Wavelet Based Multi-scale Coarse Graining Approach For DNA Molecules

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Molecular dynamics simulation has traditionally been used to investigate the mechanical and physical properties of biopolymer systems. However, molecular dynamics simulation of biopolymer systems in practical medical applications requires a unmanageable large simulation model, both in space and in time. To bridge the gap between manageable atomistic simulations and the typical biology events observed by experiment, a coarse grained model that retains a close connection to the underlying atomistic representation is essential [1].

In this work, a coarse graining technique is developed for multi-scale modeling of DNA molecules based on a multi-scale wavelet projection method [2]. Based on the linear hat function, a set of scaling and wavelet functions and their corresponding wavelet transformation matrices are constructed. The wavelet-based multi-scale transformation is utilized to hierarchically filter out the high scale components of the characteristic function while retaining the most essential scales of the characteristics for the construction of a coarse grained model.

In this coarse-graining construction, the center of mass of a group of atoms is chosen as the super-atom position. From the fine-scale atomistic simulation results of the representative DNA segment, the distribution functions between centers of mass of two groups of atoms are obtained, and the effective potential at fine-scale level is calculated. These fine-scale effective potentials are then homogenized using the multi-scale wavelet projection to yield the coarse-scale potentials between superatoms. These coarse-scale effective potentials are utilized to parameterize the force field of the coarse grained model. To verify the proposed method, molecular dynamics simulations using fine-scale and coarse grained DNA models are performd, and the predicted distribution functions are compared. The coarse grained simulation is shown to be in good agreement with the fine-scale simulation results, whereas only 1/1000 of the CPU time for fine-scale simulation is needed in the coarse grained simulation.

References

[1] W. Tschop, K. Kremer, J. Batoulis, T. Burger and O. Hahn, "Simulation of polymer melts. I. Coarse-graining procedure for polycarbonates," *Acta Polymer.*, **49**, 61–67, 1998.
[2] S. Mehraeen and J.S. Chen, "Wavelet-based multi-scale projection method in homogenization of heterogeneous media," *Finite Elements in Analysis and Design.* **40**, 1665–1679, 2004.

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