INTERDISCIPLINARY CENTRE FOR
ADVANCED MATERIALS SIMULATION

The ICAMS Seminar presents

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Computer simulations of critical phenomena and phase behaviour of fluids

Computer simulation techniques such as Monte Carlo (MC) and Molecular Dynamics (MD) methods yield numerically exact information (apart from statistical errors) on model systems of classical statistical mechanics. However, a systematic limitation is the restriction to a finite (and often rather small) particle number N (or box linear dimension L, respectively). This limitation is particularly restrictive near critical points (due to the divergence of the correlation length of the order parameter) and for the study of phase equilibria (possibly involving interfaces, droplets, etc.). Starting out with simple lattice gas (Ising) models, finite size scaling analysis have been developed to overcome this limitation. These techniques work for both simple Lennard-Jones fluids and their mixtures, including generalizations to approximate models for quadrupolar fluids such as carbon dioxide, benzene etc. and various mixtures, whose phase behaviour can be predicted. A combination of MC and MD allows the study of dynamic critical phenomena, and specialised techniques (umbrella sampling plus thermodynamic integration) yield the surface free energy of droplets as function of droplet size. Thus, computer simulation has become a versatile and widely applicable tool for the study of fluids.