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Knotting of long DNA molecules confined to nanochannels close to the persistence length KEVIN DORFMAN, AASHISH JAIN, Univ of Minn - Minneapolis — Understanding the confinement of long DNA within a nanochannel close to its circa 50 nm persistence length is important for genome mapping, an emerging genomics method that complements next-generation sequencing. Knotting of the DNA inside a nanochannel poses a challenge to genome mapping, since the topological complexity of the chain can scramble the labels used to identify the genomic sequence of the DNA. To date, simulations of the knotting of DNA in nanochannels have tended to focus on short chains, likely due to the computational costs to simulate and analyze long chains in narrow channels. However, practical applications involve long DNA, typically in excess of 150 kilobase pairs, confined in narrow channels with sizes less than 50 nm. We have studied the equilibrium ensemble of such chains using pruned-enriched Rosenbluth method (PERM) simulations of a DNA model confined in channels between 30 nm and 50 nm in width. We will present results on the location and size of knots in confined DNA as a function of channel size and knot type. Our results provide new insights into the complexity of knotting of very long DNA, including the presence of multiple knots on single chains and very complex knots. We will also provide a comparison with experiments.

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