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Density fluctuations in the geometric cluster algorithm JIWEN LIU, Department of Materials Science and Engineering, University of Illinois at Urbana-Champaign, Urbana, Illinois 61801, NIGEL B. WILDING, Department of Physics, University of Bath, Bath BA2 7AY, U.K., ERIK LUIJTEN, Department of Materials Science and Engineering, University of Illinois at Urbana-Champaign, Urbana, Illinois 61801 — We have extended the recently-developed geometric cluster Monte Carlo algorithm[1] to study the critical properties of fluid systems. Density fluctuations are introduced by exchanging clusters of particles between two identical cells. This allows the system to decompose into two coexisting phases of different densities. We exploit a mapping on the grand-canonical order-parameter distribution function to systematically locate the critical point. The method is illustrated for the standard Lennard-Jones fluid. Remarkably, even away from the percolation threshold, our cluster algorithm is able to suppress critical slowing-down, leading to a considerable efficiency improvement compared to grand-canonical Monte Carlo simulations already at moderate system sizes. Owing to the non-local nature of the geometric cluster moves, we anticipate that our method becomes particularly advantageous in the study of critical properties of fluids containing components of widely different sizes.

[1]J. Liu and E. Luijten, Phys. Rev.Lett. **92**, 035504 (2004).

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