Generalized ensemble computer simulations for structure formation of semiflexible polymers

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Abstract:

Over the last decade generalized ensemble Monte Carlo computer simulation studies, especially multicanonical, Wang–Landau, and replica exchange (or parallel tempering) simulations, have emerged as a strong tool to study the statistical mechanics of polymer chains. Phase diagrams of single chains in bulk as well as attached to surfaces and the aggregation behavior of a few polymers have been investigated in large-scale simulations. In this talk, I will first present the theoretical background for these methods, assess their performance and show that they are perfectly suited for a microcanonical analysis, which has been recognized as a powerful concept. As an illustration, I give an overview of systems investigated with these methods, focusing on studies of coarse-grained models for semiflexible polymers, which show a rich variety of structural motifs including hairpins, toroids, knots and twisted bundles.