Computer Simulation of the Dynamics of Two Polymers Under Box-like Confinement

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In this project, computer simulations employing the Brownian dynamics method were used to study the equilibrium dynamics of a system of two confined, linear polymers. The polymers were modeled as bead-spring chains and were confined to a rectangular box with very strong confinement in one dimension. This work is relevant to a recently published paper in which the dynamics of polymers, such as λ-DNA, were examined (Capaldi et al., Soft Matter 14, 8455 (2018)). In that experimental study, a theoretical approximation was used to analyze the mean-square displacement of the polymers. In this approximation, the polymers were modeled as hard circular objects free to diffuse around the box. In order to gain a better understanding of the system and to examine its behaviour under different degrees of confinement, we used computer simulations to measure the time dependence of the mean-square displacement. By analyzing this data, the model used in the experimental study was critically examined.