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A NOVEL FAST SOLVER FOR POISSON'S EQUATION WITH NEUMANN BOUNDARY CONDITION

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Abstract—In this paper, we present a novel fast method to solve Poisson's equation in an arbitrary two dimensional region with Neumann boundary condition, which are frequently encountered in solving electrostatic boundary problems. The basic idea is to solve the original Poisson's equation by a two-step procedure. In the first stage, we expand the electric field of interest by a set of tree basis functions and solve it with a fast tree solver in $O(N)$ operations. The field such obtained, however, fails to expand the exact field because the tree basis is not curl-free. Despite of this, we can retrieve the correct electric field by purging the divergence-free field. Next, for the second stage, we find the potential distribution rapidly with a same fast solution of $O(N)$ complexity. As a result, the proposed method dramatically reduces solution time compared with traditional FEM methods. In addition, it is the first time that the loop-tree decomposition technique has been introduced to develop fast Poisson solvers. Numerical examples including electrostatic simulations are presented to demonstrate the efficiency of the proposed method.

1. INTRODUCTION

There are a variety of physical situations and engineering problems described by elliptic partial differential equations (PDEs) such as Poisson's equation:

$$\nabla^2 u(\mathbf{r}) = f(\mathbf{r}). \tag{1}$$

Examples of this equation are encountered in low-frequency dielectric or conductivity problems [1, 2]. This equation is often solved in

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micro and nanoelectronic device physics: it is also found in electronic transport and electrochemistry in terms of the Poisson-Boltzmann equation [3, 4]. Moreover, in electrostatics, Eq. (1) is a crucial analysis tool for electrical engineers. Hence, finding a robust and efficient solution has attracted considerable interests.

Over the past few decades, several kinds of fast methods for solving Poisson's equation have been proposed. One popular fast Poisson solver is based on Fourier analysis and accelerated by FFT [2]. However, this method has generally been limited to regular geometries, such as rectangular regions, 2D polar and spherical geometries [5], and spherical shells [6].

Multigrid methods are generally accepted as among the fastest numerical methods [7–9]. These methods take advantage of fine mesh and coarse mesh. Multigrid methods can be used in irregular domains and also be extended to other partial differential equations. Moreover, it has been proven effective for a number of applications including graphics application [10]. But it is difficult to implement multigrid methods in a robust fashion because they demand a hierarchy of grids of different density, which are not convenient in many real world problems.

The fast multipole method (FMM) [11–13] has been developed to solve Poisson problems with $O(N \log N)$ complexity. This method is applied to integral equation derived via the Green's function rather than differential equation methods where Poisson's equation is discritized directly. It also can be incorporated in a domain decomposition method using local spectral approximation to acquire a direct adaptive Poisson solver [14]. FMM solvers are particularly well suited for problems with large region of homogeneity.

In this paper, we will solve Poisson's equation with Neumann boundary condition, which is often encountered in electrostatic problems, through a newly proposed fast method. Instead of discretizing Poisson's equation directly, we solve it in two sequential steps: a) We first find the electric field of interest by a set of tree basis functions whose coefficients can be solved with a fast method in $O(N)$ operations (we call this fast method as fast tree solver in this paper); This field, however, cannot represent the desire field uniquely since the tree basis is not completely curl-free; Then we use a systematic divergence free field removal procedure to retrieve the exact electric field. b) In the second step, we obtain the electric potential ϕ from $-\nabla\phi = \mathbf{E}$, which can be solved for by a fast tree solver of $O(N)$ complexity. Consequently, the proposed method dramatically reduces solution time comparing with traditional FEM with iterative method and almost linear complexity has been observed in our numerical tests.

In contrast with the traditional finite element method (FEM), the proposed method solves the electric field in the first step, and then finds the electric potential in the second step. Furthermore, it introduces the loop-tree decomposition technique — which has been applied widely in integral equations within the computational electromagnetics (CEM) community for decades — to solve Poisson's equation arising from electrostatic problems for the first time.

