321a Frontiers of Molecular Simulation

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Over the past two years we have developed a novel class of Monte Carlo methods that permits calculation of the free energy of complex systems as a function of appropriately chosen order parameters. The usefulness and limitations of our proposed approach will be discussed in the context of three applications. The first is concerned with the study of biological membranes. Results will be presented for on the phase behavior of several model bilayer membranes, using both coarse-grained and atomistic force fields. The second application is concerned with the study of liquid-crystal based biosensors. Results from multi-scale simulations of liquid-crystal based biosensors will be presented, including a description of the relaxation of defects over microscopic length scales and the role of hydrodynamics in that process. The third application is concerned with the stability of model proteins on surfaces or in confined geometries. Results from order-parameter Monte Carlo simulations will be presented that illustrate the effect of surfaces and different types of confining walls on the free energy of a variety of proteins.