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A Fast Method for Evaluating Green's Function in Irregular Domains with Application to Charge Interaction in a Nanopore

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Abstract. We develop a fast meshless algorithm for electrostatic interaction in an irregular domain with given potential boundary conditions, which is of importance in many applications such as electrochemical energy and electric structure calculations. The algorithm is based on an approximation of the Green's function using two-level image charges, in which the inner-layer charges are located nearby the boundary to eliminate the singularity of the induced polarization potential, and the outer-layer charges with fixed positions approximate the long-range tail of the potential. We find the number of inner-layer image charges can be very small and thus the total complexity of the algorithm is less expensive and potentially suitable for use in particle simulations. The numerical results show the performance of the algorithm is attractive. We also use the algorithm to investigate the electrostatic interaction for particles in a cylindrical nanopore and show that the electrostatic interaction within the pore has an exponential decay.

AMS subject classifications: 31B10, 65M80, 78A30
Key words: Poisson's equation, image charge methods, meshless algorithm, electrostatic many-body phenomena, Green's function.

1 Introduction

Electrostatics at interfaces has been the central theme for nanoscale systems such as colloidal suspensions, biomolecules, electrochemical energy devices, and nanoparticle self-assembly [1]. Particle simulations for these systems require a convenient calculation for

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the Green's function of Poisson's equation with specified boundary or interface conditions, which gives the electrostatic interaction between particles. The image-charge method (ICM) is unique to provide an analytical representation for given boundary or interface conditions [2]. The ICM has been widely applied in particle simulations for dielectric effects near interfaces [3, 4], but it only exists in very limited boundary geometries such as planar interfaces and spheres. The use of the Green's function for irregular boundaries is often avoided in literature, and one solves the Poisson's equation by the grid-based method such as boundary integral method [5–7] in order to do particle simulations with irregular surfaces, which is computationally intensive and is only available for small systems.

In this work, a meshless fast algorithm is proposed for numerical approximation of the Green's function for Poisson's equation in irregular domains with Dirichlet boundary condition. Since the induced potential due to a point source is a harmonic function, we approximate its boundary data by potential functions from fictitious point sources outside the boundary (image charges), and determine the coefficients by requiring the error minimization on the boundary. Historically, this idea with fictitious point sources has been widely discussed as the method of fundamental solutions (MFS) for boundary value problems of differential equations in engineering applications, particularly, for Laplace's equation [8, 9], which keeps attracting the latest attention in computational science [10, 11]. The new development in the present work is the use of a two-layer ICM approximations for assignment of image-charge locations, and the inner-layer images are determined through an adaptive manner by a nonlinear least squares fitting. Since in the Green's function problem, the induced charge is only singular when the source approaches the boundary, it is found that only a small number of inner-layer images can effectively eliminate the singularity, and thus the nonlinear optimization can be performed rapidly due to the low dimensions. As usual as the MFS, the outer-layer images have fixed locations distributed on a regular surface, and their strengths are determined by solving a linear problem. We show the two-layer algorithm provides very rapid calculations of Green's functions, and thus it is potentially useful for particle simulations of charged systems, which will be the objective of our ongoing work.

The new algorithm is used to investigate the interaction force between ionic particles in nanopores. This problem is of great importance in electrochemical energy devices as the electrode is often made of porous materials and the understanding of ionic interaction within nanopores is essential to enhance the capacitance of the electrode [12]. It is observed that ionic pairwise interaction is exponentially decaying within the nanopore and the decaying rate is comparable to the pore size. This implies that a nanopore is accessible by a large number of likely charged ions and the capacitance is then maximized due to appropriate pore sizes, in agreement with many experimental and simulational suggestions [13–15].

The organization of this paper is as follows. In Section 2, we present the boundary integral expressions for the Green's function with conducting boundary condition on physical boundary and extended boundary, and discuss the numerical algorithm. In