

A High-Accurate Fast Poisson Solver Based on Harmonic Surface Mapping Algorithm

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Abstract. Poisson's equations in a cuboid are frequently solved in many scientific and engineering applications such as electric structure calculations, molecular dynamics simulations and computational astrophysics. In this paper, a fast and highly accurate algorithm is presented for the solution of the Poisson's equation in a cuboidal domain with boundary conditions of mixed type. This so-called harmonic surface mapping algorithm is a meshless algorithm which can achieve a desired order of accuracy by evaluating a body convolution of the source and the free-space Green's function within a sphere containing the cuboid, and another surface integration over the spherical surface. Numerical quadratures are introduced to approximate the integrals, resulting in the solution represented by a summation of point sources in free space, which can be accelerated by means of the fast multipole algorithm. The complexity of the algorithm is linear to the number of quadrature points, and the convergence rate can be arbitrarily high even when the source term is a piecewise continuous function.

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Key words: Fast algorithm, Poisson's equation, boundary integral method, image charge, mixed boundary condition, fast multipole method.

1 Introduction

The solution of Poisson's equation plays an essential role in scientific computing as well as many physical and engineering applications such as molecular simulations, electric structure calculations, computational astrophysics, and fluid dynamics for both particle simulations [1–4] and continuum-theory calculations [5–8]. The development of efficient

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method for the Poisson's equation in these fields remains an important theme for simulations using high-performance computing. A great deal of numerical approaches have been developed, subject to different geometry and boundary conditions such as grid-based methods based on finite element or finite difference discretizations [9]. To reduce the number of grid elements, the boundary integral/element method [10–12] reformulates the Poisson's equation into a Fredholm integral equation of the second kind and can be accelerated through the fast multipole method (FMM) [13, 14].

Despite many advances on complex domains, fast numerical solvers for Poisson's equation of constant coefficient in a cuboidal domain remain to be an important theme due to its significance in many applications. Various numerical approaches especially for large scale parallel solvers have been proposed for this problem which are extensively used in practice. Most of the algorithms have second order of accuracy and $\mathcal{O}(n \log n)$ computational complexity, with n being the total number of grid points, such as the finite difference method with fast Fourier transform (FFT) or geometric multigrid, and the finite element method with proper preconditioning strategy [15]. Higher order schemes are also available by using high-order elements. When the source term and boundary conditions are sufficiently smooth, the spectral method based on orthogonal polynomials could converge exponentially while the computation cost remains to be expensive, and efficient implementations can achieve $\mathcal{O}(n^{3/2})$ for two dimensions and $\mathcal{O}(n^{4/3})$ for three dimensions using Legendre or Chebyshev polynomials [16, 17]. For certain type of boundary conditions, the pseudospectral Fourier method with polynomial subtraction technique to eliminate the Gibbs phenomenon can also achieve high order accuracy [18, 19]. For specific boundary conditions in a regular domain, the method of image can be used to represent the solution into an infinite sum or integral over the whole 3D space [20, 21]. The solution of Poisson's equation in the whole 3D space can be written as the convolution of the free-space Green's function and the source term. This convolution can be efficiently evaluated with high order accuracy through the FMM-based methods [20, 22], the method of local corrections [23, 24], or the FFT-based methods [25, 26].

Recently, a harmonic surface mapping algorithm (HSMA), which combines the method of image charges and the boundary integral method to calculate the Green's function, has been proposed and applied to particle systems [27, 28]. Its basic idea is that an auxiliary surface is introduced such that the contribution of image charges outside the surface is represented by image charges distributed over the surface. The harmonic surface mapping is a procedure to transform the local expansion from the exterior contribution into the surface integral which can be discretized into a sum of image charges. This algorithm is efficient to calculate the infinite sum for particle interaction in a box with various boundary conditions, especially non-periodic conditions when the FFT-based lattice summation cannot be directly applied.

The algorithm developed in this work is the extension of the HSMA, aiming to solve the Poisson's equation in a rectangular domain with mixed-type boundary conditions, which also introduces the auxiliary surface and uses a surface integral to represent the integral outside the surface. The main difficulty of this extension is the treatment of sin-