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The Geometric Cluster Algorithm: Rejection-Free Monte Carlo Simulation of Complex Fluids

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The study of complex fluids is an area of intense research activity, in which exciting and counter-intuitive behavior continue to be uncovered. Ironically, one of the very factors responsible for such interesting properties, namely the presence of multiple relevant time and length scales, often greatly complicates accurate theoretical calculations and computer simulations that could explain the observations. We have recently developed a new Monte Carlo simulation method[1] that overcomes this problem for several classes of complex fluids. Our approach can accelerate simulations by orders of magnitude by introducing nonlocal, collective moves of the constituents. Strikingly, these cluster Monte Carlo moves are proposed in such a manner that the algorithm is rejection-free. The identification of the clusters is based upon geometric symmetries and can be considered as the off-latice generalization of the widely-used Swendsen–Wang and Wolff algorithms for lattice spin models. While phrased originally for complex fluids that are governed by the Boltzmann distribution, the geometric cluster algorithm can be used to efficiently sample configurations from an arbitrary underlying distribution function and may thus be applied in a variety of other areas. In addition, I will briefly discuss various extensions of the original algorithm, including methods to influence the size of the clusters that are generated and ways to introduce density fluctuations.

[1]J. Liu and E. Luijten, Phys. Rev. Lett.**92**, 035504 (2004); see also Physics Today, March 2004, pp. 25–27.