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New Distributed Multipole Methods for Accurate Electrostatics for Large-Scale Biomolecular Simultations

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An accurate and numerically efficient treatment of electrostatics is essential for biomolecular simulations, as this stabilizes much of the delicate 3-d structure associated with biomolecules. Currently, force fields such as AMBER and CHARMM assign "partial charges" to every atom in a simulation in order to model the interatomic electrostatic forces, so that the calculation of the electrostatics rapidly becomes the computational bottleneck in large-scale simulations. There are two main issues associated with the current treatment of classical electrostatics: (i) how does one eliminate the artifacts associated with the point-charges (e.g., the underdetermined nature of the current RESP fitting procedure for large, flexible molecules) used in the force fields in a physically meaningful way? (ii) how does one efficiently simulate the very costly long-range electrostatic interactions? Recently, we have dealt with both of these challenges as follows. In order to improve the description of the molecular electrostatic potentials (MEPs), a new distributed multipole analysis based on localized functions – Wannier, Boys, and Edminston-Ruedenberg – was introduced, which allows for a first principles calculation of the partial charges and multipoles. Through a suitable generalization of the particle mesh Ewald (PME) and multigrid method, one can treat electrostatic multipoles all the way to hexadecapoles all without prohibitive extra costs. The importance of these methods for large-scale simulations will be discussed, and examplified by simulations from polarizable DNA models.