

Knots in DNA, Chromosomes and Polymer melts

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After a general introduction into the topic of entanglements and knots in natural sciences, I will focus on three recent projects:

(1) 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.

(2) Recent developments have for the first time allowed the determination of 3d structures of individual chromosomes (see Figure containing two knots) and genomes in nuclei of single haploid mouse embryonic stem (ES) cells based on Hi-C chromosome conformation contact data. We further analyse these structures and provide first evidence that G1 phase chromosomes are knotted, consistent with the fact that plots of contact probability vs sequence separation show a power law intermediate between that of a fractal globule and an equilibrium structure.

(3) 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 at the Theta-point, which in turn are not well-represented by random walks either.

