BROWNIAN DYNAMICS SIMULATIONS OF A ROUSE CHAIN IN AN UNCROSSABLE GRID

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Entanglements contribute to fascinating properties of polymers such as viscoelasticity and memory. The most successful model for treating entangled polymers is the reptation/tube model1,2. Most of the theoretical approaches are based on this model3,4 . Nevertheless, some basic assumptions of the tube theory lack a microscopic foundation. In this project, we are interested to find out if the tube theory can adequately describe our simulation model, whether the tube theory has to be modified accordingly, and how to find the parameters of the tube. The model is a Brownian dynamics simulation of a single chain in an array of obstacles, a grid. The intrachain interactions are described by the Rouse model and a non-crossability algorithm is used to prevent the chain from crossing the grid, thereby preserving the topological constraints. This allows us to study well entangled systems as compared to melt simulations. The method preserves the Gaussian statistics of the chains at all time and length scales, so that equilibrium configurations can be generated with no effort. The results of both linear chains and stars will be compared to the tube theory.

References,

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