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Geometric cluster algorithm for anisotropic particles DANIEL W. SINKOVITS, University of Illinois at Urbana-Champaign, ERIK LUIJTEN, Northwestern University — Complex fluids typically contain components of different sizes. In simulations of such systems, the relaxation time increases strongly with the size ratio, effectively limiting the type of fluids that can be studied. The geometric cluster algorithm is a Monte Carlo method that eliminates this limitation for mixtures of particles with isotropic interaction potentials, but cannot be applied to anisotropic particles. We present an elegant modification of the geometric cluster algorithm which has the ability to efficiently relax the rotational degrees of freedom of anisotropic particles in a rejection-free manner. This greatly expands the applicability of this method, as is illustrated by means of simulations of self-assembly in a multicomponent mixture of nanoparticles and non-adsorbing polymer.

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