2024-12-06

**kMC Model Improvements**

1. Everyone runs the same script for 3 num\_averages, and then we compare to see how many averages we must do in the larger computations.
2. Ideas of improving the existing code structure:
   1. Implement nearest neighbours, and next nearest neighbours dictionaries instead of computing those positions at every time step
   2. [Optional] Diffusion Radius
   3. Time propagation adjusting on the rates of the transitions (I’ll upload a paper here)
   4. Markov Chain steps in the Wasserstein space (depends a bit on step 1.)
3. Implement anisotropic diffusion based on nearest neighbours to model intermolecular interactions.