From Particle Condensation to Polymer Aggregation

W. Janke, J. Zierenberg, and P. Schierz

Abstract:

A new simulation method to study temperature-driven droplet formation is discussed that allows a shape-free determination of free-energy barriers [1]. Combined with theoretical considerations for nucleation in particle systems, this leads to finite-size scaling predictions for the barrier at fixed density. Using parallelized multicanonical Monte Carlo computer simulations [2], this approach is first validated for a Lennard-Jones particle gas and then generalized to bead-spring polymers. Our results suggest an analogy of polymer aggregation with particle condensation, when the macromolecules are interpreted as extended particles. The talk concludes with a brief comment on the role of kinetic energy [3], which is commonly neglected in Monte Carlo simulations.

References:

[1] J. Zierenberg, P. Schierz, and W. Janke, Canonical free-energy barrier of particle and polymer cluster formation, Nat. Commun. 8 (2017) 14546.

[2] J. Zierenberg, M. Marenz, and W. Janke, Scaling properties of a parallel implementation of the multicanonical algorithm, Comput. Phys. Commun. 184 (2013) 1155.

[3] P. Schierz, J. Zierenberg, and W. Janke, First-order phase transitions in the real microcanonical ensemble, Phys. Rev. E 94 (2016) 021301(R) (Editors' Suggestion).