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Coarse-grained simulations of highly driven DNA translocation from a confining nanotube

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Driven DNA translocation through a nanoscopic pore has been the focus of many studies in recent years both due to its importance in biological processes and as a promising new technology to probe single DNA molecules. However, the simple process of driving monodisperse DNA chains through a pore often leads to surprisingly wide distributions of translocation times. In the regime where the driving force is high, such that translocation occurs much faster than the time required for the chain to relax, the different conformations that a DNA chain can have at the initiation of the translocation is a major contributor to this broadening. As an effort to reduce the broad distribution of translocation times, we test a situation where the DNA is placed inside a small nanotube whose purpose is to limit the range of initial conformations. We present the results of coarse-grained Langevin Dynamics simulations where the DNA is confined inside both infinitely long tubes and finite-length end-capped tubes. We demonstrate that the results for both tube geometries can be reproduced by a theoretical Tension-Propagation model. Since the end-capped tube contains an extra degree of freedom compared to the semi-infinite tube, we show how both cases need different strategies in order to minimize the coefficient of variation, and obtain tighter distributions of the translocation time.

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