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A new multilevel method for electrostatic problems through hierarchical loop basis

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ABSTRACT

We present a new multilevel method for calculating Poisson's equation, which often arises from electrostatic problems, by using hierarchical loop basis. This method, termed as hierarchical Loop basis Poisson Solver (hieLPS), extends previous Poisson solver through loop-tree basis to a multilevel mesh. In this method, Poisson's equation is solved by a two-step procedure: first, the electric flux is found by using loop-tree basis based on Helmholtz decomposition of field; second, the potential distribution is solved rapidly with a fast solution of $O(N)$ complexity. Among the solution procedures, finding the loop part of electric flux is the most critical part and dominates the computational time. To expedite this part's convergent speed, we propose to use hierarchical loop basis to construct a multilevel system. As a result, the whole solution time has been noticeably reduced. Numerical examples are presented to demonstrate the efficiency of the proposed method.

1. Introduction

Numerical solutions of Poisson's equation have been found to be of great importance in various scientific and engineering problems, such as nanodevice design, fluid dynamics, and electrochemistry [1–3].

At the present time, existing numerical methods for Poisson's equation are grouped into two categories: direct and iterative solvers. Within direct methods, the multifrontal method is one of the most efficient algorithms. In [4], a superfast multifrontal method has been developed to take advantage of hierarchical tree structures of both hierarchically semiseparable (HSS) matrices and the classical multifrontal idea. It leads to a total complexity of $O(N^2)$. However, $O(N^2)$ is still unacceptable for large problems. As for iterative solvers, the multigrid method [5–9] is the most popular one because it could achieve nearly optimal complexity in theory.

Recently, a novel Poisson solver has been proposed to solve 2D problems [10,11]. This method affords a new way to solve Poisson's equation that is faster than the traditional finite element methods (FEM). Moreover, almost linear complexity has been observed when the stopping criterion is not less than 1×10^{-3}. However, the solution time could deteriorate as more accurate results are required.

To enhance the efficiency of this method, a method based on multilevel analysis of differential operators provides a good option. One important multilevel approach is the hierarchical linear Lagrangian basis (nodal basis) method that was proposed by Yserentant about two decades ago [12]. In this method, the FEM basis is changed from a single-level one to a multilevel basis that spans the same space. Deuflhard et al. soon afterwards reported an adaptive multilevel FEM code [13] achieving the same kind of computational complexity without use of standard multigrid techniques. Moreover, in [14,15], a hierarchical vector-valued basis on triangular mesh has been proposed to solve the electric field integral equation (EFIE) with method of moment (MoM). This basis can be further decomposed into the solenoidal part and irrotational part and the solenoidal part comprises hierarchical loop basis.

Another important category of multilevel methods is that based on the wavelet theory. In the last few decades, wavelet methods [16–18] have been developed as a powerful tool in numerous areas of mathematics, engineering, computer science, statistics, physics, etc. For example, in electronic applications, wavelet-based

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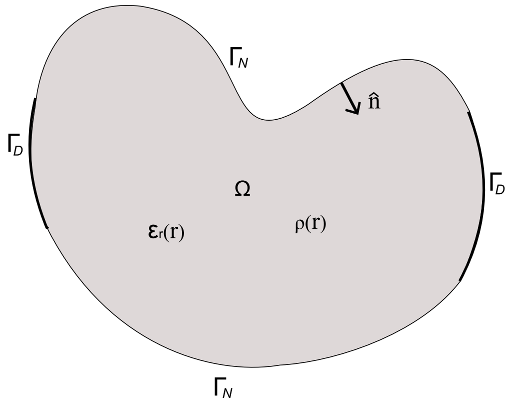

Fig. 1. Schema for a typical Poisson problem.

methods have been used for electromagnetic wave problems [19] and device modeling [20]. Moreover, the hierarchical loop basis, in view of [14], could be considered as a special kind of wavelet functions.

In this paper, we propose to extend our previous loop-tree-based Poisson solver to a multilevel method by using the hierarchical loop basis that has been used for EFIE before. It can speed up the iteration process and then reduce the solution time of our Poisson solver. As compared with multilevel multigrid method, this method is attractive because it is simpler to implement. In addition, this method is more friendly to parallel computing since all computations are local.

The organization of this paper is as follows. In Section 2, we introduce the formulation arising from electrostatic analysis and derive the corresponding Poisson's equation. In Section 3, we briefly outline the algorithm of previous Poisson solver that use normal loop-tree basis. Next, the hierarchical loop basis functions are presented in Section 4. Finally, in Section 5, we will validate the method and illustrate the efficiency of the new method. Conclusions will be drawn in Section 6.

