A Coarse-Grained DNA Model for Bubble Formation and Dynamics

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Understanding the supercoiled state is key to resolving the structure-function relationship in the DNA molecule. The supercoiled state is a result of under or over twisting, and is stabilized by the formation and dynamics of bubbles along the DNA molecule. In recent years, several experimental and theoretical studies have been focused on characterization and analysis of the supercoiled state. The theoretical models, such as Peyrard-Bishop model, are generally over simplified. Full atomistic computational models are only feasible for only short chains (10-15 base-pairs). In this study, a coarse-grained model has been developed, which would be simple enough for the simulation of long-chain systems, and still be able to represent the double helical nature of the DNA molecule. In this model each base-pair is represented by four superatoms, two central superatoms for the bases, and the other two for the sugar group and phosphate backbone on each strand. The bonded, angular, and dihedral interactions among these superatoms are obtained by Iterative Boltzmann method. Full-atomistic simulations of the target molecule are analyzed to obtain the probability distributions of the degrees of freedom of interest. The inverse of the probability distributions are used to obtain mean interaction potentials for the superatoms. Our coarse-grained model successfully mimics the local geometric structure of the DNA molecule, such as the 3'-5' directionality, major-minor groove structure, and the helical pitch. The persistence length, and melting temperature behavior of the coarse-grained model is also compared with the experimental and theoretical results. We will also present some preliminary results about formation of supercoiled DNA structures and bubble dynamics.