Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Toward multiscale modeling of the chromatin fiber: a coarse grain model for DNA ALEXEY SAVELYEV, GAREGIN PAPOIAN, Department of Chemistry, University of North Carolina at Chapel Hill, Chapel Hill, NC 27599-3290 — In eukaryotic cells DNA is compacted a million-fold into a chromatin. Understanding the mechanism of chromatin folding is of great biological importance. All-atom Molecular Dynamics (MD) simulations could provide crucial insights into the electrostatic and structural mechanisms of chromatin folding. However, because of the enormous size of even short chromatin fiber segment and long folding timescales, atomistic simulations are computationally impractical. Our long-term aim is to build an accurate coarse-grain (CG) model of the chromatin, derived systematically from all-atom simulations of its smaller parts. Here we report the development of the CG model for a linear DNA chain, playing the role of a linker DNA segment in the chromatin. We derived CG inter-DNA electrostatic potential from atomistic simulations with explicit solvent and mobile ions, instead of relying on the standard models of continuum electrostatics, which are inadequate at small intermolecular distances. In addition, we used the ideas of renormalization group theory to construct an optimization scheme for parameterizing the CG force field. This novel approach is designed to accurately reproduce correlations among various CG degrees of freedom. The implementation of these correlations was left as an open question in the prior studies of CG polymer models.

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Date submitted: 22 Nov 2007 Electronic form version 1.4