The differences of the proposed method with aforementioned fast methods are twofold. First, the proposed method is based on differential equations while FMM based methods are using boundary integral equations. Second, compared with multigrid methods, the proposed method does not need the multilevel mesh.

The remainder of the paper is organized as follows. In Section 2, we outline the problem arising from electrostatics that we seek to solve. In Section 3, details of the proposed method will be described, in which two sequential steps of this method will be presented by two subsections. Next, in Section 4, we demonstrate and validate the efficiency by applying several numerical examples. Finally, the conclusions are drawn in Section 5.

2. ELECTROSTATIC BOUNDARY VALUE PROBLEM

A typical electrostatic boundary value problem (BVP) is stated in terms of its governing equation over a domain Ω:

$$\begin{aligned} \nabla \times \mathbf{E}(\mathbf{r}) &= 0 \\ \nabla \cdot \mathbf{D}(\mathbf{r}) &= \rho(\mathbf{r}), \end{aligned} \tag{2}$$

where $\mathbf{E}(\mathbf{r})$, $\mathbf{D}(\mathbf{r})$ denote the electric field and the electric flux density vector, respectively, and $\rho(\mathbf{r})$ is the electric charge density. In the following, $\mathbf{D}(\mathbf{r})$ is denoted by electric flux for short. The region Ω is a two dimensional bounded and simple connected domain with boundary Γ as shown in Fig. 1.

Given the assumption of linear, isotropic media, $\mathbf{D}$ is linked to $\mathbf{E}$ through the constitutive relation

$$\mathbf{D}(\mathbf{r}) = \epsilon_r(\mathbf{r})\epsilon_0\mathbf{E}(\mathbf{r}), \tag{3}$$

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

We can introduce the electrostatic scalar potential, ϕ, so that the electric field can be computed from

$$\mathbf{E} = -\nabla\phi, \tag{4}$$

which is due to the irrotational nature of the electric field under static conditions.

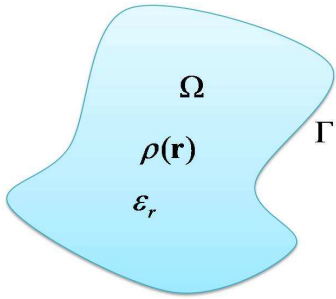


Figure 1. Schema of the electrostatic problem.

Use of (4) in the second of the equations in (2) yields Poisson's equation for the electrostatic potential,

$$\nabla \cdot \epsilon_r(\mathbf{r}) \nabla \phi(\mathbf{r}) = -\frac{\rho(\mathbf{r})}{\epsilon_0}. \tag{5}$$

To ensure the uniqueness of the solution, appropriate boundary conditions must be imposed on all boundaries in solution region. More specifically, on the boundaries of interested domain, the tangential component of the electric field must be specified on one portion of the boundary, while the normal component of electric flux must be specified on the remaining portion. In fact, these two kinds of conditions correspond to Dirichlet boundary condition and Neumann boundary condition, respectively. For the sake of convenience, we only focus on those problems with Neumann boundary condition. Moreover, we further assume that the media is linear, isotropic and homogeneous throughout. Hence, the boundary value problem is described by:

$$\begin{aligned} \nabla^2 \phi(\mathbf{r}) &= -\frac{\rho(\mathbf{r})}{\epsilon_r \epsilon_0} \quad \mathbf{r} \in \Omega \\ \hat{n} \cdot \nabla \phi(\mathbf{r}) &= -\frac{\rho_s(\mathbf{r})}{\epsilon_r \epsilon_0} \quad \mathbf{r} \in \Gamma, \end{aligned} \tag{6}$$

where $\rho_s(\mathbf{r})$ is two dimensional surface charge density, and $\hat{n}$ is the norm pointing to the solving region.

