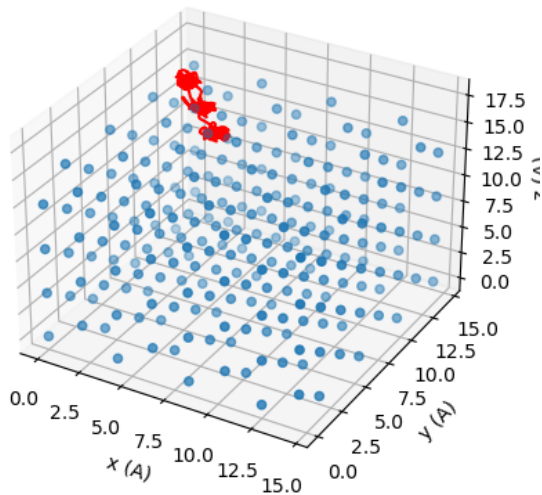


PBC, initial temperature

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

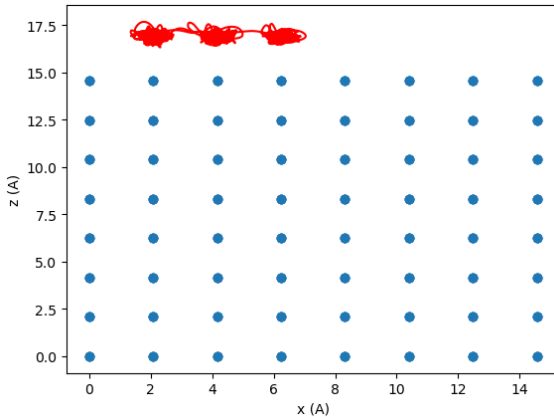


Extra atom trajectory, $T = 1000\text{ K}$



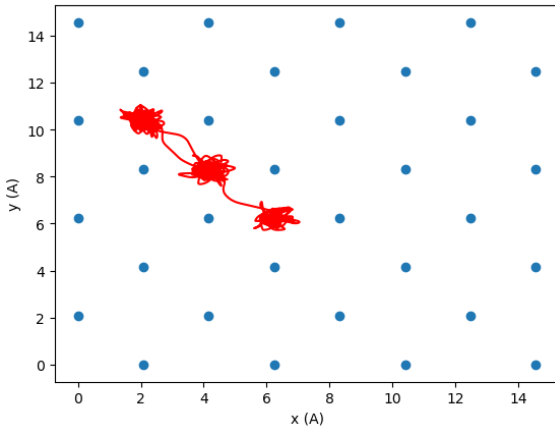
Extra atom trajectory, $T = 1000\text{ K}$

Lateral view

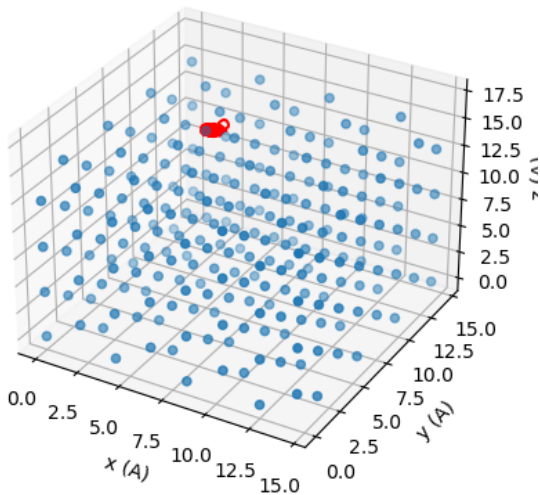


Extra atom trajectory, $T = 1000\text{ K}$

View from above with only first layer

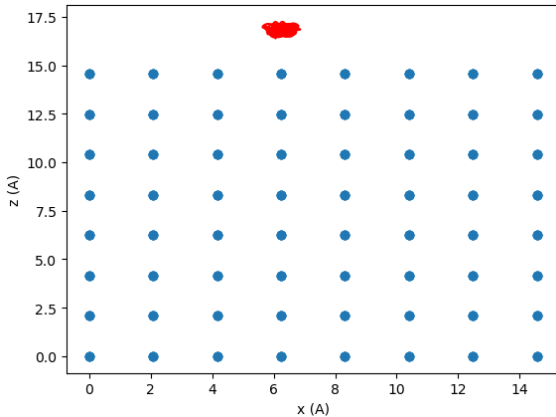


Extra atom trajectory, $T = 600\text{ K}$



Extra atom trajectory, $T = 600\text{ K}$

Lateral view



Extra atom trajectory, $T = 600\text{ K}$

View from above with only first layer

