

Knots in DNA, Chromosomes and Polymer melts

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In this talk I will mainly focus on three of our more recent projects: First, I will present recent results on using knots as a gauge for the development of coarse-grained models for DNA and polymers. We show that single DNA chains exceeding 250,000 base pairs in physiologically relevant salt conditions tend to be knotted in agreement with recent experiments. The analysis is motivated by the emergence of DNA nanopore sequencing technology, as knots are a potential cause of erroneous nucleotide reads in nanopore sequencing devices and may severely limit read lengths in the foreseeable future. Recent developments have for the first time allowed the determination of three-dimensional structures of individual chromosomes and genomes in nuclei of single haploid mouse embryonic stem (ES) cells based on Hi-C chromosome conformation contact data. In this project, we further analyse these structures and provide the first evidence that G1 phase chromosomes are knotted, consistent with the fact that plots of contact probability vs sequence separation show a power law dependence that is intermediate between that of a fractal globule and an equilibrium structure. Finally, we investigate the occurrence of knots in polymer melts. In polymer physics it is typically assumed that chains in melts can be described by effective random walks without excluded volume interactions. We show that this idea is problematic as the latter severely overrate the occurrence of knots. Interestingly, we find that the structure of a chain in a melt is very similar to the structure of a single chain undergoing a collapse transition at the Theta-point, which in turn are not well-represented by random walks either.