It should be noted the above Poisson problem of (6) is a special case where Neumann boundary condition is imposed in the entire region. In this case, the uniqueness is guaranteed apart from an additive constant. This implies we need to impose a reference potential to the particular problem of interested, which will be address in our numerical test in Section 4.

3. SOLUTION METHOD

In order to solve the Poisson problem of (6), one can discretize Eq. (6) directly and then solve it by the traditional finite element method. With FEM, the electric potential is obtained first while the interested electric field then can be computed from Eq. (4).

In contrast, our proposed method finds the electric field **E** first. This can be done by utilizing loop-tree decomposition that stems from CEM applications. In the CEM community, the low frequency problem has attracted intense interest for the last decade. When the frequency is low, the current **J** naturally decomposes into a solenoidal (divergence-free) part and an irrotational (curl-free) part. Moreover, these two parts are not balanced for low frequency. Hence, there is a severe numerical problem when solving integral equations in which RWG basis is normally used. One remarkable remedy for this low frequency breakdown is the well known loop-tree decomposition [15–19]. The RWG basis set is decomposed into the loop basis, which has zero divergence, and the tree basis, which has non-zero divergence.

The well-known Helmholtz decomposition [20] states that any sufficiently smooth, rapidly decaying vector field in three dimensions can be resolved into the sum of an irrotational (curl-free) vector field and a solenoidal (divergence-free) vector field. By this theory, an electric field arising from dynamic electromagnetic problems definitely can be decomposed into two orthogonal parts: curl-free one and divergence-free one[†]. If one expands this electric field in the RWG space and resolves it into tree basis part and loop basis part (here and throughout we also call them tree space and loop space), the loop basis will approximately represent the divergence-free part whereas the tree basis will not expand the curl-free part uniquely. This is because the tree basis itself is not curl-free. Moreover, the tree basis is not unique since one can construct different of tree structures from a RWG space. From this point of view, the loop-tree decomposition is a quasi-Helmholtz decomposition.

An electric field resulting from electrostatic problems, on the other hand, is curl-free. Although the tree basis alone cannot expand this electric field uniquely, the electric field such obtained is related to charge density because its complement, the loop space one, does not bring in any charge density due to its divergence-free nature. Therefore, we can solve Poisson's equation with the tree basis alone first. By so doing, we can take advantage of a fast method that exploits the topological information and is of $O(N)$ complexity. Having found the tree space part of electric field, we purge the solution of divergence

[†] Orthogonality here is defined in the inner product space where $\langle \mathbf{A}, \mathbf{B} \rangle = \int \mathbf{A} \cdot \mathbf{B} d\mathbf{r}$

free field to retrieve the desired electric field. Details of this solution procedure will be delineated.

3.1. Solution of the Tree Space Part of Electric Field

Borrowing the idea of loop-tree decomposition, we can use a tree basis to expand the tree space part of electric field as

$$\mathbf{E}_t = \sum_{i=1}^{N_t} t_i \mathbf{T}_i(\mathbf{r}), \tag{7}$$

where $\mathbf{T}_i$ is the i-th tree basis whose coefficient is t_i, and N_t is the total number of tree basis functions. It is equal to the number of patches minus one for a triangular mesh. We then use the pulse basis to expand the charge density ρ, namely

$$\rho(\mathbf{r}) = \sum_{i=1}^{N_p} c_i P_i(\mathbf{r}), \tag{8}$$

where N_p stands for the patch number. The pulse function is defined as

$$P_i(\mathbf{r}) = \begin{cases} 1, & \text{if } (\mathbf{r}) \in i\text{-th patch}, \\ 0, & \text{otherwise.} \end{cases} \tag{9}$$

