

Fast multipole boundary element method for the solution of 3D electrostatic field problems

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Abstract

Direct and indirect boundary element methods are applied to the numerical solution of electrostatic field problems. The fully populated matrix of the system of linear equations is compressed by the fast multipole method along with a significant reduction of computational costs and memory requirements. With some modifications and enhancements the fast multipole method yields to accurate results even for adaptive meshes and mixed boundary conditions. Besides the efficient solution of the system of linear equations the fast multipole method abridges the postprocessing time noticeably. Emphasis is placed on an implementation of the fast multipole method into existing BEM software.

Keywords: electrostatics, fast multipole methods, Galerkin methods, Laplace equations, matrix compression techniques.

1 Introduction

The application of the fast multipole boundary element method (FMBEM) to the solution of electrostatic problems is very advantageous. Only the surfaces of linear, piecewise homogeneous media have to be discretized and the surrounding infinite space is taken into account exactly. By the use of the fast multipole method (FMM), Greengard and Rokhlin [1], the fully populated matrix of the system of linear equations of the classical BEM is compressed very efficiently. Both the memory requirements and the computational costs are reduced to approximately $O(N)$, where N is the number of unknowns. In the context of an indirect BEM formulation based on surface charge densities, Rao *et al* [2], the FMM is similar to the original approach for particle interactions Nabors and White [3]. An extension of the FMM to treat both Dirichlet and Neumann



boundary conditions with a high accuracy and numerical stability is shown in this paper. Furthermore a direct BEM formulation based on Green's theorem is discussed, especially the computation of so-called double-layer potentials with the FMM. In practice higher-order elements with partly extremely varying size of the elements are often used. Enhancements of the FMM algorithm are presented to achieve a high accuracy and high compression rates even in such cases. The numerical examples show the efficiency of the FMBEM and its applicability to practical problems.

2 Classical formulation

Electrostatic field problems with linear, isotropic and piecewise homogeneous media are considered. A Dirichlet boundary condition is the given potential on the conductors. The continuity of the normal component of the electric displacement at interfaces between two dielectrics is a Neumann boundary condition. To numerically solve the problem the surfaces of the conductors and the dielectrics are discretized with second order, quadrilateral eight-noded elements. A system of linear equations is obtained by an application of the Galerkin method. The system of linear equations is solved iteratively with generalized minimal residual solver (GMRES) and a Jacobi preconditioner Axelsson [4] and Barrett *et al* [5].

In an indirect formulation the nodal values are the free surface charge densities on conductors and polarization charge densities on dielectrics. To compute the potential u in an arbitrary point an integral over all surface charge densities σ must be evaluated

$$u(\mathbf{r}) = \frac{1}{4\pi\epsilon_0} \int_A \frac{\sigma(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} dA'. \quad (1)$$

All surfaces belong to a single computational domain. This simplifies the application of the method.

A direct formulation is based on Green's theorem

$$c(\mathbf{r})u(\mathbf{r}) = \oint_A \frac{\partial u(\mathbf{r}')}{\partial n'} \frac{1}{|\mathbf{r} - \mathbf{r}'|} dA' - \oint_A u(\mathbf{r}') \frac{\partial}{\partial n'} \frac{1}{|\mathbf{r} - \mathbf{r}'|} dA'. \quad (2)$$

It is applied to closed domains. Different domains are coupled at their interfaces. In electrostatics a direct formulation is very attractive for interior problems, e. g. steady current flow field problems.

To obtain a system of linear equations the Galerkin method is applied. The computation of the potential with eqn. (1) becomes then

$$\int_{A_i} N_i(\mathbf{r}) u(\mathbf{r}) dA = \frac{1}{4\pi\epsilon_0} \sum_j \sigma_j \int_{A_j} N_i(\mathbf{r}) \int_{A_j} \frac{N_j(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} dA' dA \quad (3)$$

in discretized form. For each node i on a surface with a given Dirichlet boundary condition $u(\mathbf{r})$ eqn. (3) is used to determine the unknown surface charge densities σ_j . N_i are the shape functions of the elements.

