Commun. Comput. Phys.
doi: 10.4208/cicp.230813.291113a

Vol. **20**, No. 5, pp. 1381-1404
November 2016

A Novel Efficient Numerical Solution of Poisson's Equation for Arbitrary Shapes in Two Dimensions

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Received 23 August 2013; Accepted (in revised version) 29 November 2013

Abstract. Even though there are various fast methods and preconditioning techniques available for the simulation of Poisson problems, little work has been done for solving Poisson's equation by using the Helmholtz decomposition scheme. To bridge this issue, we propose a novel efficient algorithm to solve Poisson's equation in irregular two dimensional domains for electrostatics through a quasi-Helmholtz decomposition technique—the loop-tree basis decomposition. It can handle Dirichlet, Neumann or mixed boundary problems in which the filling media can be homogeneous or inhomogeneous. A novel point of this method is to first find the electric flux efficiently by applying the loop-tree basis functions. Subsequently, the potential is obtained by finding the inverse of the gradient operator. Furthermore, treatments for both Dirichlet and Neumann boundary conditions are addressed. Finally, the validation and efficiency are illustrated by several numerical examples. Through these simulations, it is observed that the computational complexity of our proposed method almost scales as $\mathcal{O}(N)$, where N is the triangle patch number of meshes. Consequently, this new algorithm is a feasible fast Poisson solver.

AMS subject classifications: 52B10, 65D18, 68U05, 68U07

Key words: Fast Poisson solver, loop-tree decomposition, electrostatics.

1 Introduction

The Poisson's equation occurs in the analysis and modeling of many scientific and engineering problems. In electrostatics, Poisson's equation arises when finding the electrostatic potential of an electric field in a region with continuously distributed charges.

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It is often solved in micro- and nano-electronic device physics [1], as well as in electronic transport and electrochemistry problems in terms of the Poisson-Boltzmann equation [2]. In fluid dynamics, Poisson's equations are solved to find the velocity potential in a steady-state potential flow of an incompressible fluid with internal sources or sinks [3]. Moreover, Poisson's equation is also encountered in finding the steady-state temperature in an isotropic body with internal sources [4].

An accurate and efficient solution of Poisson's equation is critical in various areas. For example, in design optimization of nano-devices where quantum effects are significant, a widely used scheme is to solve the coupled Schrödinger-Poisson system self-consistently [5–9], in which Poisson's equation is solved repeatedly, and concomitantly with the Schrödinger's equation. Consequently, the computational load for solving Poisson's equation is always of concern.

There are two main classes of solvers for linear systems from Poisson's equation: direct and iterative. One of the direct solvers is the fast Poisson solver based on fast Fourier transform (FFT) [10]. Indeed, this method is extremely efficient when the solution regions are simple and regular geometries with regular grids, such as rectangular regions, 2-D polar and spherical geometries [11], and spherical shells [12]. Since practical problems usually involve complex geometries, there have been many research works on seeking alternative methods. The multifrontal method with nested dissection ordering [13] is the most efficient direct method that can deal with complex geometries. Its key idea relies on partitioning the domain using a nested hierarchical structure and generating the LU decomposition from bottom up to minimize fill-ins. Typically, the computational complexity of the multifrontal method is of $\mathcal{O}(N^{1.5})$ in two dimensions where N is the dimension of the matrix.

For the other class of solvers, the iterative ones are more favorable when large systems are solved. This kind of methods often collaborate with acceleration algorithms or preconditioning techniques. A popular one is the approach based on integral equation techniques and accelerated by the fast multipole method (FMM) [14–17]. By expanding the system Green's function using the multipole expansion, this method can speed up the calculation of long-range interaction. As a result, it can achieve $\mathcal{O}(N)$ complexity when the underlying Green's function is available and amenable to factorization. Other than the FMM, the Multigrid (MG) method is one of most effective preconditioning strategies for iterative Poisson solvers. Since the pioneering work of Achi Brandt in 1970s [18], the multigrid method has been developed as a powerful tool for various computational problems. Hence, it spawns a large number of documents on the classic multigrid method [19–23] or specific aspects of multigrid techniques.

Apart from seeking fast solvers, much research in recent years has focused on the interface problems with discontinuous coefficients and singularities due to the demand from many applications. For example, dielectric constants of different components in metal oxide semiconductor field effect transistors (MOSFETs) vary dramatically, leading to typical problems with material interfaces. Since Peskin introduced the immersed boundary method (IBM) [24], a number of strategies have been developed to deal with