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Driving proteins and DNA with mechanical forces: Pushing, pulling, and squeezing molecules using computer simulations.[1]

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In living organisms, proteins and other biopolymers are often subjected to mechanical forces. Some of those forces are strong enough to cause proteins to unfold. For example, proteins driven across transmembrane pores may only enter the pores after they are mechanically denatured. Mechanically driven protein unfolding is often a non-equilibrium, irreversible process; Nature often takes advantage of the energy dissipation associated with such irreversible phenomena. For example, the ability of certain protein domains to dissipate large amounts of energy in the process of their mechanical unfolding is exploited in natural fibers and adhesives, which, as a result, display a remarkable combination of toughness and strength that is rarely achieved in artificial materials. In this talk, I will report on theoretical studies and computer simulations of several types of mechanical processes involving biopolymers. Examples include mechanical unfolding of proteins pulled at their ends, translocation of polymers across transmembrane pores, and stochastic dynamics of knots in tensioned polymer chains. I will discuss some of the computational challenges associated with the disparity between the time scales of simulation and experiments, comment on the molecular origins of high mechanical resistance displayed by some proteins, and compare our results with single-molecule pulling experiments.

[1]NSF, Welch Foundation