Contribution to the Workshop on "Computational and Theoretical Biology"
MSU, 24 April 1999

Self-assembly, folding and unfolding of polymers

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During the past 10 years, members of the MSU Cluster Science Collaboration [1] have been actively involved in studying the self-assembly mechanism of complex finite systems in Nature. The twofold emphasis of this project has been on the dynamics of formation and restructuring at finite temperatures, and on the equilibrium structure of these systems.

Results of our molecular dynamics simulations, which will be presented as a movie, show the microscopic mechanism of formation, folding and and stepwise unfolding of polymers in viscous media. These results, obtained for a model system of soft spheres with an anisotropic dipole-dipole interaction [2], are believed to be universal for a large range of polymers in liquids.

The nontrivial problem of finding the most stable isomers of very long, entangled polymers, is being addressed using the Genetic Algorithms technique. Unlike in previous studies, we optimize the structure by modifying the genotype rather than the phenotype of the structure. This approach provides a sampling of the configurational phase space which is superior to any other technique, and is also capable of recognizing frequently occurring structural and dynamical patterns.

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[1] CSC URL on the web: `http://www.pa.msu.edu/cmp/csc/`

[2] P. Jund, S.G. Kim, D. Tománek, and J. Hetherington, Phys. Rev. Lett. **74**, 3049 (1995).