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A Fast Adaptive Multipole Algorithm for Calculating Screened Coulomb (Yukawa) Interactions

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The screened Coulomb (Yukawa or Debye–Hückel) potential, $\Phi = \exp(-\kappa r)/r$, where r is the separation distance and κ is the Debye–Hückel screening parameter, gives a good description of the electrostatic interactions in a variety of biologically and physically important charged systems. It is well known that the direct calculation of the energy and forces due to a collection of N charged particles involves the pairwise summation of all charged particle interactions and exhibits an $O(N^2)$ computational complexity which severely restricts maximum problem size. This has prompted the development of fast summation algorithms that allow the electrostatic energy and forces to be obtained in only $O(N \log N)$ operations. To date, however, practically all such implementations have been limited exclusively to pure Coulombic potentials ($\kappa = 0$), and the central contribution of the present method is to extend this capability to the entire range of the inverse Debye length, $\kappa \geq 0$. The basic formulation and computational implementation of the spherical modified Bessel function-based multipole expansions appropriate for the screened Coulomb kernel are first presented. Next, a simple model system consisting of a single source charged particle is studied to show that the maximum electrostatic energy error incurred by an M-order multipole expansion for the Yukawa potential is bounded above by the error of the equivalent multipole expansion for the Coulombic potential. Finally, timing and accuracy studies are presented for a variety of charged systems including polyelectrolyte chains, random distributions of charges inside a cube, and face-centered-cubic lattice charge configurations containing up to 103,823 charges.

Key Words: electrostatics; Yukawa potential; Debye–Hückel potential; screened Coulombic interactions; fast multipole method; polyelectrolyte.

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