

Simulating Large-Scale Chromatin Fibers

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Understanding chromosome tertiary organization and its role in control of gene expression represents one of the most fundamental open biological challenges. Chromatin structure and gene expression are intimately related because the complex nature and dynamics of protein-bound DNA folding in the living cell regulates gene activity at a large range of spatial and temporal scales. Recent advances in experimental studies of chromatin using nucleosome structure determination, ultra-structural techniques, single-force extension studies, and analysis of chromosomal interactions have revealed important chromatin characteristics under various internal and external conditions. Modeling studies, anchored to high-resolution nucleosome models, have explored many related questions systematically. In this talk, I will describe recent findings regarding chromatin structure and function using a combination of coarse-grained modeling and large-scale all-atom molecular dynamics simulations of chromatin fibers. In particular, I will describe how such multiscale modeling can successfully address questions regarding the effects of epigenetic chemical modifications and the structure of condensed chromosomes in the metaphase cell cycle.

Of possible interest:

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