Biomolecular Dynamics
Stock Lab

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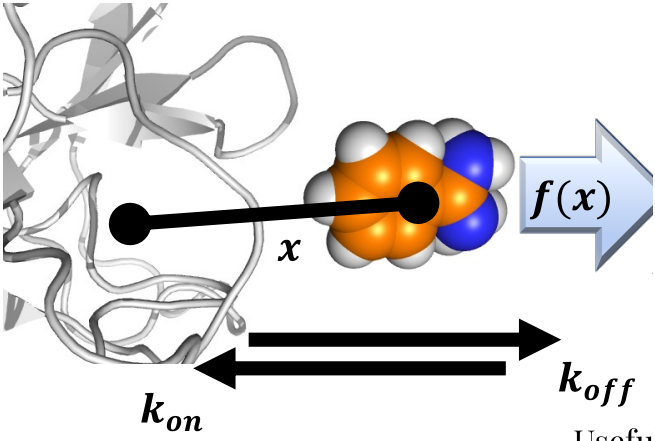
Bachelor/Master Project

Pulling harder and harder: Convergence of free energy calculations

The calculation of free energies is one of the central applications of molecular dynamics simulations. Often, the investigated complexes such as drug molecules bound to their target protein that effects their action are too stable to see them binding or unbinding spontaneously in simulations.
To allow predictions of the free energy of unbinding, we have developed an approach called dissipation-corrected targeted MD, where drug-protein unbinding is enforced by a constant velocity constraint. However, a constraint is a concept that is not compatible with experimental single molecule pulling approaches such as atomic force microscopy, which uses a Hookian spring for the same purpose. Here we check the applicability of employing a corresponding potential harmonic for pulling simulations and its effect on data analysis in dissipation-corrected MD.



Useful information

Wolf, S., & Stock, G. (2018). Targeted Molecular Dynamics Calculations of Free Energy Profiles Using a Nonequilibrium Friction Correction. J. Chem.Theory Comput. 14, 6175–6182.

Meyer, H., Wolf, S., Stock, G., & Schilling, T. (2020). A Numerical Procedure to Evaluate Memory Effects in Non-Equilibrium Coarse-Grained Models. Adv. Theory Simul., 111, 2000197.

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