Dynamics of Polymers in a good solvent - a Molecular Dynamics Study using the Connection Machine

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In recent times the use of molecular dynamics simulations has become an important tool in modelling and understanding the dynamics of interacting many-body systems. With recent advances in computing power it is now feasible to perform modelling of systems which contain a large number of interacting particles, and thus to simulate the behaviour of real systems reasonably. Motivated by our earlier discoveries of anomalous corrections to scaling behaviour of the Edward's polymer[1,2], we apply this approach to study the dynamical behaviour of two dimensional polymer systems - either a single chain immersed in a fluid, a pure polymer melt, or with any concentration of polymers in the fluid. By choosing a suitable interaction potential between the fluid particles and the monomers, we are able to study the experimentally observable time dependent structure factor of polymers in a good solvent. Simulations were performed using the Connection Machine CM5 supercomputer at the ANU which due to its fast multi-processor nearest neighbour communications facility, enables us to easily model large systems of at least 3000 fluid plus monomer particles. Our study is based on a finite difference solution of Newton's equations of motion i.e. the Verlet algorithm, and the results are used to test current theories of polymer dynamics[3,4], which were based primarily on the earlier models proposed by Rouse(1953) and Zimm (1956). In particular dynamical scaling predictions is scrutinised to examine the effects due to the anomalous corrections-to-scaling behaviour found in an earlier work[1] using finite-size scaling analysis of Monte-Carlo data and now understood via a new perturbation concept[2].

References

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