Technical article

Efficient Boundary Element Solutions of Electrostatic Fields Using the Fast Multipole Method

Introduction

A wide spread method for the solution of electrostatic problems is the boundary element method (BEM). The surrounding infinite space is taken into account exactly and only the surfaces of linear, isotropic media have to be discretized. To overcome the full populated matrix of the resulting system of linear equations fast and efficient methods like the fast multipole method (FMM) [1] can be used. When assembling the system matrix or postprocessing the solved problem, singular or nearly singular integrals must be computed. To calculate these integrals with a high accuracy efficient integration techniques were developed [2, 3]. The focus of this paper is on direct and indirect boundary element formulations and their application to the solution of electrostatic problems. Especially the efficient solution of the system of linear equations and the fast postprocessing using the fast multipole method is considered.

Direct and indirect boundary element formulations

Boundary element formulations can be summarized into two formulations, the direct and the indirect method [4]. A main property of the direct method is, that the potential in an arbitrary evaluation point inside a domain is calculated from its values and normal derivatives on the boundary of the domain. In contrast to this in the indirect method the potential in an arbitrary evaluation point is obtained from sources on the boundary, which are charges in the case of electrostatic problems.

Normally the direct method is based on Green's theorem, which must be modified for evaluation points on the boundary

$$c(\boldsymbol{r})u(\boldsymbol{r}) = \oint_A \frac{\partial u(\boldsymbol{r}')}{\partial n'} \frac{1}{|\boldsymbol{r}-\boldsymbol{r}'|} \mathrm{d}A' - \oint_A u(\boldsymbol{r}') \frac{\partial}{\partial n'} \frac{1}{|\boldsymbol{r}-\boldsymbol{r}'|} \mathrm{d}A' . \quad (1)$$

The so-called singularity coefficient $c(\boldsymbol{r})$ becomes 2π on a smooth boundary [4]. Actually (1) can only be applied to closed domains, but the surrounding infinite space can be treated as a closed domain, too, since the boundary in infinity makes no contribution to the integrals in (1) [5].

As mentioned above in the indirect method the potential in an arbitrary evaluation point is computed from the surface charge densities $\sigma(\boldsymbol{r})$ on the boundaries

$$u(\boldsymbol{r}) = \frac{1}{4\pi\varepsilon_0} \int_A \frac{\sigma(\boldsymbol{r}')}{|\boldsymbol{r}-\boldsymbol{r}'|} \mathrm{d}A' . \quad (2)$$

In contrast to the direct method, when applying (2) no distinction between different domains is necessary, that means for each evaluation point the integration has to be performed over all surface charge densities.

Description of the problem and discretization

A general electrostatic problem consists of conductors embedded into multiple dielectrics (Fig. 1). It is assumed, that the linear and isotropic dielectrics are piecewise homogeneous. The conductors' potential can be known or can be left unknown.

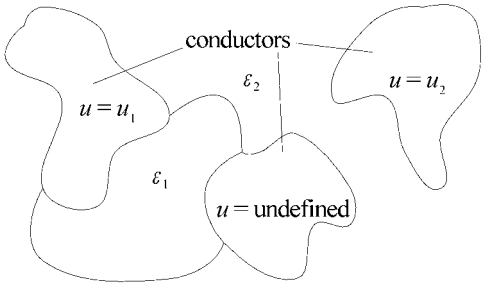

Fig. 1 Conductors embedded in multiple, piecewise homogeneous dielectrics

In the case of piecewise homogeneous, isotropic and linear dielectrics, it suffices to describe the dielectrics with boundary values. That means only the surfaces of the dielectrics and the conductors must be discretized and the boundary element method can be used. Commonly used surface elements are triangular and quadrilateral elements with Lagrangian polynomials for the interpolation between the nodes of the elements, the so-called shape functions $N_i(\boldsymbol{r})$. The usage of linear polynomials simplifies the numerical treatment but on the other hand a relative large number of elements is needed for a good approximation of geometry and sources. Therefore often second order elements are preferred.

Conventional solution of the problem

To numerically solve an electrostatic problem with the boundary element method the collocation or the Galerkin method can be used. Assembling the system of linear equations is relative simple, when the collocation method is applied, but often the Galerkin method is more suitable. Not only the number of elements can be reduced to obtain a comparable accuracy as the collocation method, but also numerical problems at the computation of the singularity coefficients or of the normal component of the electric field in corners or on edges are overcome.

