Grid projection techniques for modelling fixed charges in Poisson-Boltzmann solvers

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For solvation problems, one of the most used models is the Poisson-Boltzmann (PB) formalism which takes into account the solvent implicitly, as a dielectric continuum and electrostatics interactions are approximated at mean-field level. A variant of the PB formalism, called Dipolar Poisson-Boltzmann-Langevin (DPBL) model, has been recently proposed in order to improve physical accuracy by including some aspects of the discrete nature of the problem (neglected in PB model): explicit treatement of the solvent molecules (modelled as dipoles) and of the ion − solvent interactions. For the DPBL model, rigourous mathematical derivations have already been given and an open source simulation code (AquaSol) has been previously developed [1]. This code has proved to have interesting numerical behaviour and to be in good agrement with experimental results for some simple configurations. However, two main issues remain that are related to the use of Cartesian meshes and were not yet completely solved: the treatement of fixed point charges and of molecular surface.

This study is devoted to analyze several techniques for the treatement of fixed charges in PB and DPBL formalisms from mathematical and numerical points of view and is detailed in [2]. These techniques include trilinear interpolation for point charge representation model and direct grid projection for uniform spheric charging model which were already implemented in AquaSol code. In addition, we consider other grid projections : the antialiasing improvement for uniform spheric charging model [3] and projections for gaussian-like charge representation models as used for instance in [4]. Their numerical implementation in finite volume framework of AquaSol code is described and the obtained results for some configurations (including calculations of Born ion solvation energies) are compared.

Références

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