2. Problem formulation

Assume inhomogeneous dielectric materials occupying a two-dimensional bounded and simply connected region, Ω, with boundary Γ and normal $\hat{\mathbf{n}}$ that points to the solution region as shown in Fig. 1. Consider a typical electrostatic problem which is governed by the following equations

$$\begin{aligned} \nabla \times \mathbf{E}(\mathbf{r}) &= 0 \\ \nabla \cdot \mathbf{D}(\mathbf{r}) &= \rho(\mathbf{r}), \end{aligned} \tag{1}$$

where $\mathbf{E}(\mathbf{r})$, $\mathbf{D}(\mathbf{r})$ denote the electric field and the electric flux, respectively, and $\rho(\mathbf{r})$ is the electric charge density. Under the assumption of linear, isotropic media, the electric flux $\mathbf{D}(\mathbf{r})$ relates the electric field by

$$\mathbf{D}(\mathbf{r}) = \epsilon(\mathbf{r})\mathbf{E}(\mathbf{r}), \tag{2}$$

where the permittivity $\epsilon(\mathbf{r}) = \epsilon_0\epsilon_r(\mathbf{r})$. ϵ_0 is the permittivity of free space, while the relative permittivity $\epsilon_r(\mathbf{r})$ is position dependent generally.

By introducing the electrostatic scalar potential in Eq. (1) such that

$$\mathbf{E} = -\nabla\phi, \tag{3}$$

we have Poisson's equation as follows:

$$\nabla \cdot \epsilon_r(\mathbf{r})\nabla\phi(\mathbf{r}) = -\frac{\rho(\mathbf{r})}{\epsilon_0}. \tag{4}$$

To ensure the uniqueness of the solution, appropriate boundary conditions must be imposed on all boundaries. Suppose that the boundary Γ is composed of two parts: the first one, Γ_D, is imposed by the Dirichlet boundary condition and the other part, Γ_N, comprises the Neumann boundary condition. Suppose that the Dirichlet boundary consists of finite M distinct boundaries, $\Gamma_D = \bigcup_{i=1}^{M} \Gamma_D^{(i)}$, then a fixed potential $\phi_0^{(i)}$ is prescribed on the boundary $\Gamma_D^{(i)}$ for $i = 1, 2, \ldots, M$. Moreover, to complete the description of a well-posed problem, the Neumann boundary data $g(\mathbf{r})$ must be a square integrable function over the corresponding boundary [21].

3. Poisson solver through loop-tree bases

In [11], a novel Poisson solver using loop-tree bases has been developed. We briefly describe this method here.

The point of departure for this method is to expand the electric flux by

$$\mathbf{D}(\mathbf{r}) = \mathbf{D}_l(\mathbf{r}) + \mathbf{D}_t(\mathbf{r}) = \sum_{i=1}^{N_l} l_i\mathbf{L}_i(\mathbf{r}) + \sum_{i=1}^{N_t} t_i\mathbf{T}_i(\mathbf{r}), \tag{5}$$

where $\mathbf{D}_l$ and $\mathbf{D}_t$ are the loop-space part and the tree-space part respectively, $\mathbf{L}_i(\mathbf{r})$ is a loop expansion function such that $\nabla\cdot\mathbf{L}_i(\mathbf{r}) = 0$, and $\mathbf{T}_i(\mathbf{r})$ is a tree expansion function such that $\nabla\cdot\mathbf{T}_i(\mathbf{r}) \neq 0$ [22,23], the numbers of the loop basis functions and the tree basis functions are N_l and N_t, respectively.

3.1. Solution procedures for Neumann problems

In order to find the electric flux and then solve Poisson's equation (4) with given Neumann boundary conditions, we need to go through the following three steps:

1. **Acquire the tree space part of electric flux**:
   Since the loop space part is divergence free, using Eq. (5) into the second equation of (1) leads to
   $$\nabla\cdot\mathbf{D}_t(\mathbf{r}) = \rho(\mathbf{r}). \tag{6}$$
   As a result, the tree space part, $\mathbf{D}_t$, can be solved for from the above by expanding $\mathbf{D}_t$ with tree basis functions and ρ with pulse functions. Then $\mathbf{D} = \mathbf{D}_l + \mathbf{D}_t$.
2. **Find the loop space part of electric flux**:
   It is well known that the electric field, $\mathbf{E}$, is curl-free. Thus, the electric field is orthogonal to the loop space, namely,
   $$\mathbb{P}_L\mathbf{E} = 0,$$
   where $\mathbb{P}_L$ denotes the projection operator onto the loop space. Applying the projection operator $\mathbb{P}_L$ to a vector field results in its loop space component. This operation amounts to extracting the loop space part from a given E field. Furthermore, this orthogonality implies that the electric field is orthogonal to any loop basis function: $\langle\mathbf{L}_i, \mathbf{E}\rangle = 0$. Using the relation of Eq. (2), we have
   $$\left\langle \mathbf{L}_i(\mathbf{r}), \frac{\mathbf{D}_l(\mathbf{r}) + \mathbf{D}_t(\mathbf{r})}{\epsilon(\mathbf{r})} \right\rangle = 0. \tag{7}$$
   Having $\mathbf{D}_t$ in hand, the above can be transformed to a matrix system, from which one can find the loop space part $\mathbf{D}_l$.
3. **Obtain the potential**:
   Finding the potential amounts to solving the following equation
   $$-\nabla\phi = \frac{\mathbf{D}(\mathbf{r})}{\epsilon(\mathbf{r})}. \tag{8}$$
   As shown in [10], one merit of this method is that the solution of Eq. (8) can be achieved by using the same fast tree solver because the del operator (∇) is the transpose of the divergence operator ($\nabla\cdot$).