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### **Electrostatics in Biomolecular Interactions: a Surface Charge Method**

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Biomolecular interactions determine how transcription factors recognize their DNA binding sites, how proteins interact with each other, and consequently how a biological system functions. Since both proteins and DNAs are significantly charged, electrostatic interactions are among the most important when studying biomolecular interactions. 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 the electrostatic 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 energetic calculations of such a system are still very crude and lack systematic control of accuracy. To establish a scheme where accuracy of the computation can be controlled systematically, we have established a new formulation where the surface charge distribution is used as a new variable. The surface charge has the advantage of reducing the number of degrees of freedom (from 3D to 2D), can accommodate the presence of ions, and is applicable to arbitrary geometrical shapes. The Poisson-Boltzmann equation is currently the most popular approach in dealing with ionic effects. This approach, unfortunately, suffers from several drawbacks. In this talk, I will describe these drawbacks in slightly more detail, and describe possible methods to circumvent these problems. The solution for general geometrical shapes can be obtained numerically by choosing a tiling of the surface and solving a corresponding set of linear algebraic equations (the finite-element method). These equations can be efficiently solved numerically for use in molecular dynamics simulations.