3-D electromagnetic scattering analysis of electrically large dielectric objects using MLFMA

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Abstract — **In this contribution we use the volume integral equation (VIE) to model the full-wave electromagnetic scattering from 3-D inhomogeneous dielectric objects. To reduce the computational cost and memory requirements the multilevel fast multipole algorithm (MLFMA) is used. For the geometries, typically encountered in inverse problems, this is an $\mathcal{O}(N)$-method, N being the number of unknowns. However, additional efforts are to be made to reduce the rather large prefactor. This method may be a more flexible and competitive alternative to the FFT methods.**

1 INTRODUCTION

The first step in solving an inverse scattering problem, in our case a complex permittivity reconstruction, is the choice of a forward-modeling method. Since we do not want to make any sacrifices concerning accuracy, we choose to take the full physics of the electromagnetic scattering from inhomogeneous dielectric objects into account, by using the volume integral equation (VIE). To handle the VIE numerically, we can discretize it with a classical method of moments (MoM). The inverse problem is solved by means of a non-linear optimization technique which leaves us two options. We can either solve a forward problem in every iteration (when the cost function is expressed in terms of the dielectric contrast only [1]) either use the relation between contrast and fields as a constraint in the optimization with respect to both fields and contrasts [2]. Either way the VIE has to be imposed several times and since we discretized it, this comes down to performing a lot of matrix-vector products.

If this matrix-vector product is carried out with a full matrix, this requires $\mathcal{O}(N^2)$ operations. To store the matrix we need $\mathcal{O}(N^2)$ memory. This is too expensive for large problems. The conjugate gradient fast Fourier transform method (CG-FFT) [3] is often used to overcome this burden. This method uses a uniform grid with cuboidal cells to model the object and then exploits the Toeplitz property of the interaction matrix by performing the matrix-vector product with a 3-D FFT. Also there is no need to store the full matrix. This reduces the computational complexity to $\mathcal{O}(NlogN)$ and the memory use to $\mathcal{O}(N)$.

The FFT methods use the fact that the Green's function is in fact a convolution operator. Beyond this, however, no physical information contained in this Green's function is exploited. Fast multipole methods (FMM)[4] on the other hand use physical information to a large extent to reduce the cost of calculating fields radiated by certain sources in remote observation points. For dense volume scatterers (e.g. a quasi-equilateral cuboid), this leads to an $\mathcal{O}(N)$-algorithm both in computational complexity as in memory use.

In the following sections we adress the integral formulation of the scattering problem and give a brief description of the MLFMA. Next we consider some extra modifications to reduce the prefactor. Finally we present a numerical validation and some further remarks.

2 FORMULATION

The problem will be formulated in the frequency domain and the time factor $e^{j\omega t}$ will be suppressed.

2.1 Formulation of the VIE

We consider an inhomogeneous dielectric object with complex permittivity $\epsilon(\mathbf{r})$ and permeability μ_0 that is situated in an infinite homogeneous background medium with parameters ϵ_0 and μ_0, which we will denote as free space. The incident electric field $\mathbf{e}^i(\mathbf{r})$ is defined as the field in absence of the object. Using the equivalence principle, we replace the dielectric object by a contrast current distribution in free space

$$\mathbf{J}(\mathbf{r}) = j\omega\frac{\epsilon(\mathbf{r}) - \epsilon_0}{\epsilon(\mathbf{r})}\mathbf{d}(\mathbf{r}) = j\omega\chi(\mathbf{r})\mathbf{d}(\mathbf{r}). \quad (1)$$

Here $\mathbf{d}$ is the electric flux density. $\chi(\mathbf{r})$ will be called the contrast function. The contrast charge ρ is given by $\rho = -\frac{1}{j\omega}\nabla\cdot\mathbf{J} = -\nabla\chi\cdot\mathbf{d} - \chi\nabla\cdot\mathbf{d}$. We now can write the volume integral equation:

$$\mathbf{e}^i(\mathbf{r}) = \frac{\mathbf{d}(\mathbf{r})}{\epsilon(\mathbf{r})} - \mathbf{e}^s(\mathbf{r}), \quad (2)$$