Firstly the assembly of the system of linear equations for the indirect method is described. On the surfaces of the conductors a Dirichlet boundary condition, the known potential, must be fulfilled and (2) can be discretized

$$\int_{A_i} N_i(\boldsymbol{r}) u(\boldsymbol{r}) \mathrm{d}A = \frac{1}{4\pi\varepsilon_0} \sum_j \sigma_j \int_{A_i} N_i(\boldsymbol{r}) \int_{A_j} \frac{N_j(\boldsymbol{r}')}{|\boldsymbol{r}-\boldsymbol{r}'|} \mathrm{d}A' \mathrm{d}A \,, \quad (3)$$

where i is a node on the conductor and the summation over j must be performed over all nodes. On a surface between two dielectrics the normal component of the dielectric displacement is continuous, what can be formulated as Neumann boundary condition. The corresponding integral equation is

$$\begin{aligned} &\frac{\varepsilon_2-\varepsilon_1}{(\varepsilon_2+\varepsilon_1)4\pi\varepsilon_0} \sum_j \sigma_j \int_{A_i} N_i(\boldsymbol{r}) \int_{A_j} N_j(\boldsymbol{r}') \frac{(\boldsymbol{r}-\boldsymbol{r}')\cdot\boldsymbol{n}}{|\boldsymbol{r}-\boldsymbol{r}'|^3} \mathrm{d}A' \mathrm{d}A \\ &+ \frac{1}{2\varepsilon_0} \sum_s \sigma_s \int_{A_i} N_i(\boldsymbol{r}) N_s(\boldsymbol{r}) \mathrm{d}A = 0 \end{aligned} \quad .(4)$$

Computing the integrations in (3) or in (4) the surfaces A_i and A_j coincide for $i=j$ and the integrand becomes singular. In both cases the integrals are weakly singular [5]. Singular integrals cannot be calculated with standard Gaussian quradrature techniques, instead improved integration methods are needed. An approach for the efficient and accurate integration of weakly singular integrals is, to perform a coordinate transformation. The singular point is then the origin of a cylindrical coordinate system. A consequence of that coordinate transformation is the resulting Jacobian, which regularizes the singularity. If the surface A_i is close to the surface A_j the integral in (4) becomes nearly strong singular. Then additionally to the coordinate transformation a Taylor's series expansion of the integrand must be calculated to regularize the integral [2, 3].

When the direct method is applied, the assembly of the system matrix is more complicated. A distinction between different domains is necessary. Furthermore the different domains must be coupled on their boundaries. The basic integral equation applying Galerkin method has the form

$$\begin{aligned} &\sum_j \left(\frac{\partial u}{\partial n}\right)_j \int_{A_i} N_i \int_{A_j} N_j \frac{1}{|\boldsymbol{r}-\boldsymbol{r}'|} \mathrm{d}A' \mathrm{d}A \\ &= 2\pi u_i \int_{A_i} N_i \mathrm{d}A + \sum_j u_j \int_{A_i} N_i \int_{A_j} N_j \frac{\partial}{\partial n'} \frac{1}{|\boldsymbol{r}-\boldsymbol{r}'|} \mathrm{d}A' \mathrm{d}A \end{aligned} \quad . \quad (5)$$

Depending on the known boundary conditions the left and right hand side of the system of linear equations are varying. Two domains are coupled by replacing the boundary values of the potential and its normal derivative of one domain by the corresponding values of the other domain.

LU-decomposition is a direct solver for the system of linear equations for both the direct and the indirect method. An advantage of such a solver is, that the system matrix is inverted once and can then be applied to several right hand sides. However the computational costs are of $O(N^3)$, where N is the number of unknowns. A preconditioned iterative solver reduces the computational costs to approximately $O(N^2)$. In most cases the problem size is limited by the needed memory for the matrix storage, since the memory requirements are of $O(N^2)$.

Efficient solution of the problem

To reduce the memory requirements of the full populated system matrix fast methods like the fast multipole method are applied. Additionally these fast methods also reduce the computational costs. However then the usage of an iterative solver is required, but this is not a restriction. In the following the fast multipole method is exemplary described for the indirect method.