From loop-tree decomposition, it is obvious that the irrotational (non-divergence free) part of electric field, which corresponds to the charge density, is only associated with the tree space part. Hence, we can substitute Eqs. (7) and (8) into the first of Eq. (6) and test it with the same set of pulse functions as in the Galerkin's method. This procedure leads to

$$\bar{\mathbf{K}} \cdot \mathbf{I_t} = \mathbf{V}_\rho \tag{10}$$

where

$$\left[\bar{\mathbf{K}}\right]_{ij} = \int P_i(\mathbf{r}) \nabla \cdot \mathbf{T}_j(\mathbf{r}) \, \mathrm{d}\mathbf{r}, \tag{11}$$

$$\left[\mathbf{V}_\rho\right]_i = \int P_i(\mathbf{r}) \rho(\mathbf{r}) / (\epsilon_0 \epsilon_r) \, \mathrm{d}\mathbf{r} = c_i / (\epsilon_0 \epsilon_r). \tag{12}$$

It should be emphasized that, in order to satisfy the boundary condition, one can introduce the known surface charge density into the matrix system, and then subtract the corresponding coefficients from the right hand side of Eq. (10).

The matrix equation system of (10) can be solved in $O(N)$ operations with a fast tree solver described in [17, 21]. We will outline this fast method as below.

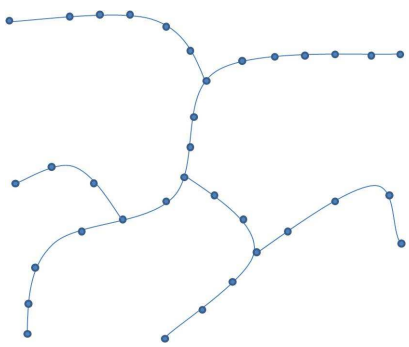


Figure 2. Schematic of a general tree.

3.1.1. Fast Tree Solver

The basic idea of fast tree solver is as follows. In the first place, a tree is found to span the domain where Poisson's equation is solved. This tree corresponds to a set of RWG basis functions complementary to the loop basis. Fig. 2 shows a typical tree structure. Each node of the tree represents the center of a patch, which is related to the triangle patch of the RWG basis. Each line between two nodes can be associated with the current that flows between two patches. Furthermore, the patch unknown associated with a tip of the dendritic branch is only related to one current unknown. Therefore, starting from the branch tips, the unknowns can be solved for recursively until a junction is reached. Noticing that a junction node cannot be connected more than three neighboring nodes for the case of RWG functions, we can solve for the unknowns of junctions when the unknowns on two associated open branches have been solved. Hence, all unknowns can be solved for in $O(N)$ operations.

3.2. Divergence-free Field Removal

It is well known that the tree basis is not curl-free and non-unique. This property makes representing the desired electric field by $\mathbf{E}_t$ inaccurate. Alternatively, it implies that some solenoidal components contaminate it.

Since $\mathbf{E}$ is curl-free, the correct electric field, $\mathbf{E}$, can be obtained by projecting $\mathbf{E}_t$ onto the curl-free space. To this end, one has to find a set of completely curl-free basis functions. Few research work has devoted to it [22]. Thus, it is formidable to find a completely curl-free basis in the RWG space.

Another way to circumvent this obstacle is to remove the

complementary solenoidal (divergence-free) part that is orthogonal to the curl-free space. This is practical because the divergence-free part, unlike its curl-free counterpart, could be expanded by the loop basis that is living on the space spanned by RWG functions. Since the loop basis has divergence-free property, it can then expand the divergence-free space. Therefore, we can first project $\mathbf{E}_t$ onto the divergence free space using a set of loop basis function. Once the projection has been done, the pure curl-free part of $\mathbf{E}_t$ can be obtained by subtracting the divergence-free components.

Mathematically, $\mathbf{E}_t$ can be expressed by

$$\mathbf{E}_t(\mathbf{r}) = \sum_{i=1}^{N} a_i \mathbf{f}_i(\mathbf{r}) + \sum_{i=1}^{N_l} l_i \mathbf{L}_i(\mathbf{r}), \tag{13}$$

where the first term on the right side is pure curl-free part of $\mathbf{E}_t$, while the second one is the divergence-free part. Moreover, $\mathbf{f}_i$ refers to RWG basis functions whose total number is N, and $\mathbf{L}_i$ denotes the loop basis functions with total number of N_l.