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where $\mathbf{e}^s$ is the scattered field, given by:

$$\mathbf{e}^s(\mathbf{r}) = -j\omega\mu_0 \int \bar{\bar{G}}(\mathbf{r}-\mathbf{r}') \cdot \mathbf{J}(\mathbf{r}')\mathrm{d}V'. \quad (3)$$

$\bar{\bar{G}}$ is the Green's tensor

$$\bar{\bar{G}}(\mathbf{r}-\mathbf{r}') = (\bar{\mathbf{I}} - \frac{1}{k_0^2}\nabla\nabla)\left(\frac{e^{-jk_0|\mathbf{r}-\mathbf{r}'|}}{4\pi \mid \mathbf{r}-\mathbf{r}' \mid}\right), \quad (4)$$

in which $k_0 = \omega\sqrt{\epsilon_0\mu_0}$ is the wavenumber of free space. Equation (2) states that the incident electric field is the difference between the total electric field and the field generated by the contrast currents only, the so-called scattered field.

2.2 Discretization of the VIE

In order to solve (2) numerically, we have to choose a mesh to model the scatterer and a type of basisfunction to represent the unknown field. The MLFMA can be used on all sorts of basis functions with limited support, so the choice of mesh type is completely free. Suppose we have defined a mesh and have chosen a set of (vectorial) basis functions, the n-th of which we will denote as $\mathbf{f}_n$. On a tetrahedral mesh we could for instance take the Schaubert-Wilton-Glisson basis functions. We then write

$$\mathbf{d}(\mathbf{r}) = \sum_{n=1}^{N} D_n \mathbf{f}_n(\mathbf{r}), \quad (5)$$

where N is the number of unknowns. Furthermore we take the contrast function χ to be constant over each mesh element.

By substituting (5) into (2) and applying Galerkin testing, we arrive at a set of N lineair equations.

2.2.1 MLFMA

Since in classical MoM we have to calculate the interactions between each pair of basis functions, we end up with an $\mathcal{O}(N^2)$ algorithm if we solve the system iteratively. The fast multipole method (FMM) only considers interactions between groups of basis functions and reduces the computational cost of the matrix-vector product.

The basis of FMM is formed by the following expansion of the Green's tensor [4]:

$$\bar{\bar{G}}(\mathbf{r}-\mathbf{r}') \approx \frac{-jk_0}{(4\pi)^2}\int \mathrm{d}\hat{k} e^{-j\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}_\lambda)} T_{\lambda\lambda'}(\hat{k})(\bar{\bar{I}}-\hat{k}\hat{k}) e^{j\mathbf{k}\cdot(\mathbf{r}'-\mathbf{r}_{\lambda'})}, \quad (6)$$

where $\mathbf{k} = k_0\hat{k}$ and where

$$T_{\lambda\lambda'}(\hat{k}) = \sum_{l=0}^{L}(-j)^l(2l+1)h_l^{(2)}(k_0 r_{\lambda\lambda'})P_l(\hat{k}\cdot\hat{r}_{\lambda\lambda'}) \quad (7)$$

is called the translation operator. The approximation in (6) is caused by the truncation of the series in (7). $h_l^{(2)}$ is the spherical Hankel function of the second kind, P_l is the Legendre function of order l and $\mathbf{r}_{\lambda\lambda'} = \mathbf{r}_\lambda - \mathbf{r}_{\lambda'}$. In addition $r_{\lambda\lambda'} > d$ with $\mathbf{d} = (\mathbf{r}-\mathbf{r}_\lambda) - (\mathbf{r}'-\mathbf{r}_{\lambda'})$. Let S_m be the support of $\mathbf{f}_m$. Using (6) we can write down the scattered field due to the current associated with $\mathbf{f}_n$ and weighted with $\mathbf{f}_m$:

$$\int_{S_m} \mathbf{f}_m \cdot \mathbf{e}_n^s \mathrm{d}V = \frac{k_0^2}{\epsilon_0} D_n \int_{S_m} \mathrm{d}V \mathbf{f}_m(\mathbf{r}) \cdot \int_{S_n} \mathrm{d}V' \chi(\mathbf{r}') \bar{\bar{G}}(\mathbf{r}-\mathbf{r}') \cdot \mathbf{f}_n^{\pm}(\mathbf{r}') = \frac{-jk_0}{(4\pi)^2}\int \mathrm{d}\hat{k} \mathbf{D}_{m,\lambda}(\hat{k}) \cdot T_{\lambda\lambda'}(\hat{k}) \mathbf{U}_{n,\lambda'}(\hat{k}), \quad (8)$$