In each iteration step the product of the system matrix with the current solution, which corresponds to the current surface charge density, is computed

$$\{y\} = [A]\{x\} \,, \quad (6)$$

where it's not necessary to store the matrix $[A]$ explicitly.

A truncated series expansion of Green's function in spherical harmonics

$$\frac{1}{|\boldsymbol{r}-\boldsymbol{r}'|} = \begin{cases} \sum_{n=0}^{L} \sum_{m=-n}^{n} \frac{r^n}{r'^{n+1}} Y_n^m(\vartheta,\varphi) Y_n^{-m}(\vartheta',\varphi'), & r < r' \\ \sum_{n=0}^{L} \sum_{m=-n}^{n} \frac{r'^n}{r^{n+1}} Y_n^m(\vartheta,\varphi) Y_n^{-m}(\vartheta',\varphi'), & r' < r \end{cases} \quad (7)$$

is the basis of the fast multipole method, where $Y_n^m(\vartheta,\varphi)$ are normalized spherical harmonics [1]. When (7) is applied, a strict distinction between the source domain and the domain with the evaluation points is required. Since spherical coordinates are used, these domains are described by spheres. Before the interactions between the elements can be computed, all elements are arranged in a hierarchical grouping scheme. In the first step of the multipole algorithm the surface charge densities on the elements are replaced by equivalent multipoles in the domains. The interactions between domains far from each other are calculated for large domains and only for domains lying close to each other the interactions are computed for small domains. If the distance between two elements is too small for the application of (7), conventional integrations (3) or (4) are evaluated. This hierarchical algorithm reduces the memory requirements and the computational cost to approximately $O(N)$ and with it very large problems can be solved [6].

An alternative method to the fast multipole method is the adaptive cross approximation technique (ACA) [7], there the matrix is approximated by low rank matrices. This reduces the computational costs and the memory requirements for the system matrix to approximately $O(N)$, too. An advantage of the ACA is, that it can be applied easily to different kernels of integral equations.

Postprocessing

After the solution of the system of linear equations the potential or the electric field in an arbitrary point is computed by integrating over all surface charge densities

$$u(\boldsymbol{r}) = \frac{1}{4\pi\varepsilon_0} \sum_j \sigma_j \int_{A_j} \frac{N_j(\boldsymbol{r}')}{|\boldsymbol{r} - \boldsymbol{r}'|} \mathrm{d}A' \tag{8}$$

and

$$\boldsymbol{E}(\boldsymbol{r}) = \frac{1}{4\pi\varepsilon_0} \sum_j \sigma_j \int_{A_j} N_j(\boldsymbol{r}') \frac{\boldsymbol{r} - \boldsymbol{r}'}{|\boldsymbol{r} - \boldsymbol{r}'|^3} \mathrm{d}A' . \tag{9}$$

If the direct method is used, surface integrals over the boundary values of the considered domain have to be calculated

$$\begin{aligned} u(\boldsymbol{r}) = & \frac{1}{4\pi} \sum_j \left(\frac{\partial u}{\partial n} \right)_j \int_{A_j} N_j \frac{1}{|\boldsymbol{r} - \boldsymbol{r}'|} \mathrm{d}A' \\ & - \frac{1}{4\pi} \sum_j u_j \int_{A_j} N_j \frac{\partial}{\partial n'} \frac{1}{|\boldsymbol{r} - \boldsymbol{r}'|} \mathrm{d}A' \end{aligned} . \tag{10}$$

For large problems with a large number of elements the evaluation of (8), (9) or (10) can be very time consuming, especially when the field in many evaluation points is calculated. To reduce the computational costs, the fast multipole method can be applied, as well [8].

Numerical Examples

All presented examples were computed on a Digital AlphaServer 1200 5/533 with 2 GByte memory. A commercial meshing tool was used for the discretization of the surfaces with eight-noded quadrilateral second order elements. The system of linear equations is obtained by the application of the Galerkin method and solved with GMRES and a Jacobi preconditioner [9]. The accuracy of the residual in GMRES is set to 10^{-7}.

The first example consists of two electrodes (Fig. 2). One of the electrodes is coated with a dielectric with $\varepsilon_r = 10$. The potential of the coated electrode is 1 V and the potential of the other electrode –1 V. For a numerical solution of the problem, the surfaces are discretized with 4068 elements.

