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Calculating free energy profiles and identifying the underlying dynamics in systems with memory effects from bi-directional pulling processes JIONG ZHANG, IOAN KOSZTIN, University of Missouri-Columbia — A proper description of the effective dynamics of a biomolecular system along a relevant reaction coordinate (RC) requires not only the determination of the corresponding free energy profile (potential of mean force or PMF) but also the correct identification of the underlying stochastic model. While there exist several methods for determining the PMF from fast non-equilibrium pulling processes, for simplicity reasons, it is generally assumed that the dynamics along the RC is that of a simple overdamped Brownian particle with known diffusion coefficient. However, in general, the dynamics along the RC is non-Markovian and can be modeled with a generalized Langevin equation characterized by a friction memory kernel. Here we propose and demonstrate a method that permits the simultaneous determination of both PMF and friction memory kernel from fast bi-directional (forward and time-reversed) pulling processes. As a result, one can identify whether the diffusion along the RC is normal or anomalous (e.g., subdiffusion). The proposed method provides a novel approach for identifying and characterizing the underlying dynamics along a RC of a biomolecular system studied by either single-molecule force microscopy or steered molecular dynamics simulations.

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