in which

$$\mathbf{U}_{n,\lambda'} = \frac{k_0^2}{\epsilon_0} D_n \int_{S_n} \chi(\mathbf{r}') e^{j\mathbf{k}\cdot(\mathbf{r}'-\mathbf{r}_{\lambda'})}(\bar{\bar{I}} - \hat{k}\hat{k})\mathbf{f}_n \mathrm{d}V' \quad (9)$$

$$\mathbf{D}_{m,\lambda} = \int_{S_m} e^{-j\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}_\lambda)} \mathbf{f}_m \mathrm{d}V. \quad (10)$$

From (8) the principle of FMM can be seen. First we divide the basis functions into groups, for example group $G_{\lambda'}$, centered around $\mathbf{r}_{\lambda'}$. We then calculate the radiation pattern $\mathbf{U}_{\lambda'}$ of $G_{\lambda'}$ by summing the radiation patterns $\mathbf{U}_{n,\lambda'}$ for all $\mathbf{f}_n \in G_{\lambda'}$. This involves only single integrals. We then shift this pattern by multiplication with $T_{\lambda\lambda'}$ to the center $\mathbf{r}_\lambda$ of G_λ where it is projected onto the basis functions by $\mathbf{D}_{m,\lambda}$. The radiation patterns turn out to be quasi band limited, which allows us to reconstruct them using only a minimal amount of samples $\hat{k}_s$. If this procedure is repeated for every pair of groups, the number of operations is reduced compared to the calculation of every interaction between pairs of basis functions.

Unfortunately the accuracy of the expansion (6) breaks down when L grows too large. This is called the *low frequency breakdown* and therefore the used algorithm is a *high frequency* (HF) FMM. The breakdown is caused by a numerical instability when l exceeds the argument of $h_l^{(2)}$. For nearby groups this happens before the summation in (7) has converged to the desired accuracy. This means

that we still have to calculate some interactions following the classical MoM-scheme, the so-called *near interactions*. We call the groups for which we can use the expansion *well-separated*.

The FMM can be extended to a multilevel algorithm resulting in the MLFMA [4], which yields a $\mathcal{O}(N)$ computational complexity and memory use in case of dense volume scatterers.

3 REDUCTION OF THE PREFACTOR

The MLFMA has already earned its stripes in problems involving surface integral equations (SIE). Its application to the VIE, however, shows some difficulties, especially in memory use. This is due to the fact that a volume discretization results in more unknowns per FMM group than a mesh containing only surface patches. Since we look at dense volume scatterers in particular, we end up with a huge number of unknowns even for problems of moderate electrical size.

The calculation of the radiation pattern of an FMM group can be cast into a matrix operation in which we multiply the vector containing the unknowns in the group with a so-called *aggregation matrix*. Likewise the projection of the shifted patterns onto the basis functions in another group happens by multiplication with a *disaggregation matrix*. These matrices have dimensions $(N_u \times N_s)$ with N_u the number of unknowns in the group and N_s the number of samples needed to represent the radiation pattern of the group. When N_u is large, storage of the aggregation and disaggregation matrices requires a lot of memory. Also the interaction matrices between nearby groups, the *near interaction matrices*, are large memory consumers. The memory use is still assymptotically of the form cN, but the prefactor c is very large.

While the geometry of our specific problem causes these problems, it also offers a way to solve them. Indeed, since we are interested in inverse problems, most of the time we don't know the exact bounderies of the scatterers. We merely put them into a large box and discretize this box with a mesh which we suppose to be fine enough. We then can contruct this box or whatever shape we use for the inversion domain by building it from a number of identical blocks stacked in a uniform grid. These blocks are also the FMM-groups on the lowest level. Since the FMM-groups now all have exactly the same geometrical appearance, it is possible to rewrite the aggregation, disaggregation and near interaction stages using matrices which can be reused to a large extent. This reduces the prefactor of the memory use significantly.

