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Simulating Charged Systems with the Geometric Cluster Algorithm STEPHEN BARR, ERIK LUIJTEN, University of Illinois at Urbana-Champaign — The recently introduced generalized geometric cluster algorithm (GCA) for colloidal suspensions [J. Liu and E. Luijten, Phys. Rev. Lett.**92**, 035504 (2004)] is extended to systems with electrostatic interactions. The Ewald summation is used to determine the pair potentials. However, the resulting pair potentials cannot be used directly in the GCA because the long range nature of the electrostatic potential causes all particles to be included in a cluster. In our new method, the cluster size is therefore controlled by using only the real-space part of the potential during cluster construction, then accepting or rejecting the cluster move based on the part of the internal energy that is computed in Fourier space. Although the resulting algorithm is, in contrast with the original approach, no longer rejection-free, it is possible to perform collective nonlocal moves while maintaining a significant acceptance ratio. The method is particularly beneficial for systems containing components with large size asymmetries, such as suspensions of charged colloids in the presence of salt.

Stephen Barr
University of Illinois at Urbana-Champaign

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