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The role of Nucleosome Positions on Chromatin Structure: A multi-scale approach JOSHUA LEQUIEU, ANDRES CORDOBA, JUAN J. DE PABLO, University of Chicago — Nucleosomes compose the basic unit of chromatin, and their locations are central to the regulation and compaction of eukaryotic genomes. In this work, we examine the coupling between different length scales within chromatin by examining the influence of nucleosome positions on three-dimensional chromatin structure. First, using a detailed molecular model of DNA and proteins, we predict the one-dimensional positioning of nucleosomes and the repositioning mechanisms of nucleosomal DNA. We demonstrate that this mechanism is strongly dependent on DNA sequence and that DNA slides around the histone proteins by either a screw-like or loop-like rearrangement. Next, we couple this detailed model to a coarsened model of chromatin and examine the impact of DNA sequence on chromatin's three-dimensional structure. We show that both the locations of nucleosomes and the mechanisms by which they move have a significant impact on higher-order chromatin structure and that variations in DNA sequence lead to "open" or "closed" regions of chromatin. This approach represents an efficient tool towards understanding the higher order structure of chromatin and how various aspects of chromatin structure are coupled together.

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