We already mentioned the fact that the near interaction matrices tend to be large matrices. Also in a 3-D volumetric FMM there are quite a lot of near interactions per group. This makes the near interaction stage (multiplying the near interaction matrices with the corresponding vectors) the most time consuming step in the iterations. We cannot reduce the number of near interactions beyond a given point due to the breakdown of expansion (6). Therefore we reduce the workload by performing a truncated factorization on the near interaction matrices. To this end we can for instance use a singular value decomposition (SVD) or a rank-revealing QR factorization (RRQR). For both methods the error on the truncation is controllable. Suppose we factorize a $(m \times n)$-matrix A into a $(m \times k)$-matrix Q and a $(k \times n)$-matrix R, with $k < min(m, n)$. We then have a gain $(mn)/(k(m+n))$ both in storing the matrix and in the cost of multiplying it with a vector.

4 NUMERICAL VALIDATION

In this section we will present some numerical results which demonstrate the correctness and efficiency of the method. For all the examples to follow we used a tetrahedral mesh. First of all we present the time for one matrix-vector multiplication as a function of the number of unknowns in figure 1. The geometry consists of a cube, built from elementary blocks as depicted in figure 5. In this case the blocks each contain 736 unknowns. The background wavelength is taken $\lambda_0 = 2\pi$ m. To increase the number of unknowns, more blocks are used. There clearly is a cross-over point with the classical MoM around $N = 10000$ and for large N the $\mathcal{O}(N)$ behaviour sets in. In figure 2 the memory use is given for the same geometries. Clearly classical MoM would not allow simulation of problems this big on a simple PC.

Next we show the scattering from a homogeneous dielectric sphere with radius $1.5\lambda_0$ and permittivity $\epsilon = 2\epsilon_0$ in figure 3. The structure is illuminated by a plane wave $\mathbf{e}^i(\mathbf{r}) = e^{-jk_0 z}\hat{x}$. The x-component of the scattered field is measured on a semicircle with radius $r = 10\lambda_0$ in the yz-plane. We modeled the sphere by a spheroidal contrast distribution in a larger cube. Since our actual approximation to the sphere is rather spiky (figure 6), we get some discrepancy with the exact Mie-series solution. The boundaries of a cube can be modeled exactly, so we present the results for a cube with side $4\lambda_0$ in figure 4 were the comparison is made with the solution obtained with a weak form BCGS-FFT code [5],[6],[7].

It has to be noted that for the geometries con-

sidered here (which are dense volume scatterers) the FFT-method is still much faster. However, our method offers more flexibility since the scatterer (or multiple scatterers) can be modeled with an arbitrary stacking of elementary mesh blocks whereas in the FFT code, the object has to be enclosed in one large cuboidal box. One could divide this box further into smaller identical boxes to obtain the same kind of flexibility and consider the interactions between these boxes also by using FFT's. However, when two such boxes are well-separated it is advantageous to use the FMM in order to physically reduce the needed information. Currently, we are working on a further reduction of the cost of the near interaction stage. We strongly believe that the methods can be made competitive.

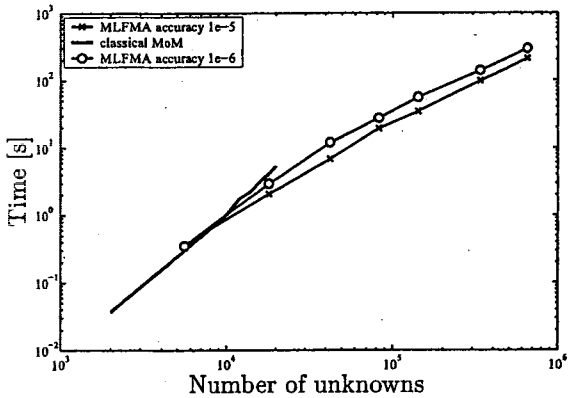

Figure 1: Time for 1 matrix-vector multiplication versus the number of unknowns. The different curves correspond to a different accuracy.

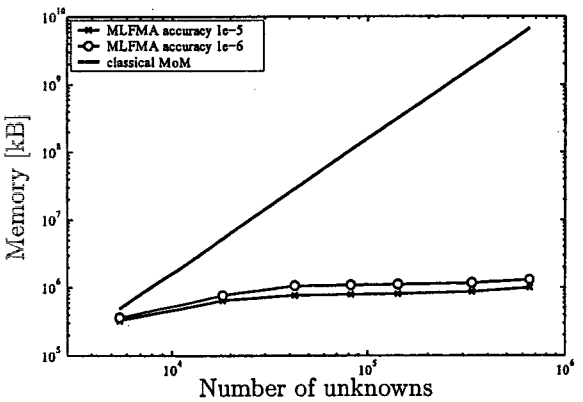

Figure 2: Memory requirements.

