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Long-time diffusivity of DNA chains in nanochannels: A Brownian dynamics study AASHISH JAIN, KEVIN DORFMAN, Univ of Minn - Minneapolis — The simplest approach to calculate the diffusivity of any polymer chain is to use the double sum Kirkwood formula, which is based on preaveraging approximation of diffusion tensor. The error due to the preaveraging approximation has been reported by a number of researchers in the context of free solution by computing both Kirkwood diffusivity $D^{(K)}$ (also known as short-time diffusivity) and long-time diffusivity D_L. In nanochannels, the main approach to compute the diffusivity is the Kirkwood formula. However, the error due to the preaveraging approximation is not known in a confined system. We use Brownian dynamics simulation algorithm with excluded volume and hydrodynamic interactions to calculate both short-time and long-time diffusivities of DNA chains in nanochannels, and compare them for a range of channel sizes and DNA chain sizes. Our results indicate that the long-time diffusivity is always smaller than the short-time diffusivity, which is consistent with the result obtained in free solution using linear response theory $D_L < D^{(K)}$ [M. Fixman, Macromolecules **14**, 1710 (1981)]. We show that this preaveraging error decreases as channel size decreases. Even for weakly confined channels, errors are found to be about 1 % for chains up to 40 μm.

Aashish Jain
Univ of Minn - Minneapolis

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