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Mathematical Structure of Electrostatic Interactions Among Biomolecules: Many Interacting Charged Dielectric Objects TIMOTHY P. DOERR, National Center for Biotechnology Information, NLM, NIH, YI-KUO YU, National Center for Biotechnology Information, NLM, NIH — The electrostatic force is one of the more important forces acting on each atom in a biomolecular system. Although the fundamental equations for electrostatics are known, the solution in low symmetry situations with a high dielectric constant solvent (e.g. water) can be difficult to obtain in an appropriate form and with an acceptable degree of accuracy and amount of computation. In order to compute this force, each atom is usually modeled as a dielectric sphere with a point charge at its center. Even the case of two spheres is non-trivial. The case of many spheres (necessary for any realistic biomolecule) can be constructed from the most general two sphere case with appropriate mathematical machinery for handling rotations between the global "laboratory" coordinate system and the local coordinate system of each pair of atoms (defined to have its z axis along the line connecting the centers of the two spheres). We provide an intuitive explanation of the machinery involved in carrying out this process. Ions can be included, as well. The solution for surfaces more general than the union of the surfaces of many spheres can be obtained numerically by choosing a tiling of the surface and solving a corresponding set of linear algebraic equations (the finite-element method).

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