Special Issue

Multiscale Simulation of DNA: From Atoms to Chromosomes

Message from the Guest Editors

In the past few years, there has been a renewed interest in modeling and simulating the structure, conformation, and dynamical behavior of biological systems containing DNA, a key molecule of life. Boosted by recent developments in refined all-atom force fields (parmbsc1, ol15, c36), the standardization and universalization of genome-wide experiments (deep sequencing, 3C technologies, etc.), and advances in high-resolution microscopy coupled to gene-painting techniques, dozens of new models and hundreds of new applications have come to light. Fueled by the increasing computational power available, simulations of nucleosomes at atomic resolution have reached the microsecond timescale. Simultaneously, several coarse-grained models of chromatin derived from first principles (bottom-up) have reached maturity, allowing the simulation of chromatin fibers in different epigenetic states. Finally, a huge variety of top-down mesoscopic models have emerged based on constrained simulations that leverage spatial information derived from the experiments mentioned above.

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