Computer simulation of nucleic acids: across scales and across methods.

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Deoxyribonucleic acid (DNA) and ribonucleic acid (RNA), despite their importance to genetics, biochemistry and molecular biology, are much less studied than proteins by computational methods. The huge size of a typical DNA molecule, the structural and conformational variability of the RNA and the extremely delicate interplay of electrostatics, hydrogen bonds and solvation effects make the simulation of nucleic acids much more challenging than the simulation of proteins or even membranes. In nucleic acids, there is a hierarchy of complex interactions at different length and time scales, but on the other hand the interactions with small molecules depend strongly on the local details of the structure. The computational study requires therefore a range of methods, from explicit atomistic classical (or even quantum-mechanical) simulations, through coarse-grained simulations until mesoscopic models. The current advances in the simulation of nucleic acids will be presented, with emphasis to the multi-scale methods, such as the Adaptive Resolution Simulation Scheme (AdResS), which couples simultaneously two regions of the system, described by different levels of resolution. This multi-resolution method allows the continuous interchange of particles between the different levels of resolution, minimizing many artifacts present in the fixed dual-scale simulation methods.