CRITICAL POINT ESTIMATION OF THE LJ PURE FLUID AND BINARY MIXTURES

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The Lennard-Jones fluid is considered a reference model for the analysis of new methodologies. In addition, it can be used as a model for atomic fluids and has been the subject of many numerical studies. In recent years, many works have been carried out to investigate the critical regions of fluids. A common approach has been the use of MC algorithms such as the Gibbs ensemble to obtain the subcritical coexistence data, and then a power law to extrapolate to the critical point. More detailed studies have also been carried out using histogram reweighting methodologies combined with finite size scaling techniques. In the present study, we exploit the properties of the 4th order cumulant (Binder parameter) calculation to accurately locate critical points and calculate near-critical coexistence data. We have compared the combination of mixed-field theory with finite size scaling with the intersection of the Binder parameter for different system sizes. Furthermore, we propose the use of the universal Ising value of the Binder parameter as an estimation of the system-size dependent critical point. The applications of these three methods allows us to estimate the infinite volume critical point. We have calculated the critical point of the pure LJ fluid and a binary mixture selected in order to allow for comparison with previous works. We have obtained excellent agreement between the methodologies confirming the 4th order cumulant as an interesting method to obtain a high level of accuracy for the critical point location. In addition, the proposed combination of the Binder parameter with finite size scaling techniques is straightforward to apply since it does not require the fitting process of the mixed field theory. As a consequence, this calculation allows also for the calculation of the line of critical points for binary mixtures. Finally, as has recently been shown [1], we have obtained near-critical coexistence data for the pure fluid through the study of the Binder parameter minima identified at the coexistence densities.

[1] Kim YC, Fisher ME, Luijten E. **Phys Rev Lett 91 (6)**, 065701 (2003).