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An iterative boundary potential method for the infinite domain Poisson problem with interior Dirichlet boundaries ☆

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Abstract

An iterative method is developed for the solution of Poisson's problem on an infinite domain in the presence of interior boundaries held at fixed potential, in three dimensions. The method combines pre-existing fast multigrid-based Poisson solvers for data represented on Cartesian grids with the fast multipole method. Interior boundaries are represented with the embedded boundary formalism. The implementation is in parallel and uses adaptive mesh refinement. Examples are presented for a smooth interior boundary for which an analytical result is known, and for an irregular interior boundary problem. Second-order accuracy in L_1 with respect to the grid resolution is demonstrated for both problems.
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1. Introduction

The Poisson problem is central to a wide variety of applications in computational physics, from electrostatics to projection methods for incompressible flow. For gridded data, or grid-mediated point data (*e.g.*, the particle-in-cell method) the easily implemented boundary conditions are Dirichlet, Neumann, or periodic. However, for many problems the most appropriate choice, on physical grounds, is the infinite domain condition. Solutions to the infinite domain problem have been estimated using the easily implemented boundary conditions in conjunction with very large computational domains, or with stretched grids, employed to remove the boundary from the region of interest. Of course such approaches are only approximate, and can be very demanding of resources especially in 3D. More rigorous boundary potential methods have been developed that determine the inhomogeneous Dirichlet conditions on a finite domain that are consistent with the desired

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infinite domain properties [22,14,12,23,1,16]. These methods exploit the free space Green's function to construct a boundary potential from a set of screening charges.

This work is concerned with an extension of boundary potential methods to infinite domain Poisson problems that contain also surfaces with fixed potential. One possible solution to this combined problem is the superposition of the solution of an external Dirichlet Laplace problem (*e.g.*, [19]) with the solution to an infinite domain Poisson problem constructed without interior boundaries. Such external Dirichlet Laplace problems involve quadrature of a codimension 1 Fredholm equation with singular kernel, integrated over the interior boundary. This results in a dense matrix equation for the charge density on the interior surface [15,19], and is similar to the 2D capacitance matrix method of Hockney and Eastwood [7]. Instead of pursuing such non-iterative approach, an iterative method based on existing fast solvers is developed.

Consider a three dimensional rectangular domain Ω_{dom} which contains space charges prescribed through the charge density ρ, and one or more closed regions Ω_{int} with prescribed surface potentials ϕ_{int}. The objective is the solution Φ to the Poisson problem

$$\Delta\Phi = \rho \tag{1a}$$

$$\Phi = \phi_{\text{int}} \quad \text{on } \partial\Omega_{\text{int}} \tag{1b}$$

$$\Phi(\mathbf{x}) \sim -\frac{Q}{4\pi|\mathbf{x}|} \quad \text{as } \mathbf{x} \to \infty, \tag{1c}$$

where Q is the sum of all charges in Ω_{dom}, consisting of space charges ρ, and also surface charges on $\partial\Omega_{\text{int}}$. After [22,14,12] we decompose Φ as sum of two fields, $\Phi = \phi + \Psi$, where ϕ is given by

$$\Delta\phi = \rho \tag{2a}$$

$$\phi = \phi_{\text{int}} \quad \text{on } \partial\Omega_{\text{int}} \tag{2b}$$

$$\phi = 0 \quad \text{on } \partial\Omega_{\text{dom}}, \tag{2c}$$

and $\phi = 0$ everywhere outside Ω_{dom}. It is possible to express ϕ as a free space Green's function convolution over the space charge density ρ and surface charges densities ϱ:

$$\phi(\mathbf{x}) = {}_{\Omega_{\text{dom}}} dV' G(\mathbf{x}|\mathbf{x}')\rho(\mathbf{x}') + \int\int_{\partial\Omega_{\text{int}}} dS' G(\mathbf{x}|\mathbf{x}')\varrho_{\text{int}}(\mathbf{x}') + \int\int_{\partial\Omega_{\text{dom}}} dS' G(\mathbf{x}|\mathbf{x}')\varrho_{\text{dom}}(\mathbf{x}'). \tag{3}$$

Here the surface charge densities ϱ_{int} and ϱ_{dom} are implicit functions given by (3) with the boundary conditions (2b) and (2c). Alternatively, Green's second theorem may be written

$$\begin{aligned}\phi(\mathbf{x}) = {}_{\Omega_{\text{dom}}} dV' G(\mathbf{x}|\mathbf{x}')\Delta'\phi(\mathbf{x}') - \int\int_{\partial\Omega_{\text{int}}} d\mathbf{S}' \cdot \nabla'\phi(\mathbf{x}')G(\mathbf{x}|\mathbf{x}') + \int\int_{\partial\Omega\ \text{int}} d\mathbf{S}' \cdot \nabla' G(\mathbf{x}|\mathbf{x}')\phi(\mathbf{x}') \\ - \int\int_{\partial\Omega_{\text{dom}}} d\mathbf{S}' \cdot \nabla'\phi(\mathbf{x}')G(\mathbf{x}|\mathbf{x}') + \int\int_{\partial\Omega_{\text{dom}}} d\mathbf{S}' \cdot \nabla' G(\mathbf{x}|\mathbf{x}')\phi(\mathbf{x}')\end{aligned} \tag{4}$$

from which, using (2c) and comparing with (3), one may deduce

$$\varrho_{\text{dom}}(\mathbf{x}) = -\mathbf{n} \cdot \nabla\phi\mathbf{x} \quad \text{on } \partial\Omega_{\text{dom}}. \tag{5}$$

The correction field Ψ must solve

$$\Delta\Psi = -\int\int_{\partial\Omega_{\text{dom}}} dS'\delta(\mathbf{x} - \mathbf{x}')\varrho_{\text{dom}}(\mathbf{x}') \tag{6a}$$

$$\Psi = 0 \quad \text{on } \partial\Omega_{\text{int}} \tag{6b}$$

$$\Psi \sim -\frac{Q'}{4\pi|\mathbf{x}|} \quad \text{as } \mathbf{x} \to \infty, \tag{6c}$$

where Q' is the sum of boundary charges on $\partial\Omega_{\text{int}}$ and $\partial\Omega_{\text{dom}}$. The right hand side of (6a) is $-\varrho_{\text{dom}}$ expressed as a space charge density, required by the condition that $\Phi = \phi + \Psi$ have no charge density on the artificial boundary $\partial\Omega_{\ \text{dom}}$. As a convolution over the free space Green's function, Ψ may be written