A novel implementation of anisotropic electrostatics in the CHARMM simulation package

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Most molecular dynamics simulations are carried out using isotropic atom-atom potentials to model non-bonded interactions. Such potentials can be insufficient to accurately represent a variety of physical properties present in biologically relevant molecules. A proper description of the anisotropy of the electrostatic interactions is of particular importance, as it directly affects a variety of structural and transport properties such as hydrogen bonding and diffusion. We have recently developed and implemented a novel, algorithm to efficiently calculate Coulombic forces in the CHARMM simulation package using an arbitrary order multipole expansion. Using spherical harmonics, in conjunction with the quasi-internal reference frame, this algorithm formally scales more efficiently than all current multipole based electrostatic implementations, allows the inclusion of arbitrary order interactions (implemented through hexadecapole-hexadecapole), and is compatible with standard long range electrostatic approximations (Particle Mesh Ewald). In practice, our method is approximately one-third faster than the fastest Cartesian implementation through the quadrupole level. Additionally, our implementation can also take full advantage of molecular symmetry, yielding considerable savings when modeling explicit solvent. We present details of the algorithm, implementation and initial calculations enabled by this work.