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Mechanical unfolding of proteins: reduction to a single-reaction coordinate unfolding potential, and an application of the Jarzynski Relation PETER OLMSTED, DANIEL WEST, EMANUELE PACI, School of Physics and Astronomy & Astbury Centre for Structural Biology, University of Leeds — Single molecule force spectroscopy (AFM, optical tweezers, etc) has revolutionized the study of many biopolymers, including DNA, RNA, and proteins. In this talk I will discuss recent work on modelling of mechanical unfolding of proteins, as often probed by AFM. I will address two issues in obtaining a coarse-grained description of protein unfolding: how to project the entire energy landscape onto an effective one dimensional unfolding potential, and how to apply the Jarzynski Relation to extract equilibrium free energies from nonequilibrium unfolding experiments.

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