

Title: Coarse-grained Simulations of DNA knotting in coned geometries

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Abstract:

An indirect indication of how DNA is packaged in bacteriophages is provided by the spectrum of knots that are formed by DNA upon circularization inside the viral capsids. The experimental knot spectrum of the P4 bacteriophage DNA is here compared to results of coarse-grained simulation of DNA knotting in confined volumes. Specifically, we present recent results from extensive stochastic sampling of confined self-avoiding and semi-flexible circular chains with volume exclusion. The salient physical parameters of the DNA model (contour length, cross section and bending rigidity) have been set to match those of P4 DNA. By using advanced sampling techniques, involving multiple Markov chain pressure-driven confinement combined and thermodynamic reweighting techniques, we characterise the knot spectrum of the circular chains for increasing confinement. Our investigation indicates that confinement favours chiral knots over achiral ones, as found in the P4 experiments. However, no significant bias of torus over twist knots is found, contrary to what found in P4 experiments. To advance the understanding of the discrepancy, further studies are being carried for reaching higher packing densities in the simulations as well as for ascertaining the relevance of out-of-equilibrium mechanisms.