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A Well-Conditioned Hypersingular Boundary Element Method for Electrostatic Potentials in the Presence of Inhomogeneities within Layered Media

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Abstract. In this paper, we will present a high-order, well-conditioned boundary element method (BEM) based on Müller's hypersingular second kind integral equation formulation to accurately compute electrostatic potentials in the presence of inhomogeneity embedded within layered media. We consider two types of inhomogeneities: the first one is a simple model of an ion channel which consists of a finite height cylindrical cavity embedded in a layered electrolytes/membrane environment, and the second one is a Janus particle made of two different semi-spherical dielectric materials. Both types of inhomogeneities have relevant applications in biology and colloidal material, respectively. The proposed BEM gives $\mathcal{O}(1)$ condition numbers, allowing fast convergence of iterative solvers compared to previous work using first kind of integral equations. We also show that the second order basis converges faster and is more accurate than the first order basis for the BEM.

AMS subject classifications: 31B05, 92C05, 65Z05

Key words: Poisson Boltzmann equation, Layered electrolytes and dielectrics, Janus particles, ion channels, explicit/implicit hybrid solvation model.

1 Introduction

Electrostatic interactions are recognized as important and dominant forces in various applications, including protein folding, stability of biomolecules, other biological processes, colloidal material sciences, and engineering devices such as nanoelectronics and near field optics [5]. In many of these applications, we are faced with a difficult task of finding

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the electrostatic fields in the presence of inhomogeneous media and/or layered structures. For instance, for ion transport through a biological membrane, the dynamics of the ions are closely related to the electrostatic forces of the permanent charges in the residues of ion proteins and the surrounding layered dielectric environment. In the application of drug designs, a drug molecule's binding with a virus protein depends greatly on the complicated geometry and the electrostatic potential distribution of the former. On the other hand, for the study of colloidal media involving Janus particles [21], the inhomogeneous polarization of the particles can be the key to creating novel electric, magnetic, and self-assembling phenomena for various engineering applications.

Finding the electrostatic potential in non-homogeneous media requires the solutions of the Poisson and/or Poisson-Boltzmann equation if ionic materials are involved [12]. There are two basic approaches in obtaining the solutions, either by analytic methods, such as image charge methods [6, 23] or generalized Born approximations [20], or by grid-based numerical methods [5]. While the former is easy to implement and computationally less intensive, it does not produce a high-accuracy solution when modeling an ion channel [15]. The latter consists of finite difference, finite element methods using 3-D mesh discretization of the PDEs in the medium, and by boundary element methods (BEMs) based on boundary integral equations, which give the polarization charges on the boundary of the molecules or the inhomogeneities. The BEMs reduce the solution domain to lower dimensional manifolds, provided a Green's function is available as in the cases of homogeneous or layered background materials wherein some isolated inhomogeneities such as a Janus particle or an ion channel may be embedded.

In this paper, we will present a hypersingular integral equation which gives a well-conditioned second kind integral equation formulation. We will employ a singularity subtraction technique due to Müller [17] and Rokhlin [19], and the hypersingularities in the integral operators from adjacent dielectric materials are canceled out and the final integral equations only contain a weakly singular integrand, ready to be treated by a simple local polar coordinate transform.

The rest of the paper will be organized as follows. In Section 2, we will briefly review the basic information on the Green's function in layered media and the computation of the Green's functions and their normal derivatives (first and second) as needed in the hypersingular operators. In Section 3, we will present the Müller hypersingular integral equations [17, 19], which have been previously used in computing electrostatics potentials of biomolecules [13, 16], and numerical discretizations. In Section 4, appropriate numerical quadrature for various singular kernels are discussed. Numerical tests are included in Section 5 for several cases, including a dielectric sphere for accuracy checking of the proposed BEM, a Janus particle with different combinations of interior dielectric constants, and finally, an ion channel model. Both first and second order basis functions will be used for these tests and the results show the advantage of higher order basis and the well-conditioning of the second kind boundary integral equations. In Section 6, a conclusion and discussion on some numerical issues are included.