Coarse grain FF for describing DNA nanostructures
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Due to an increase in computational power and more efficient algorithms, computer simulations of Bio-molecules are now able to provide insight of unprecedented resolution, producing thermodynamics and structural information that would otherwise be impossible to obtain. Most of these simulations are based on a description of these molecules at an atomistic level; force-fields used in these simulations effectively describe the crucial atom-atom interactions as understood by Newtonian Mechanics.

These simulations, while powerful and generally accurate, are fundamentally limited in their usefulness because of their very nature: the atomistic representation of the bio-molecules. Even on the most powerful of computers, current equilibrium simulations of a bio-polymer such as DNA are limited to the nano-second regime of total simulation time, a timescale that is far too small to observe many of the interesting structural transitions that occur.

Efficient codes, employing parallel computing and fast methods of computing the non-bonded interactions present in these molecules are to be credited for the increase in simulation time recently. However, in order for realistic simulations to be performed in a reasonable amount of time, there is a need to have an alternate description of these molecules, a description that is preferably based on atomistic simulations, just as most force fields for atomistic simulations are based on quantum mechanical information.

Solvent molecules can be included in molecular dynamics simulations for short DNA duplexes, but at a high computational cost. There is therefore a need not only to simplify the representation of the solvent molecules, but also decrease the number of degrees of freedom in the model for DNA itself. This simplified model of DNA (mesoscale model) will inherently not be as detailed as the atomistic model. However, the reduction in the degrees of freedom will permit the monitoring of the simulation dynamics on a much larger timescale.

We present our mesoscale model of DNA, based on a backbone-base structure, where each nucleotide is represented by three beads, depending on the nucleotide (see figure 1). The model faithfully reproduces the helical nature of the double helix for 2 microseconds and represents a simulation speedup of at about 1000 over the all atomistic system.