Structural mechanics of nucleic acids

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Abstract:

Mechanical properties of DNA and RNA molecules play an important role in their biological functioning and in nanotechnology applications. Structure and stiffness of the DNA double helix, modulated by its sequence of bases, affects binding of proteins and higher order organization of the genome. RNA molecules fold into a variety of well-defined nonhelical structural motifs found in the ribosome and in other functional complexes. These recurrent motifs also serve as building blocks in the emerging field of RNA nanotechnology. Nucleic acids are subject to allosteric effects: they change conformation upon binding of small molecules, which in turn affects subsequent binding of other ligands. Experimental information concerning nucleic acids mechanical properties is scarce, and computer simulations represent a viable alternative. Our research is focused on designing suitable coarse grained models of nucleic acid shape and stiffness. The parameters of the models are inferred from large-scale, atomic resolution molecular dynamics simulations. We applied this approach to problems such as establishing mechanical properties of DNA A-tracts and their binding to nucleosomes, investigating recurrent RNA structural motifs, or modelling allosteric effects in DNA.

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