

Abstract Submitted
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Reconstruction of bonds potentials from first passage time distributions TOM CHOU, UCLA, PAK-WING FOK, Univ. Delaware — We explore the reconstruction the functional form of the potential energy surface of a molecular bond from distributions of its rupture times. For a single measured first passage time distribution (FPTD) the inverse problem is ill-posed and only a few attributes (such as the height and width of an energy barrier) can be reconstructed. However, we find optimal temperatures and initial bond configurations that yield the most efficient reconstruction of simple potentials. Reconstruction of finer details of more complicated bond potentials can be achieved by simultaneously using two or more measured FPT distributions, obtained under different physical conditions. For example, by changing the effective potential energy surface by known amounts, through for example, externally applied forces, the additional FPT distributions render the inverse problem less ill-posed. We demonstrate the feasibility of reconstructing potential with multiple minima, motivate heuristic rules-of-thumb for optimizing the reconstruction, and discuss further applications and extensions.

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