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**Bayesian Uncertainty Quantification for Bond Energies and Mobilities Using Path Integral Analysis** PAK-WING FOK, University of Delaware, JOSHUA CHANG, Ohio State University, TOM CHOU, UCLA, UCLA-OSU-UD BIOMATH GROUP COLLABORATION — Dynamic single-molecule force spectroscopy is often used to distort bonds. The resulting responses, in the form of rupture forces and trajectories of displacements, are used to reconstruct bond potentials. Such approaches often rely on simple parameterizations of one-dimensional bond potentials and/or large amounts of trajectory data. Parametric approaches typically fail at inferring complicated bond potentials with multiple minima, while piecewise estimation may not guarantee smooth results. Existing techniques also do not address spatial variations in the diffusivity that may arise from inhomogeneous coupling to other degrees of freedom in the macromolecule. To address these challenges, we develop an empirical Bayesian approach that incorporates data and regularization terms into a path integral. All experimental and statistical parameters in our method are estimated from the data. Upon testing our method on simulated data, our regularized approach requires less data and allows simultaneous inference of both complex bond potentials and diffusivities. We show that the accuracy of the reconstructed bond potential is sensitive to the spatially varying diffusivity and accurate reconstruction can be expected only when both are simultaneously inferred.

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