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Simulations of single-molecule pulling experiments: equilibrium and non-equilibrium free-energy landscape trajectories ERIC COPENHAVER, JUTTA LUETTMER-STRATHMANN, Department of Physics, University of Akron — The response of a single molecule to an applied force is important for many biological processes. This response is often investigated via single-molecule pulling experiments, where a tension force is applied to the opposite ends of a biological chain molecule. In equilibrium conditions, the system follows a trajectory that may be predicted from the free-energy landscape. In non-equilibrium experiments, the pulling force varies too rapidly for the chain to explore all available configurations resulting in a deviation from the equilibrium trajectory. To gain a better understanding of the relationship between equilibrium and non-equilibrium processes, we investigate the effect of the pulling speed on the system's trajectory with two types of computer simulations of single-molecule experiments. We perform Wang-Landau simulations to determine the energy landscape and Langevin dynamics simulations to probe the dynamic response of the same bead-spring model of a biopolymer. After verifying that both simulation methods yield consistent equilibrium results, we study the effect of the pulling protocol on the free-energy landscape trajectories. The goal of this project is to devise an effective dynamic field that recreates the non-equilibrium pathway under equilibrium conditions.

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