Brownian dynamics simulation of bead-rod system with a general topology

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Abstract

Bead-rod model are frequently used in both numerical and theoretical studies of polymer due to its intuitive and fixed contour length properties. Brownian dynamics(BD) simulation is one of the most important methods in the study of bead-rod polymers in complex processes, such as DNA movements in the cell. However, most attention of BD simulation is on chain like polymer structure. More complex polymer topology may encounter especially in complex circumstances, and this is definite the case if we consider multi-polymers system. Here, we propose a general method to perform BD simulation on arbitrary topologies, includes the multi-polymers. The connecting topology, which can be described in the form of adjacent matrix, is linked to the metric matrix. Extensive simulation results are obtained for several typical cases with applications in biological system.