Biomolecular Dynamics
Stock Lab

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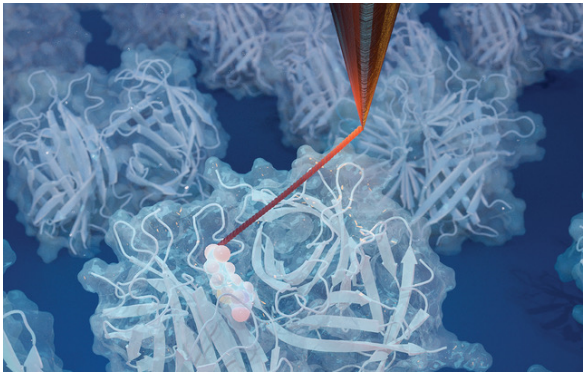
Bachelor/Master Project

hard vs. soft springs: comparing pulling in atomic force microscopy simulations

Binding and unbinding events between proteins and host molecules, e.g. drugs, are a crucial step in signalling between proteins. To understand the physics of these processes, our group has developed an approach called dissipation-corrected targeted molecular dynamics (dcTMD). This approach uses active pulling to force (un)binding and allows the parameterisation of free energy and friction profiles along the pulling distance.
Currently, dcTMD limited to pulling via a constant velocity, i.e., a „stiff“ spring. However, most molecular dynamics (MD) software packages use harmonic potentials, i.e., „soft“ springs for pulling simulations. Atomic force microscopy pulling can be approximated by such harmonic potentials.
In this project, you will perform and analyze pulling MD simulations using "soft spring" to investigate under which conditions a harmonic potential can be used for pulling to still be suitable for analysis via dcTMD, and which error it causes in the estimation of free energy and friction profiles.



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.

Cai, W., Jäger, M., Bullerjahn, J. T., Hugel, T., Wolf, S., Balzer, B. N. (2023). Anisotropic Friction in a Ligand-Protein Complex. Nano Lett 23, 4111

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