Heavily parallelized codes for the energy minimization and Monte Carlo simulation of polymer knots

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Polymer rings, also called catenanes in the chemical literature, constitute a frequently occurring motif in nature and in artificial soft matter materials. Very often in DNA and sometimes in proteins, these rings form very complicated knots. Knots are also relevant in polymer materials, for instance by increasing their breakability or altering their elastic behavior. The study of the mechanical and thermal properties of polymer knots poses several challenges and is a highly interdisciplinary problem. To obtain a satisfactory statistics, several hundreds of billions of knot conformations must be sampled during a Monte Carlo simulation. This requires the development of fast algorithms that are able to take into account the topological properties of the knot. On the other side, the energy landscape of a polymer knot is very complex. Sophisticated algorithms of energy minimization are necessary in order to explore this landscape.

In this talk the results of a recent study of the statistical mechanics of very long polymer knots will be presented. This case demands in a compelling way the application of heavily parallelized codes. In the investigation, the Wang-Landau multicanonical Monte Carlo algorithm has been used. The polymers are mainly, but not only, defined on a lattice. Some of the problems arising in Monte Carlo numerical simulations and in exploring the energy landscape of very long polymer knots will be discussed together with their solution. The results obtained in understanding the mechanical and thermal properties of these interesting physical systems will be shown.