Hybrid solvation model for electrostatic interactions in molecular dynamics simulation of ionic solvent

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Abstract

In this dissertation, we discuss the image approximation methods to the reaction field and their applications to electrostatic interactions in molecular dynamics simulations. We first introduce a 6th-order image approximation to the reaction field, employing a point charge at the classical Kelvin image point with three line charges that extend from the Kelvin image point along the radial direction to infinity. Discretizion of the line charges by point image charges and $O(N)$ complexity for potential and force field calculations are included. Numerical results demonstrate the 6th-order convergence rate of the image approximation and the $O(N)$ complexity of the fast implementation of the point image approximation. We then apply the image-based reaction field method to the calculation for electrostatic interactions in molecular dynamics simulations. A hybrid solvation model, termed the Image-Charge Solvation Model (ICSM), is extended for simulations of bioimolecules in ionic solvent, which combines the strengths of explicit and implicit solvent representations. We test our model in a simulation of sodium-chloride-water solvent. Our results demonstrate that the proposed model can faithfully reproduce many known solvation properties of sodium and chloride ions as well as many structural and dynamic properties of the water. Convergence and controlled accuracy can be achieved with only one image charge in the case of ionic solvent.

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