Hybrid All-Atom/Coarse-Grain Models for DNA Simulations in Implicit and Explicit Solvents

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Institut Pasteur de Montevideo, Mataojo 2020, CP 11400, Montevideo - Uruguay.

Complex fluids, soft matter, and biological systems are characterized by the presence of disparate size and time scales in its structural conformation and dynamics. Although all-atom simulations have proved to be very useful for the study of the structural and dynamical behavior of several types of solvents/molecules/biomolecules and the interactions between them, their capabilities are limited to small systems and short simulation times. For this reason, substantial effort has been devoted towards the implementation of simulation techniques based on the idea of coarse grained representations of the atomic systems. However, in the most challenging cases, the molecular complexity of the systems requires a multiscale computer simulation methodology capable to describe events occurring over a range of time and length scales. Multiscale methods break the calculation up into parts to be treated at different levels of accuracy.

Combining an atomistic with a lower-resolution description, we present a novel approach to explore the dynamics of DNA fragments in implicit and explicit solvents using hybrid all-atom/coarse-grain representations of DNA, waters and ions. Based on our previous implementations of coarse grained DNA and water models, this approach combines the advantages of coarse graining with those of all-atoms simulations, required to treat molecular recognition and reactive processes. Furthermore, back-mapping procedures allow recovering the fully atomistic detail at any time during the simulation. The comparison between calculated properties with those obtained with experiments and all-atom state-of-the-art molecular dynamics simulations establishes the accuracy of the model. Our combined multiscale method can be extended to the study of reactive and molecular recognition processes in systems whose characteristic size and/or time scale prevent the analysis based on all-atom molecular dynamics.