1163-92-1109 **Nicole Pagane***, npagane@rockefeller.edu, and **Devany West**, **Quinn MacPherson**, **Bruno Beltran**, **Andrew J. Spakowitz** and **Viviana I. Risca**. *Coarse-graining DNA mechanics to study mesoscale chromatin geometries and interdigitation.*

DNA behaves as a semi-flexible polymer, well described by the worm-like chain model. In order to study how the mechanical properties of DNA interact with nucleosome geometry in chromatin, we previously implemented a discretized stretchable, shearable worm-like chain model in a coarse-grained Monte Carlo simulation codebase called wlcsim. To study the mesoscale structure and fluctuations of chromatin—the stiff sub-kilobase regime with just a handful of nucleosomes—we now incorporate explicit twisting rigidity, excluded volume, and inter-nucleosome potential terms into the wlcsim code. We simulate short single and multiple chromatin fibers to assess how these pairwise repulsive and attractive terms modulate fiber geometries, compaction, and phase separation. We then characterize features of the single-fiber structure space and the multiple-fiber phase space. Lastly, we generate predicted contact matrices that enable comparison of simulated chromatin structure ensembles with experiments in cultured cells. (Received September 14, 2020)