By using the loop basis to test the above equation, Eq. (13) leads to a matrix system

$$\bar{\mathbf{G}}_l \cdot \mathbf{I}_l = \mathbf{V}_d \tag{14}$$

where

$$\left[\bar{\mathbf{G}}_l\right]_{ij} = \int \mathbf{L}_i(\mathbf{r}) \cdot \mathbf{L}_j(\mathbf{r})\, \mathrm{d}\mathbf{r}, \tag{15}$$

is the Gram matrix of the loop basis, and

$$\left[\mathbf{V}_d\right]_i = \int \mathbf{L}_i(\mathbf{r}) \cdot \mathbf{E}_t(\mathbf{r})\, \mathrm{d}\mathbf{r}, \tag{16}$$

is the projection value of $\mathbf{D}_t$ onto the loop space. In this equation, we use the relation

$$\int \mathbf{L}_i(\mathbf{r}) \cdot \sum_{i=1}^{N} a_i \mathbf{f}_i(\mathbf{r})\, \mathrm{d}\mathbf{r} = 0, \tag{17}$$

because the fact that loop basis is orthogonal to the curl free space.

The Gram matrix of loop bases, $\bar{\mathbf{G}}_l$, is highly sparse. Moreover, it is a symmetric, positive definite and diagonally dominant. Therefore, common iterators, such as CG, Bi-CGSTAB [23] and GMRES [24, 25], work efficiently for solving Eq. (14).

Consequently, the electric field desired can be retrieved by

$$\mathbf{E} = \mathbf{E}_t - \sum_{i=1}^{N_l} l_i \mathbf{L}_i. \tag{18}$$

3.3. Solution of Potential

Generally, finding the electric field **E** indicates that the pertinent Poisson's equation has been solved. In some applications, however, the electric potential is the ultimate concern. In this section, we describe a rapid solution of the electric potential as follows.

Finding the potential amounts to solving Eq. (4) with the electric field, **E**, that is obtained from previous parts. It is interesting that the solution of Eq. (4) can be achieved by using the same fast tree solver because the del operator (∇) is the transpose of the divergence operator ($\nabla\cdot$). Hence, we expand the potential ϕ in terms of pulse functions, that is,

$$\phi(\mathbf{r}) = \sum_{i=1}^{N_p} \nu_i P_i(\mathbf{r}). \tag{19}$$

With a similar method described in Section 3.1, testing this equation using a set of tree basis functions, we obtain

$$\bar{\mathbf{K}}^T \cdot \mathbf{I}_\phi = \mathbf{V}_\phi \tag{20}$$

where

$$[\mathbf{V}_\phi]_i = -\int \mathbf{T}_i(\mathbf{r}) \cdot \mathbf{E}(\mathbf{r}) \mathrm{d}\mathbf{r}, \tag{21}$$

and $[\mathbf{I}_\phi]_i = \nu_i$ which is defined in (19). The element $\bar{\mathbf{K}}^T$ is originally defined as

$$\left[\bar{\mathbf{K}}^T\right]_{ij} = -\int \mathbf{T}_i(\mathbf{r}) \cdot \nabla P_j(\mathbf{r})\, \mathrm{d}\mathbf{r},$$

which can be deduced using integration by parts as

$$\left[\bar{\mathbf{K}}^T\right]_{ij} = \int P_j(\mathbf{r}) \nabla \cdot \mathbf{T}_i(\mathbf{r})\, \mathrm{d}\mathbf{r} = \left[\bar{\mathbf{K}}\right]_{ji}. \tag{22}$$

Consequently, the resulting matrix is just a transpose of the matrix $\left[\bar{\mathbf{K}}\right]$ from Section 3.1. Hence, (20) can be solved with the fast tree solver in $O(N)$ operations.

