Surfing on the minimization schemes of the minimal chromatin model

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The rapid progress of experimental techniques boosted the development of theoretical and computational approaches for the study of chromatin dynamics. High-resolution techniques that can manipulate a single molecule are combined with three-dimensional modeling followed by simulation to understand specific aspects of chromosomes within the cell nucleus. However, the human genome has around $6x10^9$ base pairs (6 Gbp) in its linear sequence, which exceeds the current capacity of modeling and simulation with all atoms. An approach has been commonly used to circumvent this technological bottleneck that makes it possible to effectively study the organization of entire genomes at various spatial scales. The energy surface theory was employed to build a minimal chromatin model (MiChroM) by taking advantage of the maximum entropy principle and others simplifications in order to better understand the chromosome architecture and folding mechanisms. We evaluated the MiChroM minimization schemes in generating structural ensembles that reproduced the contact maps obtained by Hi-C experiments, the phase separation process of chromatin structural types and the spatio-temporal dynamics of chromatin loci.