The application of the indirect method leads to a system of linear equations with 12210 unknowns. The storage of the complete full populated system matrix would require 1137 MByte. Computing the matrix-vector-product with the fast multipole method this can be reduced to 156 MByte. The iterative solver converged after 106 iteration steps in 6408 s. For the calculation of the potential in 401 evaluation points along an axis through the dielectric and the small air gap between the electrodes only 5.8 s are required (Fig. 3). The problem can be solved with the direct method, too. Then a system of linear equations with 16280 unknowns is solved in 28334 s after 179 iteration steps. The memory requirements are 244 MByte. In Fig. 3 the potential in the dielectric and the air gap is depicted.

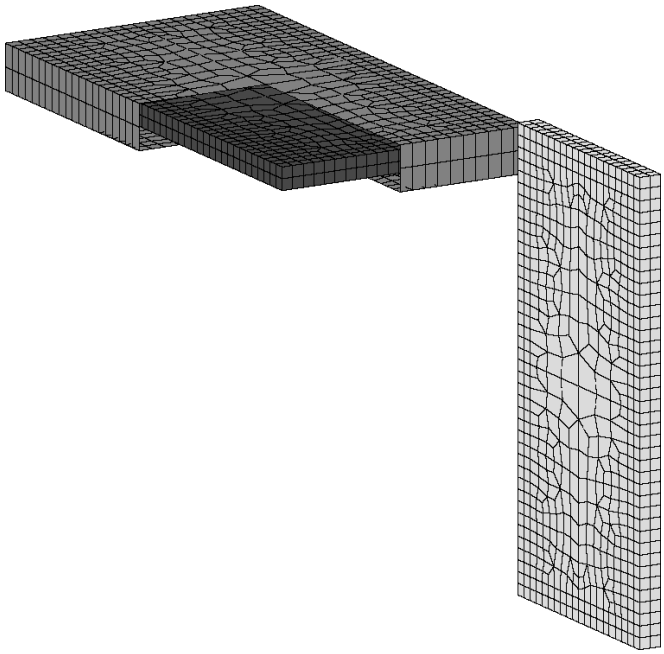

Fig. 2 Example with two electrodes, one electrode is coated with a dielectric

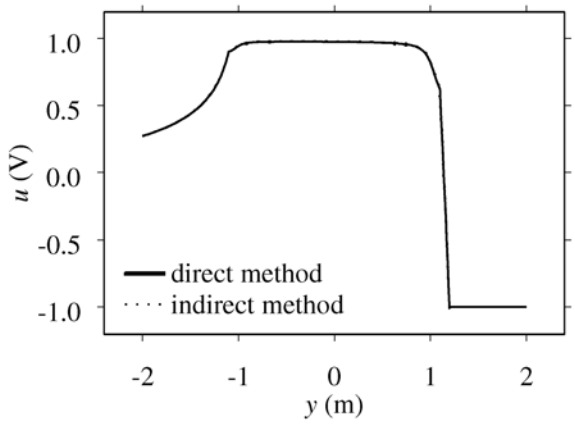

Fig. 3 Potential obtained with the indirect and the direct method in the dielectric and the air gap

As second example a model of a chip with ten pins connected to conducting paths on a printed circuit board is investigated (Fig. 4). When considering such configurations, derived field variable like the capacitance coefficients are of large interest. In this example the capacitance between the conductor, which consists of pin 1 and its conducting path, and the conductor, which is composed of pin 7 and its conducting path, is examined. All other conductors and the backside of the printed circuit board are connected together and treated as one conductor.

Since the pins of the chip are modeled as thin conductors, the indirect method is preferred for the solution of the problem. Very time consuming in this context is the computation of the free surface charge densities on the conductors from the sum of all charges, which are obtained as solution of the system of linear equations. But the applica-

tion of the fast multipole method brings the computational costs down to an acceptable level.

Discretizing the problem with 6448 elements leads to a system of linear equations with 20964 unknowns. The whole problem is solved after 24657 s and the memory requirements are 195 MByte. With this relative coarse discretization of the conductors a capacitance of 1.631 fF and 1.623 fF respectively between the examined pins is achieved.

