

Complex Computational Systems

Particles, Chains, and Sheets

R.B. Pandey

Department of Physics and Astronomy

University of Southern Mississippi, Hattiesburg, MS 39406-5046

Email: ras.pandey@usm.edu

Tel: 601 266 4485; Fax: 601 266 5149

Understanding of multi-scale phenomena of many multi-component systems remains a challenging issue. Coarsening of fundamental characteristics such as degrees of freedom, interactions, processing, and kinetics is almost unavoidable in modeling such complex systems. It is often crucial to implement effective and efficient algorithms to address difficult questions regarding cooperative properties (structure and dynamics) at desirable spatial and temporal scales. Particles, chains, and sheets are basic elements to describe many multi-component systems by coarse-grained models. Using a three dimensional discrete lattice as a host matrix, we address how a self-organizing morphology evolves in a driven mixture of immiscible particles and how its flow flux responds to pressure and field. Density profile, interface width, and surface roughness are examined as the thermodynamic equilibrium is arrested by kinetic reaction in a film growth from its hydrophobic (H) and polar (P) constituents in evaporating aqueous solvent. Relaxation of protein folding into its globular native structure is examined using an HP chain model. Conformation and dynamics of a tethered membrane are studied for a self-avoiding sheet (SAS) as well as interacting sheets in effective solvent media. Retaining the planar conformation via entropic dissipation is an important feature of SAS. Crumpling of membrane can be controlled by temperature and quality of the solvent. These examples (published in collaboration with different research groups) illustrate how computer simulation experiments can be employed to probe a range of issues and topics with appropriate coarse grained descriptions.