Abstract Submitted
for the PSF13 Meeting of
The American Physical Society

Calculating free energy profiles in systems with memory effects from bi-directional pulling processes JIONG ZHANG, IOAN KOSZTIN, University of Missouri-Columbia, Department of Physics and Astronomy — In biomolecules, in order to calculate kinetic quantities along a relevant reaction coordinate (RC), besides the corresponding free energy profile (potential of mean force or PMF), one also needs to properly identify the underlying stochastic model that best describes the dynamics along the RC. 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. Here we show that both the PDF and the features of the underlying non-Markov stochastic model (with memory effects), described by a generalized Langevin equation, can be determined simultaneously from properly designed bi-directional (forward and time-reversed) pulling processes. Besides the PMF, the proposed method determines the corresponding friction memory kernel, and identifies whether the diffusion along the RC is normal or anomalous (e.g., subdiffusion). The proposed method provides a novel way to analyze fast pulling data from molecular dynamics simulations and single molecule force microscopy.

Jiong Zhang
University of Missouri-Columbia

Date submitted: 11 Oct 2013 Electronic form version 1.4