Coupled Nanostructures of Ribonucleic Acids: Developing Discrete-Continuum Models for Large Time-Scale Simulations

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ABSTRACT

To describe many biological systems and phenomena it is often necessary to develop computationally feasible structural models that can be applied for large time-scale simulations comparable to the real time scale of biological processes. In this contribution we provide details on our recently developed coarse grained models for coupled RNA nanostructures (nanotubes) consisting of a series of nanorings [1]. With these models, we study here physical properties of RNA nanostructures as a function of the number of nanorings. The sizes vary, going up to 40 nm, and our main results, reported here, have been confirmed by molecular dynamics (MD) simulation.

In the first part of this contribution, we briefly review our earlier results, where a comprehensive analysis of different bead approximations was carried out [2,3]. Based on such an analysis, our focus in this contribution is on a three bead approximation in which a single nucleotide in the RNA nanocluster is treated by three beads. The resulting coarse grained models have been developed from the all atom MD simulation using the Boltzmann Inversion Method. The molecular dynamics simulations for these coarse-grained models have been performed by using DL-POLY. In particular, we have calculated the radial distribution functions, as well as the histograms for the bond angles and the dihedral angles. From the dihedral angles histograms we have analyzed the characteristics of the links used to build the nanotubes. Furthermore, we have also calculated the bead distances along the chains of RNA strands in the nanoclusters. The variations in these features with the size of the nanotube are discussed in detail. Then, we present the results on the calculation of the root mean square deviations for the systems analyzed with the developed coarse-grained models to demonstrate the equilibration of the systems.

Finally, we describe a new technique that allows us to move from discrete to continuum modelling in the practically important case of large RNA nanotubes. This technique provides a way to an efficient PDE-based tool for modelling RNA nanostructures, demonstrating promises for large time scales.

REFERENCES

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