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Treecode-Accelerated Boundary Integral Poisson-Boltzmann Solver

Solvation of biomolecules is a challenging problem in computational biophysics. Models that track explicit solvent molecules are extremely costly, and implicit solvent models based on the Poisson-Boltzmann (PB) equation provide an efficient alternative for computing solvent-solute interactions. Even so, PB solvers still encounter numerical difficulties stemming from the discontinuous dielectric constant across the molecular surface, the boundary condition at spatial infinity, and the presence of charge singularities representing the biomolecule. To address these issues, we present a linear PB solver employing a well-conditioned boundary integral formulation and GMRES iteration accelerated by a treecode algorithm. The accuracy and efficiency of the method are assessed for the Kirkwood sphere and a solvated protein (PDB:1A63). We compare numerical results for both the Poisson-Boltzmann and Poisson equations, using the proposed treecode-accelerated boundary integral solver, as well as the mesh-based Adaptive Poisson-Boltzmann (APBS) method. The present scheme has the features of relatively simple implementation, efficient memory usage, and straightforward parallelization.