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An adaptive fast multipole accelerated Poisson solver for complex geometries

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ABSTRACT

We present a fast, direct and adaptive Poisson solver for complex two-dimensional geometries based on potential theory and fast multipole acceleration. More precisely, the solver relies on the standard decomposition of the solution as the sum of a volume integral to account for the source distribution and a layer potential to enforce the desired boundary condition. The volume integral is computed by applying the FMM on a square box that encloses the domain of interest. For the sake of efficiency and convergence acceleration, we first extend the source distribution (the right-hand side in the Poisson equation) to the enclosing box as a C^0 function using a fast, boundary integral-based method. We demonstrate on multiply connected domains with irregular boundaries that this continuous extension leads to high accuracy without excessive adaptive refinement near the boundary and, as a result, to an extremely efficient "black box" fast solver.

1. Introduction

The solution of the Poisson equation is a critical task in many areas of computational physics. The corresponding solvers need to be able to handle complex, multiply connected geometries, to be fast, adaptive, and to yield high order accuracy. Speed is of particular importance when the Poisson equation is part of a larger system of equations or in the inner loop of an optimization process. And since the physical quantity of interest is often the gradient of the solution, rather than the solution itself [36,44,11,35,29], partial derivatives of the solution must be computable with high accuracy as well.

Integral equation techniques have the potential to address all the challenges mentioned above. Complex geometries may be handled by decomposing the solution to Poisson's equation as the sum of a particular solution v that does not satisfy the proper boundary condition in general, plus a homogeneous solution u^H that solves Laplace's equation and is chosen so that the full solution $u = v + u^H$ satisfies the proper boundary condition. Fast and accurate solvers can be designed based on this construction. Indeed, several efficient and accurate integral equation based schemes exist to compute the solution of Laplace's equation on complex geometries [21,5,6], and fast and accurate evaluation of the particular solution v on fully adaptive grids by use of the Fast Multipole Method (FMM) has also been demonstrated for Poisson's equation [14,27]. Furthermore, in integral equation formulations derivatives do not have to be computed through direct numerical differentiation. Instead, one can analytically differentiate the kernels in the integral representation of the solution, and thus

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obtain integral representations for the derivatives of the solution as well. As a result the numerical error for the derivatives often converges at the same rate as the error for the solution itself [35,27].

Remarkably, despite all the strengths described above, we are not aware of an integral equation based Poisson solver for planar problems that combines all the features at once. In [14,18], grid adaptivity and FMM acceleration are demonstrated, but only simple geometries are considered. In contrast, in [32], Poisson's equation is solved for complex geometries and with FMM-accelerated quadratures, but the solver relies on fast methods for uniform grids [30,31]. The purpose of this manuscript is to close this gap and to present an adaptive, FMM-accelerated Poisson solver for complex geometries. We achieve this in the following way. We embed the irregular domain Ω on which Poisson's equation needs to be solved in a larger square domain Ω_B. We decompose the solution to Poisson's equation as $u = v + u^H$, and compute the particular solution v on Ω_B with a fast and accurate solver for square domains [14]. In order to calculate v in this way, we need to extend the source function f on the right-hand side of Poisson's equation beyond the domain Ω where it is originally given. We show that global function extension for f, constructed by solving Laplace's equation or a higher order partial differential equation on the domain $\mathbb{R}^2 \setminus \Omega$, leads to a robust, efficient and accurate algorithm for the evaluation of v. This idea is very similar in spirit to the extension technique recently presented by Stein et al. [43] for the immersed boundary method, but quite different in its implementation. Our approach for computing u^H is standard in its formulation [19], but it relies on numerical tools developed recently for optimized performance. Specifically, we represent u^H as a layer potential whose density solves a second-kind integral equation. We use generalized Gaussian quadrature [7,8] to approximate the integrals, a fast direct solver [23] to compute the density and an FMM accelerated quadrature by expansion (QBX) algorithm [26] to evaluate u^H inside Ω.

The structure of the article is as follows. In Section 2 we present our formulation for the solution to Poisson's equation, which is based on standard potential theory. We stress its computational challenges, which are then addressed in the following sections. In Section 3, we describe an efficient and accurate algorithm for the evaluation of the particular solution v and its derivatives in a square box. While this algorithm plays a central role in our approach to the problem, the section is relatively brief because our solver relies on an implementation of the algorithm and techniques that have been discussed in detail elsewhere [14,27]. In Section 4, we explain how we use a global function extension algorithm in combination with a box Poisson solver for the computation of the particular solution v on the whole square domain Ω_B. This is a key element of our solver, which allows us to deal with complex geometries in an efficient manner. To illustrate the method, we focus on a C^0 global function extension for simplicity. As we will show, for such extensions the super-convergence property of integral equation based schemes mentioned above, in which the error in the derivatives and the solution converge at the same rate, does not hold. We explain the reason for this discrepancy and discuss what is required for a global function extension method to achieve super-convergence in Sections 4.1 and 5.4. In Section 5, we present our numerical method for calculating the homogeneous solution u^H, as well as the function extension. Both are expressed as layer potentials and are computed in very similar ways. In Section 6 we study the performance of our new solver for two Poisson problems on a multiply connected domain. We summarize our work in Section 7 and suggest directions for future work.

2. The potential theoretic approach to Poisson's equation

In this article, we consider the solution u to Poisson's equation with Dirichlet boundary conditions given by

$$\Delta u = f \text{ in } \Omega \tag{1}$$

$$u = g \text{ on } \partial\Omega \tag{2}$$

where Ω is a smooth planar domain, which may or may not be multiply connected. The standard potential theory-based approach to the solution of (1)–(2) proceeds as follows. The first step is to calculate a particular solution, i.e. a function v which satisfies only equation (1) but does in general not satisfy equation (2). A natural candidate for v is given by

$$v(\mathbf{x}) = \int_\Omega G(\mathbf{x}, \mathbf{y}) f(\mathbf{y})\, d\mathbf{y}, \tag{3}$$

where $G(\mathbf{x}, \mathbf{y})$ is the free-space Green's function for Poisson's equation. For planar problems, $G(\mathbf{x}, \mathbf{y}) = -\log(||\mathbf{x} - \mathbf{y}||)/2\pi$. This is the situation we will consider in this article. Once v has been computed, the second step is to compute a homogeneous solution with appropriate boundary conditions. Specifically, one solves the following Dirichlet problem

$$\Delta u^H = 0 \text{ in } \Omega \tag{4}$$

$$u^H = g - v|_{\partial\Omega} \text{ on } \partial\Omega. \tag{5}$$

The solution to (1)–(2) is then the sum, $u = v + u^H$. There are many options for the numerical implementation of these two steps and we will not attempt to provide an exhaustive review of them here. Instead, we focus on our new approach, which is designed to address situations for which the domain Ω may be irregular and where derivatives of the solution are also required with high accuracy. The purpose of this section is to give a short overview of our approach. This overview is divided into two subsections: subsection 2.1 concerns the computation of v, and subsection 2.2 describes the computation