3 Fast multipole method

The FMM was introduced for a fast computation of particle interactions by Greengard and Rokhlin [1]. Since an indirect BEM formulation with only Dirichlet boundary conditions and constant elements is very similar to particle interactions, the FMM can be adapted to such BEM problems relative easily Nabors and White [3]. Nevertheless the finite size of boundary elements causes some troubles in the original FMM algorithm. One possible strategy to overcome these problems was proposed by Nabors and White [3]. Nowadays the FMM is a popular compression technique for BEM matrices in a variety of static and time-dependent problems.

The FMM exploits the fact, that within an iterative solver for the linear system of equations matrix-by-vector products are evaluated only. For this operation it is not necessary to compute and store BEM matrices explicitly. That means the product of a BEM matrix with a vector, the solution vector in the current iteration step, can be provided by the FMM. In the FMM a matrix-by-vector product is split into two parts. A near-field part for element interactions between elements, which are lying close to each other, and a far-field part for the remaining element interactions

$$\{y\} = [A]\{x\} = [A_{\text{near}}]\{x\} + \{y_{\text{far}}\}. \quad (4)$$

To compute the far-field element interactions Green's function in the classical integrals is replaced by a truncated series expansion into spherical harmonics

$$\frac{1}{|\mathbf{r} - \mathbf{r}'|} = \begin{cases} \sum_{n=0}^L \sum_{m=-n}^n \frac{r^n}{r'^{n+1}} Y_n^m(\theta, \varphi) Y_n^{-m}(\theta', \varphi'), & r < r' \\ \sum_{n=0}^L \sum_{m=-n}^n \frac{r^m}{r'^{n+1}} Y_n^m(\theta, \varphi) Y_n^{-m}(\theta', \varphi'), & r' < r \end{cases}. \quad (5)$$

The accuracy of the series expansion in eqn. (5) is controlled by the order L and the distance between the spherical domains with source points $\mathbf{r}'$ and evaluation points $\mathbf{r}$. The radii of these spherical domains are the basis for a definition of the near- and the far-field of an element. To obtain a robust algorithm for the near- and far-field determination all elements are grouped by a hierarchical scheme. For three-dimensional problems a grouping scheme based on cubes is used, a so-called octree. In many cases only one element is assigned to a cube at the finest octree level. For a considered cube the near-field consists of the cube itself and all cubes, which have a common corner with the considered cube. All other cubes are assigned to the far-field.

In practice the above mentioned algorithm for a determination of the near- and far-field leads to instabilities in the series expansions. In the case of adaptive meshes the size of the elements varies extremely. That means the elements at the finest octree level normally jut out of the cube, to which they are assigned. To overcome this problem the elements can be cut at the boundaries of the cubes. This strategy works very well for constant elements. Since neighbouring second order elements are connected at their common nodes to ensure C^0 -continuity, a remeshing would be necessary. To keep the original element mesh the real



convergence radii of the cubes are taken into account Buchau *et al* [6]. Only if the convergence radii of two cubes a and b are overlapping, cube b is assigned to the near-field of cube a and vice versa. To improve the convergence of the series expansions for a fixed L the values of the convergence radii of the cubes are a little bit enlarged for this decision.

In a classical BEM eqn. (3) is evaluated for each node i . The sum at the right hand side of eqn. (3) is performed over all elements or nodes respectively. That means a classical BEM matrix is fully populated. In contrast to the classical BEM matrix the near-field matrix $[A_{\text{near}}]$ is a sparse matrix. The summation index in the right hand side of eqn. (3) runs only over all elements in the near-field of node i . In other words, $[A_{\text{near}}]$ corresponds to the original matrix, from which all far-field entries were removed. The only difference in the assembling process of the classical matrix and the near-field matrix is a different interaction list between the elements.

