

1106-92-2452

Wufeng Tian* (wtian@broward.edu), Broward College, Judson A. Samuels South Campus, Department of Mathematics, Pembroke Pines, FL 33024, and **Shan Zhao**. *A fast ADI algorithm for nonlinear Poisson equation in heterogeneous dielectric media*. Preliminary report.

Recently, a nonlinear Poisson equation has been introduced to model nonlinear and nonlocal hyperpolarization effects in electrostatic solute-solvent interaction for biomolecular solvation analysis. Due to a strong nonlinearity associated with the heterogeneous dielectric media, this Poisson model is difficult to solve numerically, particularly for large protein systems. A new pseudo-transient continuation approach is proposed in this paper to efficiently and stably solve the nonlinear Poisson equation. A Douglas type alternating direction implicit (ADI) method is developed for solving the pseudo-time dependent Poisson equation. Different approximations to the dielectric profile in heterogeneous media are considered in the standard finite difference discretization. The proposed ADI scheme is validated by considering benchmark examples with exact solutions and by solvation analysis of real biomolecules with various sizes. Numerical results are in good agreement with the theoretical prediction, experimental measurements, and those obtained from the boundary value problem approach. Since the time stability of the proposed ADI scheme can be maintained even using very large time increments, it is efficient for electrostatic analysis involving hyperpolarization effects. (Received September 16, 2014)