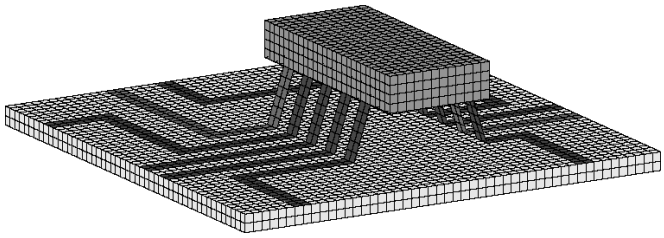

Fig. 4 Chip connected to a printed circuit board

In the third example a typical arrangement of electrodes in high voltage technique is considered. Often in high voltage systems a small conducting particle is lying on the dielectric insulators between the electrodes. If the particle is small enough, it will not disturb the operation of the system. But for long thin particles the electric field strength near the particle is too large and a breakdown will occur.

The examined experiment consists of two electrodes with a voltage of 100 kV between them (Fig. 5). To simulate the particle long needles with a small diameter are used and positioned on dielectric spacers (Fig. 6).

Near the ends of the particles high electric field strengths are expected. That's why the particle and the surrounding of the particle is fine meshed. For the rest of the problem a coarse mesh suffices. In whole the problem is discretized with 9529 elements. The system of linear equations with 28857 unknowns is solved in 41663 s after 240 iteration steps. Note, that without a preconditioner the iterative solver wouldn't converge.

Since a problem oriented mesh was used and the size of the elements is extremely varying, the memory requirements are larger than it's usual for problems with about 30000 unknowns. In this case 932 MByte were needed, of which 760 MByte are caused by the near-field matrix.

A consequence of the high electric field strength near the particle is, that the surface charge densities near the particle vary extremely (Fig. 7). Additionally it can be seen, that at the end of the particle the high surface charge density on the spacer can also be found on the half of the neighboring elements, since the elements have common nodes. To compute reliable and meaningful values for the electric field, an axis 0.6 mm above the particle was chosen for the evaluation points. As expected near the particle high electric field strengths are obtained (Fig. 8).

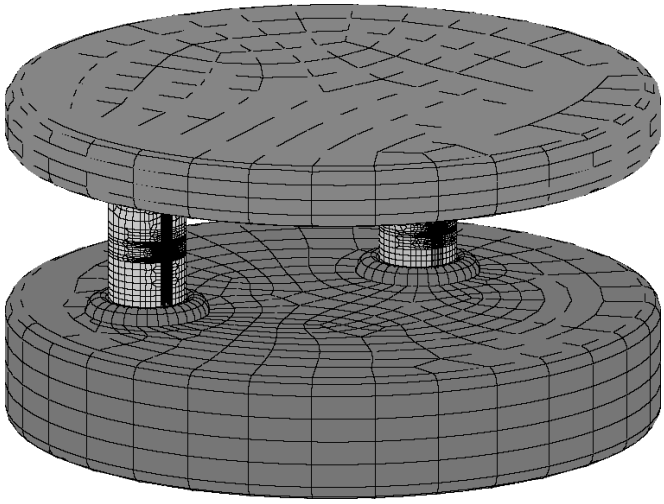

Fig. 5 Experiment in high voltage technique for the simulation of a breakdown caused by conduction particles on dielectric spacers

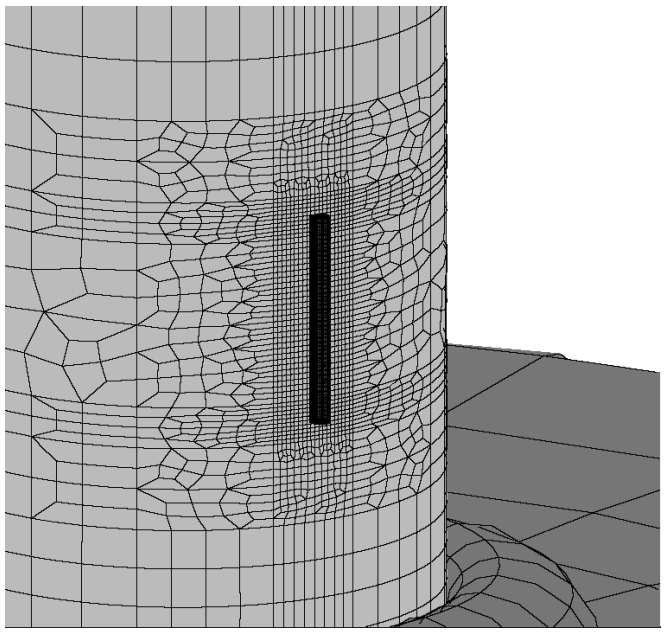

Fig. 6 Detail of Fig. 5, conducting particle on a spacer

In order to show the capability of the fast multipole method for the postprocessing the potential in 226151 evaluation points was computed (Fig. 9). This computation took 4323 s, what is larger than expected, too. The grid of the evaluation points is relative fine and many elements are relative large, so a large number of near-field interactions must be computed.

