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Simultaneous determination of the free energy profile and effective dynamics along a reaction coordinate[1] JIONG ZHANG, IOAN KOSZTIN, University of Missouri-Columbia — Often one can gain insight into the functioning of a biomolecular system by following its dynamics along a relevant reaction coordinate (RC). A proper description of the motion along the RC requires not only the determination of the corresponding free energy profile (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 it is implicitly assumed that the dynamics along the RC is a simple overdamped Brownian motion with known diffusion coefficient. However, in general, the dynamics along the RC is non-Markovian that 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 determine 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 effective dynamics along a RC of a biomolecular system studied by either single-molecule force microscopy or steered molecular dynamics simulations.

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