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Polymer physics modeling can uncover the mechanisms underlying DNA folding

Quick advances in molecular biology have shed light on the three-dimensional structure of DNA in the cell nucleus, exposing its complex, non-random nature, and its connection to gene regulation. Our challenge is to comprehend the mechanics behind such an intricate genomic architecture and how two or more genomic regions may physically connect with one another. Experiments have shown certain preferred patterns of interactions that go beyond random contacts associated with the polymeric structure of the DNA chain and imply the presence of fundamental organizing principles of folding. Polymer physics and Monte Carlo-based computational approaches are proving to be excellent tools for investigating these phenomena. Here we describe the details of the simple, yet powerful "String and Binders Switch" (SBS) polymer physics model, and its computational implementation (PRISMR). We additionally discuss some of the uses of this framework, including the prediction of chromatin structural rearrangements upon disease-associated mutations and the investigation of gene-enhancer dynamics and their connection to epigenetics.

Refs:

-Bianco S. et al. Polymer physics predicts the effects of structural variants on chromatin architecture. Nature Genetics, 2018 -Esposito A. et al. Polymer physics reveals a combinatorial code linking 3D chromatin architecture to 1D chromatin states. Cell Reports, 2022.

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