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Probing the Phase Behavior of Coarse-Grained Polymer Models with Nested Sampling KENNETH SALERNO[1], NOAM BERNSTEIN, U.S. Naval Research Laboratory — The phase behavior of polymers is not as well studied as that of atomic systems due to the highly correlated motion of polymers and resulting sampling difficulties. Nested sampling (NS) is a statistical technique that allows calculation of the partition function of physical systems by eliminating a fixed fraction of configuration space at each iteration of the algorithm. Previous studies have shown that by using NS one can directly calculate thermodynamic quantities such as heat capacity of atomic systems from the partition function. We report results from recent work extending NS to polymeric systems using Hamiltonian and Galilean Monte Carlo sampling methods. Bead-spring models of flexible and semiflexible single-chain systems that exhibit a coil to globule transition are studied. Results for thermodynamic quantities, such as the heat capacity, and chain structural quantities, like R_g, are presented. Results from physically based coarse-grained and atomistic polyethylene models are also discussed. Altogether, these results show how NS can be applied to calculate polymer phase behavior in a computationally efficient way.

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