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Multiscale simulation methods and their applications in nucleic acid studies

Wednesday, 23 December 2020 14:00 (45 minutes)

After almost seventy years from the discovery of DNA double helix structure, we know very much about nucleic acid organization and functions. However, there are still many structural and dynamical features - at different spatial and time scales - that have to be understood better. Molecular simulations are essential to understand many properties at the molecular level. With a fast increase in the computer power together with method and software development, systems over increasing sizes and longer and longer timescales can be simulated. However, studies of DNA at the atomistic level have a practical maximum size allowing a few nucleosome core particles, on the microsecond time scale to be studied. To reach larger spatial and longer temporal time scales, necessary when studying many of the biological problems involving DNA (e.g. those connected to DNA flexibility, or to chromatin folding etc.) all-atom simulations are far too expensive. It is necessary to coarsen the description of the system of interest, by removing many details non-relevant to the phenomenon under investigation [1-4]. In this talk I will present selected coarse-grain (CG) models, some of which can be applied to the double helix conformation as well as to other nucleic acid structural motifs found in the cells, like DNA quadruplexes [5-6]. Special attention will be given to the methods that can be used to study the counter-ions interactions with this highly charged poly-ion.

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