3. Efficient Monte Carlo simulation of fluid systems at low temperatures

Alexandra Valentim and Carlos E. Fiore

Universidade Federal do Paraná, Brazil

We perform Monte Carlo simulation of fluid systems at the phase transition regimes. In particular, we consider the Blume-Capel, Blume-Emery-Griffiths and Bell-Lavis liquid water models. A common feature is that at low temperatures, all of them present strong first-order transitions, a regime difficult to simulate by means of standard algorithms because the free-energy minima are separate by large barriers. Consequently standard one flip algorithms do not guarantee an ergodic simulation. In order to circumvent these difficulties, we consider the simulated tempering (ST), that consists of making the temperature as a dynamical variable: it assumes distinct values from a set { T1 < T2 < … < Tn }. The central idea is that evolution at higher T's strongly facilitates the crossing the free-energy barriers, then allowing uniform visits to the multiples regions of a fragmented phase-space. The first aim of this study consists of analyzing the role of the temperature schedule of the ST. We consider different criteria for distributing the temperatures, such as arithmetic, geometric, arithmetic progression in inverse temperature and the constant entropy method (CEM). The CEM uses the constant increase of entropy as a criterion to choose the temperature schedule. The analysis of the convergence toward the stationary from a non-typical configuration and the frequency of tunneling between phases shows that the distribution of temperatures play an important role in the visit of the phase space and the CEM criteria seems to be superior than the others, in agreement with a previous study through Parallel Tempering.