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A Coupled Discrete Element and Kernel-Independent Fast Multipole Framework

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Extended Abstract

Abstract

We present a coupling between the MercuryDPM discrete element method (DEM) code and a kernel-independent fast multipole method (KIFMM). The resulting simulation framework enables the treatment of a broad class of multiscale problems, capturing both fine-scale mechanical interactions between particles and coarse-scale long-range interactions of various physical origins. Time integration is handled by bridging the DEM time step with a larger stride for recomputing long-range forces, ensuring computational efficiency without sacrificing accuracy. This methodology supports a wide range of applications, including electrostatic interactions in powders, clays, and particulate systems; magnetic interactions in ferromagnetic granular media; and gravitational interactions in asteroid clouds. In addition, KIFMM can be readily employed to accelerate boundary integral solvers for problems involving Stokesian fluid flow or elastic solid media surrounding rigid DEM particles, as well as for modeling dielectric polarization or magnetization effects. This generality substantially broadens the scope of potential applications of the coupled framework. Furthermore, the formalism of rigid clumps is successfully integrated with KIFMM, enabling the simulation of complex long-range interactions between non-spherical particles with arbitrary charge distributions. The capabilities and versatility of the proposed approach are demonstrated through several representative application examples.

Keywords:

Discrete element method Kernel-independent fast multiple method Long-range interactions