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Force fluctuation in a semiflexible loop JAMES WATERS, HAROLD KIM, Georgia Institute of Technology, HAROLD KIM TEAM — DNA-binding proteins can regulate genetic expression by holding two sites in close proximity, forming a closed loop. Such complexes may require strong bending of DNA segments on the order of one persistence length or less. Both this elastic bending and the thermal fluctuations of the DNA molecule are necessary to describe the resulting behavior. To explore this problem, we consider a discrete model of a wormlike chain, kept in the fixed extension ensemble. By using a novel method to sample conformations in both position and momentum space, we can obtain a distribution of constraint forces as a function of chain length, extension, and flexibility. Our coarse-grained model allows us to explore the space of these parameters more efficiently than a detailed molecular dynamics approach. We find that increasing contour length decreases average force by relieving bending stress, but that the additional freedom allows fluctuations in the constraint force to increase. This implies that the probability of large forces may go up even as the mean goes down, impacting the lifetime of such bound states in a way unforeseen by purely equilibrium methods.

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