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Continuum solvation model: Computation of electrostatic forces from numerical solutions to the Poisson-Boltzmann equation. (English) Zbl 0935.78019

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Summary: A rigorous formulation of the solvation forces (first derivatives) associated with the electrostatic free energy calculated from numerical solutions of the linearized Poisson-Boltzmann equation on a discrete grid is described. The solvation forces are obtained from the formal solution of the linearized Poisson-Boltzmann equation written in terms of the Green function. An intermediate region for the solute-solvent dielectric boundary is introduced to yield a continuous solvation free energy and accurate solvation forces. A series of numerical tests show that the calculated forces agree extremely well with finite-difference derivatives of the solvation free energy. To gain a maximum efficiency, the nonpolar contribution to the free energy is expressed in terms of the discretized grid used for the electrostatic problem. The current treatment of solvation forces can be used to introduce the influence of a continuum solvation model in molecular mechanics calculations of large biological systems.

MSC:

78M20 Finite difference methods applied to problems in optics and electromagnetic theory

78A30 Electro- and magnetostatics

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electrostatic forces; Poisson-Boltzmann equation; finite-difference

Software:

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