Ex 1| d) Local moves slightly change the local polymer structure, while the large-scale shape changes only slowly. Reptation moves only affect the two ends of the polymer, and again the large-scale shape changes only after long times. In contrast, pivot moves yield uncorrelated structures much more quickly because they rapidly change the entire polymer structure.

Identical frames occur, when a move is rejected because the new configuration would have overlapped with itself.

e) Combining local, reptation and pivot moves gives large-scale and small-scale conformational changes. Lowering the temperature makes the polymer take more compact structures compared to the extended structures at $T = 4.98$.

Ex 2|, Ex 3| Jupyter notebook.

Ex 4| b) $\langle v \rangle = \int_0^\infty \left(\frac{1}{2\pi\sigma^2}\right)^{3/2} (4\pi v^2) \cdot (v e^{-\frac{v^2}{2\sigma^2}}) dv$ with $\sigma^2 := \frac{k_B T}{m}$

partial integration $= \Big[\left(\frac{1}{2\pi\sigma^2}\right)^{3/2} 4\pi v^2 \underbrace{(-\sigma^2) e^{-\frac{v^2}{2\sigma^2}}}_{=0} \Big]_0^\infty - \int_0^\infty \left(\frac{1}{2\pi\sigma^2}\right)^{\frac{3}{2}} 8\pi v (-\sigma^2) e^{-\frac{v^2}{2\sigma^2}} dv$

$= \frac{1}{\sqrt{2\pi\sigma^2}} \frac{1}{2\pi\sigma^2} 8\pi\sigma^2 \Big[-\sigma^2 e^{-\frac{v^2}{2\sigma^2}} \Big]_0^\infty$

$= \sqrt{\frac{8\sigma^2}{\pi}} = \sqrt{\frac{8 k_B T}{\pi m}}$

c) $\lambda = \frac{h}{\langle p \rangle} = \frac{h}{m\langle v \rangle} = h\sqrt{\frac{\pi}{8 k_B T m}}$, $\lambda_T = \frac{h}{\sqrt{2\pi m k_B T}}$

$\Rightarrow \frac{\lambda}{\lambda_T} = \frac{h}{h}\sqrt{\frac{\pi \, 2\pi m k_B T}{8 k_B T m}} = \frac{\pi}{2}$

d) With $m_{SiO_2} = 60\,u$ and $T = 1450\,K$ one obtains $\lambda_T \approx 5.9 \cdot 10^{-12}\,m$

This is two orders of magnitude smaller than the Si-O bond length of $1.6\,\text{Å} = 1.6 \cdot 10^{-10}\,m$.

Thus the system still behaves classically.