The evaluation of eqn. (4) is divided into two parts. In the first part the near-field matrix is multiplied with $\{x\}$. For this purpose sparse matrix libraries can be used. Then in the second part the FMM algorithm is executed to obtain the influence of the far-field $\{y_{\text{far}}\}$. The FMM algorithm consists of an upward and a downward pass. In the upward pass all sources on the elements are replaced by equivalent multipoles. These multipoles are used in the downward pass to compute a Taylor series expansion in each cube. This Taylor series expansion, also called local expansion, is applied to compute the field on the elements, which is caused by elements in the far-field.

The FMM algorithm starts at the finest octree level, the level with the smallest cubes. There the sources on each element are replaced by equivalent multipoles in the centre of the cube. The multipoles are coefficients of the so-called multipole expansions

$$u(\mathbf{r}) = \frac{1}{4\pi\epsilon_0} \sum_{n=0}^L \sum_{m=-n}^n \frac{1}{r^{n+1}} Y_n^m(\theta, \varphi) M_n^m. \quad (6)$$

The multipole coefficients are calculated directly from the source distribution on the elements, e. g. from surface charge densities in an indirect formulation

$$M_n^m = \int_A \sigma(\mathbf{r}') r'^m Y_n^{-m}(\theta', \varphi') dA'. \quad (7)$$

The potential caused by surface charge densities is a single-layer potential. In the context of a direct BEM formulation double-layer potentials of the form

$$u(\mathbf{r}) = \frac{1}{4\pi\epsilon_0} \int_A \tau(\mathbf{r}') \nabla_{\mathbf{r}'} \cdot \frac{1}{|\mathbf{r} - \mathbf{r}'|} \cdot \mathbf{n}' dA' \quad (8)$$

must be evaluated, too. Then eqn. (7) is modified Buchau *et al* [7]

$$M_n^m = \int_A \tau(\mathbf{r}') \mathbf{n}(\mathbf{r}') \cdot \nabla_{\mathbf{r}'} (r'^m Y_n^{-m}(\theta', \varphi')) dA'. \quad (9)$$

In total only one set of multipole coefficients is obtained for both single- and double-layer potentials.

In the next step the multipole coefficients at the next coarser level $l-1$ are computed from the multipole coefficients at level l . For this purpose the origin of the multipole expansion of a cube at level l is shifted to the centre of its parent



cube at level $l - 1$. The multipole expansion of a cube is obtained by a conversion of all its child cubes multipole expansions.

To compute the field inside a cube the counterpart of the multipole expansion, the local expansion,

$$u(\mathbf{r}) = \frac{1}{4\pi\epsilon_0} \sum_{n=0}^L \sum_{m=-n}^n r^n Y_n^m(\theta, \varphi) L_n^m. \quad (10)$$

is applied. The local coefficients are obtained from the multipole coefficients of the cubes in the far-field. The conversion of multipole coefficients into local coefficients is performed at different levels of subdivision. At a coarse level of subdivision the cubes are relatively large. That means the multipole coefficients of a large group of elements are transformed with a single set of operations into local coefficients of a large group of elements. At a fine level of subdivision, which consists of small cubes, the same is done for small groups of elements. The local coefficients can be converted between different levels of subdivision similar to the conversion of multipole coefficients. This hierarchical scheme reduces the computational costs and the memory requirements for the compressed BEM matrix to approximately $O(N)$.

