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Kinetics of inter-segmental contact in semiflexible polymers REZA AFRA, BRIAN TODD, Dept of Physics, Purdue University — Diffusion-limited contact between polypeptide segments is an elementary step in protein folding and this process sets an upper limit on protein folding kinetics. A common theoretical approach to calculating this "speed limit" is to reduce the high-dimensional conformational search to a one-dimensional diffusion along an effective reaction coordinate. We employed Brownian dynamic simulations to test the validity of this approximation for inter-segmental contact kinetics in the semiflexible polymer model. This model is often used to describe the unfolded protein state. We find that one-dimensional diffusion models cannot capture the correct scaling between contact dynamics and either capture radius or chain length. Our findings highlights the difficulty of describing high-dimensional protein molecules with simple kinetic theories.

Reza Afra
Dept of Physics, Purdue University

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