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An Analytical Approach to Computing Biomolecular Electrostatic Potential ANDREW FENLEY, JOHN GORDON, ALEXEY ONUFRIEV, Virginia Tech — Analytical approximations to fundamental equations of continuum electrostatics on simple shapes can lead to computationally inexpensive prescriptions for calculating electrostatic properties of realistic molecules. Here, we derive a closed form, analytical approximation to the Poisson equation for an arbitrary distribution of point charges and a spherical dielectric boundary. The simple, parameter-free formula defines continuous electrostatic potential everywhere in space and is obtained from the exact infinite series (Kirkwood) solution by an approximate summation method that avoids truncating the infinite series. We show that keeping all the terms proves critical for the accuracy of this approximation, which is fully controllable for the sphere. We apply the approximation to 580 biomolecules under realistic solvation conditions, where the effects of mobile ions are included at the Debye-Hückel level. The accuracy of the approximation as applied to the biomolecules is assessed through comparisons with numerical Poisson-Boltzmann (NPB) reference solutions. For each structure, the deviation from the reference is computed for a large number of test points placed near the dielectric boundary (molecular surface). The accuracy of the approximation is within 1 kT per unit charge for 91.5% of the individual test points.

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