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Relaxation dynamics of internal segments of DNA chains in nanochannels AASHISH JAIN, ABHIRAM MURALIDHAR, KEVIN DORFMAN, Department of Chemical Engineering and Materials Science, University of Minnesota, DORFMAN GROUP TEAM — We will present relaxation dynamics of internal segments of a DNA chain confined in nanochannel. The results have direct application in genome mapping technology, where long DNA molecules containing sequence-specific fluorescent probes are passed through an array of nanochannels to linearize them, and then the distances between these probes (the so-called DNA barcode) are measured. The relaxation dynamics of internal segments set the experimental error due to dynamic fluctuations. We developed a multi-scale simulation algorithm, combining a Pruned-Enriched Rosenbluth Method (PERM) simulation of a discrete wormlike chain model with hard spheres with Brownian dynamics (BD) simulations of a bead-spring chain. Realistic parameters such as the bead friction coefficient and spring force law parameters are obtained from PERM simulations and then mapped onto the bead-spring model. The BD simulations are carried out to obtain the extension autocorrelation functions of various segments, which furnish their relaxation times. Interestingly, we find that (i) corner segments relax faster than the center segments and (ii) relaxation times of corner segments do not depend on the contour length of DNA chain, whereas the relaxation times of center segments increase linearly with DNA chain size.

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