Multi-blob Representation of Concentrated Polymer Solutions

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A novel coarse-grained multi-blob description of concentrated solutions of interacting polymers is presented, which provides a quantitative realization of the familiar Pincus-de Gennes blob picture. Soft, transferable effective interactions between bonded and non-bonded blobs are determined from first principles, by taking appropriate averages over monomer configurations. The number of blobs is chosen such that the blob density does not exceed their overlap threshold, thus allowing polymer concentrations to be explored deep into the semi-dilute regime. This quantitative multi-blob description is shown to preserve known asymptotic scaling laws of polymer solutions, and provides accurate estimates of amplitudes, while leading to orders of magnitude increase of simulation efficiency and allowing analytic calculations of structural and thermodynamic properties.

The coarse-graining strategy is extended to polymer "brushes" grafted to a planar substrate in order to explore the regime of long polymers and high grafting densities, and to the entropically driven clustering and self-assembly of diblock copolymers into lamellar and micellar phases. It is shown that the multi-scale coarse-graining strategy allows the order-disorder transition of micelles to be observed in Monte Carlo simulations.

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