Finally the local expansion eqn. (10) is evaluated in each cube at the finest level of subdivision. The potential is obtained from the classical local expansion eqn. (10). The electric field strength can be calculated from the potential

$$\mathbf{E}(\mathbf{r}) = -\nabla u(\mathbf{r}). \quad (11)$$

One approach to compute the electric field strength with help of the local expansion in eqn. (8) is to differentiate the potential numerically Nabors and White [8]. Since this causes some numerical difficulties concerning accuracy and stability we decided to differentiate eqn. (8) analytically Buchau and Rucker [9]

$$\mathbf{E}(\mathbf{r}) = -\frac{1}{4\pi\epsilon_0} \sum_{n=1}^L \sum_{m=-n}^n \nabla(r^n Y_n^m(\theta, \varphi)) L_n^m. \quad (12)$$

The derivatives of spherical harmonics Y in eqn. (9) and in eqn. (12) are discussed in detail in Buchau and Rucker [9]. Since in the FMM for given angles θ and φ spherical harmonics are normally needed for all combinations of n and m , it is advisable to compute the numerical values of spherical harmonics with help of recurrence relations Hobson [10].

The most time consuming part in the FMM algorithm is the conversion of a multipole expansion into a local expansion. A classical approach for this transformation is of $O(L^4)$. A modified transformation reduces the computational costs significantly. Approaches for an $O(L^3)$ or an $O(L^2)$ method can be found in Cheng *et al* [11]. In the context of BEM computations the proposed $O(L^3)$ method resulted in the shortest CPU times Buchau *et al* [7]. There only transformations in z -directions are evaluated. That means the coordinate system is rotated before the actual transformation and rotated back after the transformation. The transformation of spherical harmonics under a rotation of the coordinate system is discussed in detail e. g. by Biedenharn and Louck [12].



4 Numerical results

We consider two electrostatic examples. The first example is an experiment in high voltage techniques to investigate conducting particles in gas insulated high voltage systems. In the second examples a static current flow field inside a conductor is examined. Both examples are numerically solved with a FMBEM. The surfaces are discretized with eight-noded second order quadrilateral elements and the Galerkin method is applied to obtain a system of linear equations. The problems were solved on an Intel Pentium 4 PC with a clock frequency of 3.0 GHz.

4.1 Gas insulated high voltage system

The electrode configuration depicted in fig. 1 is used to investigate the influence of a conducting particle inside a gas insulated high voltage system. The lower large electrode is grounded and the upper large electrode is set to a potential of 100 kV. Between both electrodes two dielectric spacers are mounted. At the surface of each dielectric spacer a small conducting particle is affixed. The particles are simulated by long cylindrical needles (fig. 2). For a numerical solution a potential of the needles of 30 kV and 40 kV was assumed.

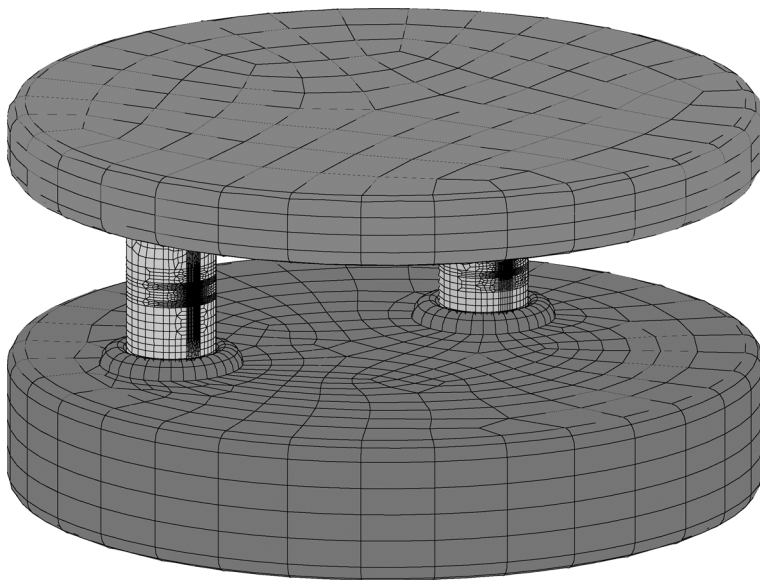


Figure 1: Discretized electrode configuration to investigate the influence of conducting particles in a gas insulated high voltage system.