For comparison reasons the same problem was discretized with 30989 elements, but a more homogeneous mesh was used, especially the large electrodes are finer meshed. Then a system of linear equations with 93409 unknowns must be solved. The memory requirements are 1.2 GByte, of which 865 MByte are needed for the near-field matrix. The problem was solved in 86385 s after 290 iteration steps and the computation of the potential took only 1062 s, since more interactions could be computed with far-field interactions.

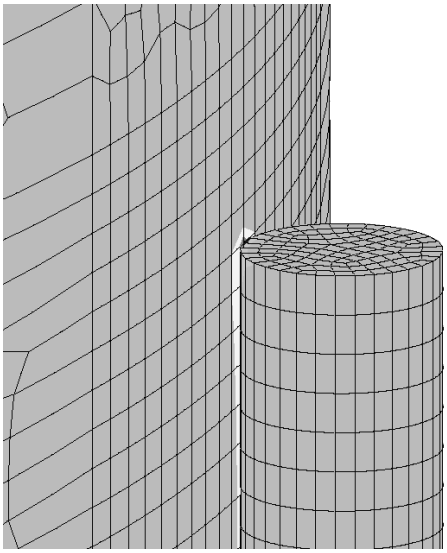

Fig. 7 Surface charge densities in the surrounding of the end of the left particle

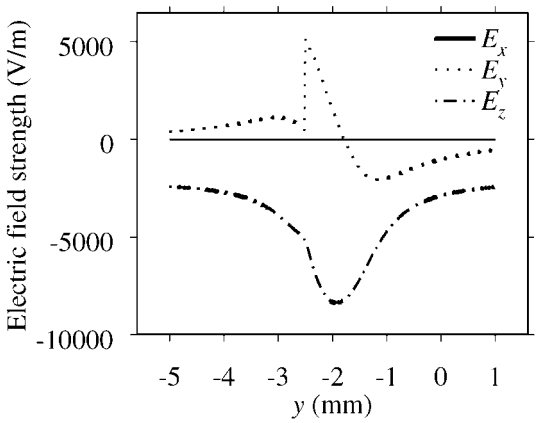

Fig. 8 Electric field strength 0.6 mm above the particle

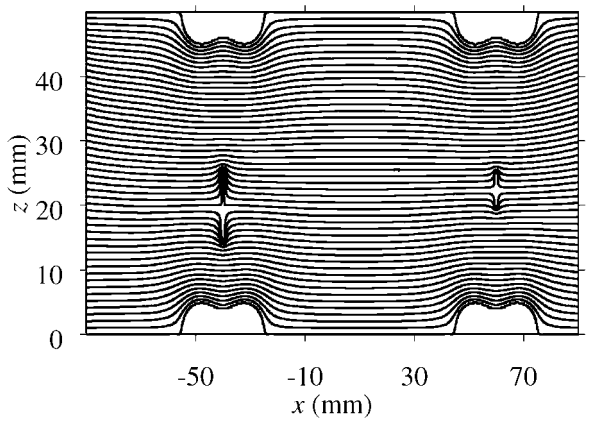

Fig. 9 Potential between the electrodes

Conclusions

Examining electrostatic problems with linear, piecewise homogeneous media the boundary element method is very attractive. Only the surfaces have to be discretized and the surrounding infinite space is taken into account exactly. In combination with an efficient method like the fast multipole method large problems can be solved on a small computer, since the memory requirements and the computational costs are only approximately proportional to the number of unknowns. The computation of field variables, even in a large number of evaluation points, can be done efficiently with the fast multipole method.

Of course, the boundary element method and the fast multipole method can also be applied to non-linear magnetostatic or eddy current problems. Then it's a good choice to couple the boundary element method with the finite element method, especially when moving bodies are considered. In the field of electromagnetic scattering problems the boundary element method in combination with the fast multipole method is applies very successfully for many years.

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