A DNA Molecule in Salt Solution: Adaptive Resolution Molecular Dynamics Simulation

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ABSTRACT

Many of the multiscale approaches are concerned with interfacing of atomistic and the continuum models of liquids. In these hybrid methods, typically molecular dynamics (MD) or a similar approach is used for simulating dynamics on the atomistic scale, whereas the Navier-Stokes equation governs the fluid dynamics on the continuum scale [1, 2]. Alternatively, multiscale schemes have been introduced using particle-based models only, e.g., atomistic and physically simplified coarse-grained (CG) molecular models. The coupling can be achieved either by a fixed resolution approach, where different resolution domains interact with each other but do not exchange molecules, or the adaptive resolution approach, where molecules change their resolution according to their current positions. Among the most advanced methods for the latter kind of simulations is the Adaptive Resolution Scheme (AdResS) [3], which allows for concurrent coupling from quantum all the way to continuum length scales of molecular liquids and soft matter.

Here, we present an adaptive resolution simulation of a DNA molecule in multiscale salt (1M NaCl) solution at ambient conditions. The DNA is always modeled at full atomistic resolution using the Amber03 force field. The solvent's level of representation changes adaptively according to distance from the DNA's center of mass from atomistic (at short distances) to coarse-grained (at larger distances) and vice versa. We observe within our error bars no differences in structural (e.g., root-mean-squared deviation and fluctuations of backbone heavy atoms, dielectric constant, and the average occupancy and residence time of sodium and oxygen atoms of water around the electronegative atoms of DNA) and dynamical properties of the DNA between the adaptive resolution and fully atomistically solvated models.

REFERENCES

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