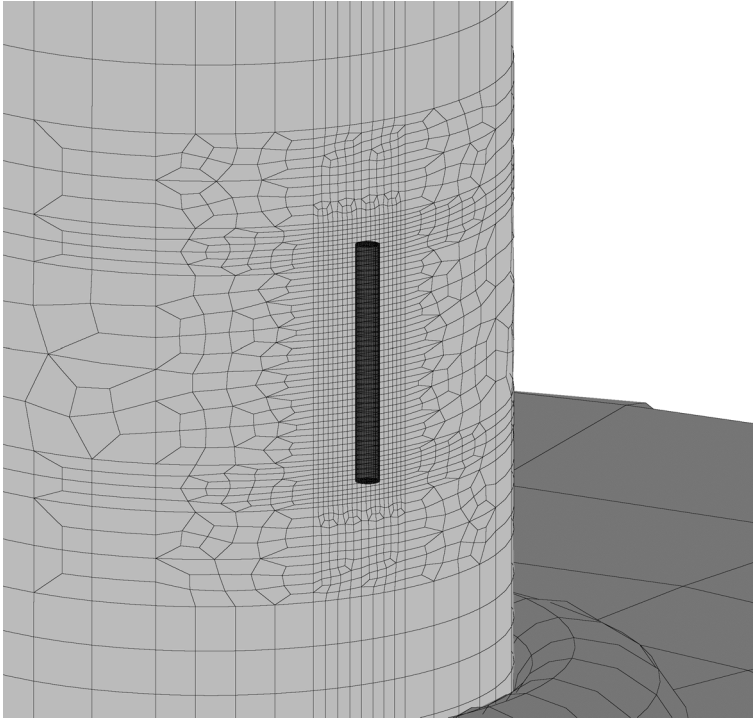


Figure 2: Cylindrical needle at the surface of a dielectric spacer, detail of fig. 1.

An indirect BEM formulation based on surface charge densities was applied. All surfaces are discretized with 9529 quadrilateral elements. To reduce the number of unknowns an adaptive mesh as depicted in fig. 1 and fig. 2 was used.

For the FMM an octree with 14 levels of subdivision was created in 2 s. In total a system of linear equations with 28855 unknowns had to be solved. The assembly of the near-field matrix took 9 minutes and 30 seconds. GMRES converged after 178 iteration steps with a residual smaller than 10^{-7} . The solution of the system of linear equations took 21 minutes and 25 seconds. The memory requirements for the system matrix were reduced from 6.2 GByte to 305 MByte. This corresponds to a compression rate for the matrix of 95 %. The field in 226752 evaluation points was computed in 161 seconds.

The influence of the particles can be seen very clearly in fig. 3. The normally relative homogeneous field between the electrodes is disturbed significantly. The density of the equipotential surfaces at the end caps of the needles is very high. That means the electric field strength is there very large. The influence of the needles to the electric field strength is shown in fig. 4. Without the needles the z -component would be constant and the other two components would vanish.

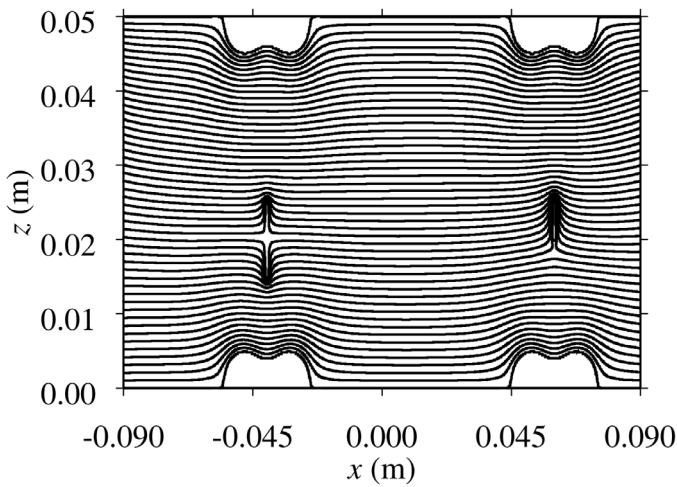


Figure 3: Equipotential surfaces between the electrodes.

