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Is DNA a non-draining, swollen coil? ABHIRAM MURALIDHAR, DOUGLAS TREE, University of Minnesota, PATRICK DOYLE, Massachusetts Institute of Technology, KEVIN DORFMAN, University of Minnesota — Double-stranded DNA has long been used as a model polymer in a wide variety of experiments, particularly in single molecule studies. However, there is little consensus about whether molecules used commonly in experiments, such as λ-DNA (48.5 kbp, kilo base pairs) and T4-DNA (169 kbp), are long enough to exhibit universal, long-chain behavior. To resolve this point of contention, we use Pruned-Enriched Rosenbluth Method (PERM) simulations to calculate static and near-equilibrium dynamic properties of DNA ranging from a molecular weight of 100 bp to nearly 1 Mbp (mega base pairs). By evaluating metrics such as the end-to-end distance, and comparing these results with renormalization group theory predictions, we show that molecules such as λ-DNA and T4-DNA are far from the swollen coil limit. Our results indicate that DNA exhibits flexible swollen coil behavior when the contour length is approximately 1 Mbp. Moreover, computation of the Kirkwood diffusivity from equilibrium configurations reveals that DNA is partially draining to chain lengths as big as 1 Mbp. We attribute this slow transition to universal behavior to the semiflexible nature of DNA, that gives rise to weak intramolecular excluded volume and hydrodynamic interactions.

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