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An efficient discretization of the Poisson-Boltzmann equation with applications to electrostatic force calculation MOHAMMAD MIRZADEH, TODD SQUIRES, FREDERIC GIBOU, University of California Santa Barbara — We present a finite difference discretization of the non-linear Poisson-Boltzmann (PB) equation over complex geometries that has second order accurracy. The level-set method is adopted to represent the interface and Octree (in three dimensions) or Quadtree (in two dimensions) data stuructures are used to generate adaptive grids. Such an approach garanties that the finest grid resolution is located near the interface where EDL forms and creates very large electric field. Several numerical experiments are carried which indicate the second order accuracy both in the case of Dirichlet and Neumann boundary conditions in L_2 and L_∞ norms. Finally, we use our method to study the electrostatic interaction of double layers between charged particles in an unbounded bulk electrolyte as well as in a channel where the channel width is of the order of Debye length.

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