Simulating nucleoprotein complexes: chromatin and ribosomes

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Abstract

Chromatin architecture plays a key role in embryonic stem cell programming, human embryo development, brain function and cancer. Specifically, epigenetic methylation and acetylation marks are thought to control gene expression by dramatically altering global chromatin architecture; however, the exact mechanism by which a single methyl group can induce a large scale conformation change of chromatin is not well understood. By examining histones in a dense nucleosome context, our long term goal is to understand the electrostatics of this crowded environment. Using coarse grain models of chromatin as a basis, we construct all atom chromatin models and simulate these in explicit solvent with the GENESIS molecular dynamics code on the large-scale high performance platforms at Los Alamos National Laboratory. The multi-disciplinary effort combined computer science, high performance computing, chip design, biophysics, structural biology, and cell biology, including researchers from RIKEN, LANL, NYU, Intel and Cray. Several performance optimizations for the KNL architecture enabled scaling to large numbers of cores. Regarding the ribosome, we have used all-atom structure-based models to simulate tRNA accommodation, revealing alternative pathways for near- cognate tRNAs.

Keywords: RNA, molecular dynamics, coarse, grain model, nucleoprotein complexes

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