

Assessment of the dipolar Poisson–Boltzmann–Langevin method to describe the ionic environment around DNA

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Deoxyribonucleic acid (DNA) is a heavily charged polyelectrolyte. It forms double helical structures that are crucial for its function. However, these structures are only stable in water, with ions to reduce the repulsion between the strands. Therefore, we should not consider the DNA double helix alone, instead we should consider the DNA double helix with its ionic environment. Experiments give a limited description of this ionic environment. A detailed description of this environment can be obtained with molecular dynamics (MD) simulations. Yet, these simulations are long to carry out, and are limited in scale. Electrostatic calculations with Poisson-Boltzmann (PB) based methods can give a detailed description of the ionic environment around DNA faster than MD, but work only on rigid solutes. The literature describes tests of several of such PB based methods with various levels of accuracy. In 2010, Koehl and Delarue implemented the resolution of the dipolar Poisson–Boltzmann–Langevin (DPBL) equation in the Aquasol solver [Koehl and Delarue, *J. Chem. Phys.* 2010]. The accuracy of the DNA ionic environment described by this methods have not been assessed so far. Hereby, we compare the DNA ionic environment described by the DPBL method on rigid DNA oligomers with the ionic environment described with MD simulations. The understanding of the method strength and limitations when working with a rigid solute is crucial to develop ways to use it with flexible ones.