4. NUMERICAL EXAMPLES

In this section, two numerical examples are shown to validate the efficiency of the proposed method. All examples have been calculated on a standard computer with 2.66 GHz CPU, 4 GB memory and Windows operating system.

4.1. Simple Neumann Problem

In order to validate the correctness of this algorithm, we solve a simple 2-D Poisson's equation as the first example. The Poisson's equation in this case is

$$\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} = -\pi \cos(\pi x) - \pi \cos(\pi y) \tag{23}$$

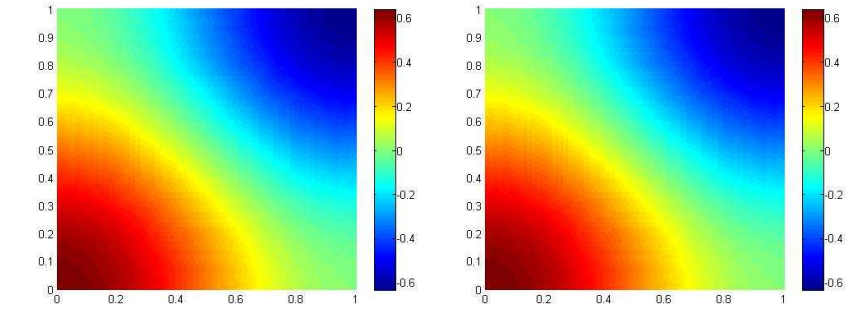
where $(x, y) \in \Omega = [0, 1] \times [0, 1]$, with the following Neumann boundary condition

$$\hat{\mathbf{n}} \cdot \left(\hat{\mathbf{x}} \frac{\partial \phi}{\partial x} + \hat{\mathbf{y}} \frac{\partial \phi}{\partial y} \right) = 0 \qquad (x, y) \in \Gamma. \tag{24}$$

As mentioned in Section 2, the Neumann problems is uniquely solvable but up to a constant; hence,we have to impose a reference potential so that the uniqueness can be guaranteed. By setting the potential as $2/\pi$ at the point $(0, 0)$, the aforementioned problem has an analytical solution

$$\phi(x, y) = \left[\cos(\pi x) + \cos(\pi y) \right] / \pi. \tag{25}$$

By utilizing the proposed method, potential distribution can be found as shown in Fig. 3, where Fig. 3(a) shows the potential distribution result while Fig. 3(b) gives the exact solution as a reference. Furthermore, in Fig. 4, we compared the value from the proposed approach with the analytic results. It is obvious that the potential distribution from this new method agrees with analytical one well.



(a) Simulation potential distribution (b) Exact potential distribution

Figure 3. Potential distribution: (a) Simulation result. (b) Exact potential distribution.

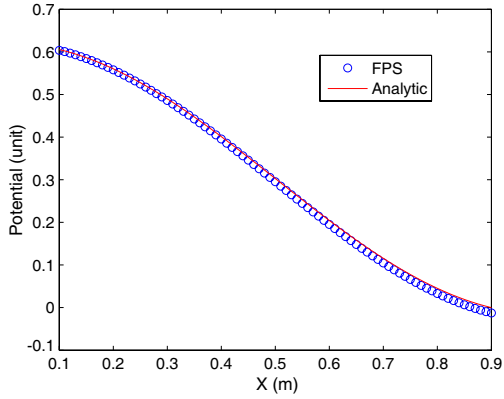


Figure 4. Comparisons of values along one line ($y = 0.1$).