5 CONCLUSIONS

We have solved the VIE by using the HF MLFMA. Compared to the CG-FFT and related methods this

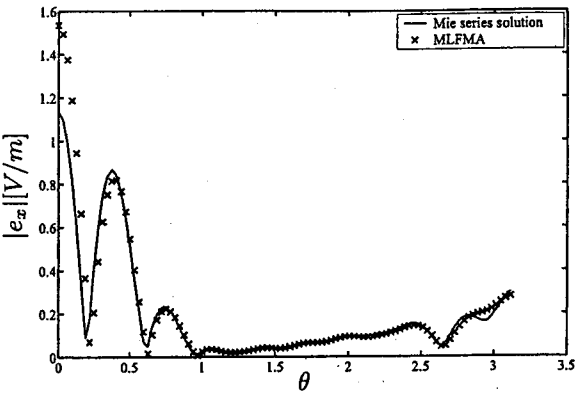

Figure 3: Scattering from the dielectric sphere of figure 6 with $\epsilon = 2\epsilon_0$: $|e_x|$ as a function of θ for $\phi = 0$ and $r = 10\lambda_0$. Comparison with Mie series.

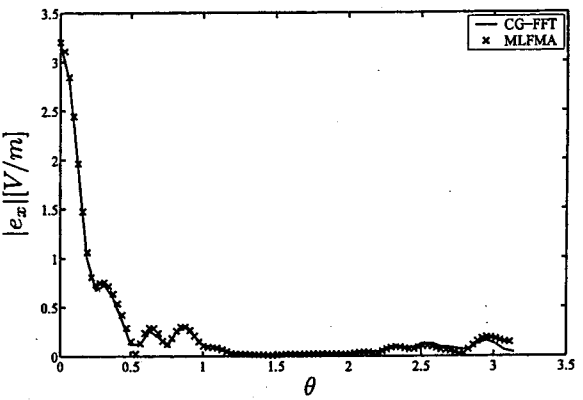

Figure 4: Scattering from a dielectric cube with $\epsilon = 2\epsilon_0$: $|e_x|$ as a function of θ for $\phi = 0$ and $r = 10\lambda_0$. Comparison with result from a Weak Form BCGS-FFT.

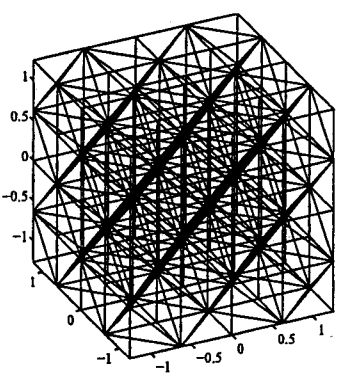

Figure 5: Elementary block of mesh. Sizes in [m].

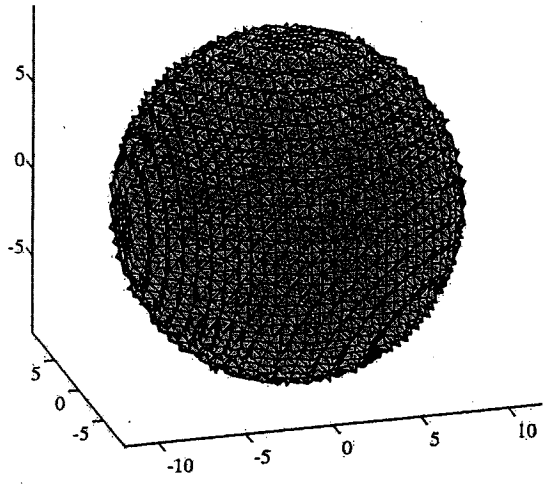

Figure 6: Approximation of sphere with radius $1.5\lambda_0$.

has the advantages of a more flexible modeling of the scatterers and a physical reduction of the workload. Moreover it reduces the computational complexity to $\mathcal{O}(N)$ in case of dense volume scatterers which are encountered frequently in inversion problems.

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