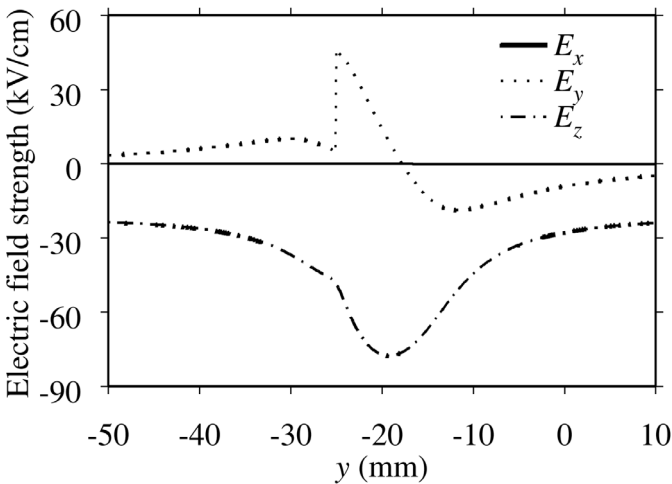


Figure 4: Electric field strength on a line very close above the right needle.



4.2 Steady current flow field problem

A detailed knowledge about electric currents inside conductors is of large interest e. g. in fabrication of resistors with a very accurate resistance. There thin film resistors are calibrated by laser cuts.

In this numerical example a simple model of a conducting path on a printed circuit board is considered (fig. 5). Potentials of 1 V, 0.2 V, and -1 V are impressed at the three ports of the conductor. For a numerical solution of the potential distribution inside the conductor a direct BEM formulation based on Green's theorem is applied. At the ports of the conductor the given potential is a Dirichlet boundary condition. At the remaining surfaces a Neumann boundary condition is set, since an electric current cannot flow out of the conductor.

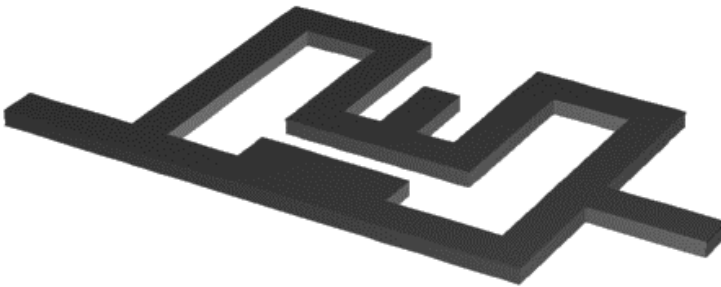


Figure 5: Model of a conducting path on a printed circuit board.



Figure 6: Potential distribution inside the conducting path of fig. 5, the potential difference between two equipotential lines is 0.1 V and the space between the two lines is coloured alternately.

The surface of the conductor was discretized with 9120 second order, quadrilateral element. This leads to a system of linear equations with 11244



unknowns. GMRES converged after 160 iteration steps in 9 minutes and 51 seconds. The assembling of the near-field matrix took 2 minutes and 46 seconds. The potential inside the conductor was computed in 49 seconds in 17220 evaluation points and is depicted in fig. 6. The matrix of the linear system of equations was compressed from originally 965 MByte to 113 MByte. This corresponds to a compression rate of 88 %.

5 Conclusion

A BEM with direct and indirect formulations was applied to the solution of electrostatic field problems. The fully populated matrix was compressed by the fast multipole method. The numerical examples show the efficiency of a BEM in combination with a compression technique. Already for relative small problems high compression rates are obtained. Therefore, computer resources are used very efficiently. Since the postprocessing is accelerated with the FMM too, the BEM becomes very attractive even for the numerical solution of large problems.

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