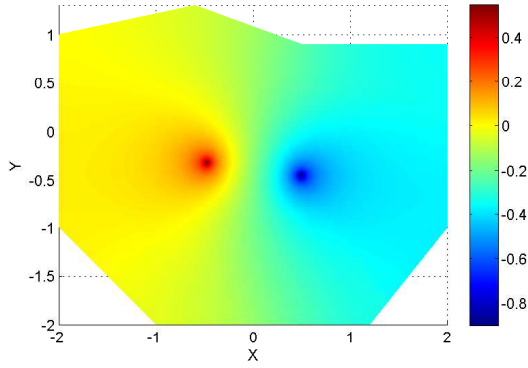


Figure 5. Potential distribution calculated by the proposed method for line sources in an arbitrary domain.

4.2. Line Source Problem

As the second example, a Poisson problem involving two line charge sources was simulated within a polygonal region. One line source was at point $(-0.475, -0.329)$ with a positive unit charge while the other one was at point $(0.494, -0.459)$ with a negative unit charge. The resultant potential distribution is shown in Fig. 5. In this case, the potential value of the up-left corner $(-2.0, 1.0)$ was set to zero as a reference potential. The result has been validated by FEM method.

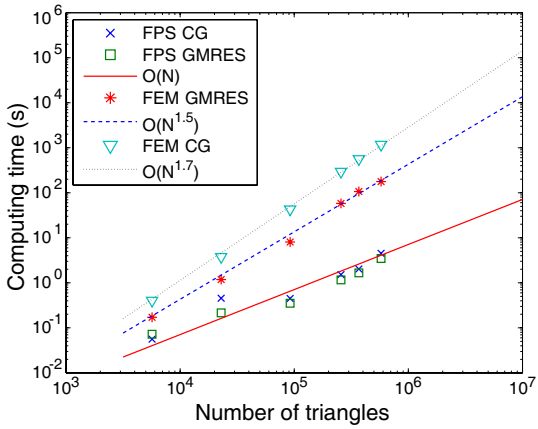


Figure 6. Complexity comparison with same stopping criterion.

4.3. Computational Complexity Analysis

To analyze the computational complexity, we have computed the problem of Section 4.1 with different mesh densities. The solution time of this algorithm consists of three parts: the first fast tree solution time for Eq. (10), the divergence free field removal time, and the second fast tree solution time for Eq. (20). As for the fast tree solution time, Zhao and Chew have proved that it is of $O(N)$ complexity [17]. Hence, the bottleneck comes from the procedure of divergence free field removal, which amounts to the iterative solution time of Eq. (14). The CPU time of this part therefore depends on iterative solver type and the required accuracy level.

In divergence free field removal part, the Gram matrix of loop basis has the form

$$\left[\bar{\mathbf{G}}_l\right]_{ij} = \int \mathbf{L}_i(\mathbf{r}) \cdot \mathbf{L}_j(\mathbf{r})\, \mathrm{d}\mathbf{r}. \tag{26}$$

Similar to the stiffness matrix of FEM, this matrix is a symmetric, positive definite one. For this kind of matrix systems, the number of iterations is proportional to the square-root of the condition number.

Figure 6 shows the computational complexity comparison between this fast Poisson solver and FEM. Both conjugated gradient (CG) and GMRES are adopted with the same stopping criterion (0.01). For GMRES, the restart parameter is 60. As can be seen from this plot, the total solution time of our proposed new method is evidently less than the one of traditional FEM, whichever CG or GMRES is adopted. In our numerical experiment, the complexity of this new

method approaches linear complexity. Moreover, GMRES methods work better than CG method in our simulations.

5. CONCLUSIONS

We have proposed and developed a new two dimensional fast Poisson solver for electrostatic problems with the Neumann boundary condition based on the loop-tree decomposition technique. This method could solve Poisson's equation rapidly with the fast tree solver. Its computational workload is evidently less than that of traditional FEM. This method promises to be a novel fast Poisson solver that can solve general Poisson's equation for electrostatics as well as other related fields. Extension of this work to Dirichlet and mix boundary condition can be carried out in a straightforward manner.

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