COUPLING OF THE GENERALIZED MULTIPOLE TECHNIQUE AND THE FINITE ELEMENT METHOD

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ABSTRACT. This paper presents a coupling of two different methods for electromagnetic scattering problems, the 3D MMP (Multiple MultiPole) code, an implementation of the Generalized Multipole Technique (GMT) and the finite element (FE) method. The coupling is performed using iterative methods. The procedure is illustrated with the solution of a benchmark problem for scattering from a three-dimensional lossy dielectric cylinder.

1. INTRODUCTION

There is an obvious interest in combining the advantages of methods for open domains, which are mostly based on analytic approaches and therefore restricted to linear and largely homogeneous domains, with methods that can handle inhomogeneous, anisotropic or nonlinear domains, but are themselves only applicable to finite domains. In the present work, such a combination is made with the 3D MMP code and a FE code. The underlying ideas are inspired by an iterative method used for solving complex problems consisting of several subproblems with the 3D MMP code [1]. The approach also closely resembles the one taken in the "field feedback formulation" [2].

2. 3D MMP CODE

The 3D MMP code [3] is an implementation of the GMT (Generalized Multipole Technique) [4]. It is a code for two- and three-dimensional time harmonic scattering problems with piecewise linear, homogeneous and isotropic domains.

An expansion for the unknown field f in each domain is made with exact solutions of the homogeneous wave equations.

$$\underline{\vec{f}} = \sum c_i \underline{\vec{f}}_i \quad \text{where} \quad \underline{\vec{f}}_i = \begin{bmatrix} \vec{E} \\ \vec{H} \end{bmatrix} \tag{1}$$

and the c_i are complex coefficients. As the name of the method suggests, the most useful expansions are multipole solutions in cylindrical or spherical coordinates, which have a strong local behavior and allow "modeling" of the field around complex domains. However, many other expansion functions, such as plane waves, waveguide modes, straight- and curved line multipoles, thin wire expansions, rooftop current-patch functions etc. are available. As a result, MMP models have in general a smaller number of unknowns than models for comparable methods.

Equations are obtained by enforcing boundary conditions or continuity conditions for the tangential and normal components of the electromagnetic field on matching points on the borders between domains. This leads to an overdetermined linear system of equations

$$\tilde{A}c_i = \tilde{b}_i \tag{2}$$

This system is solved in the least squares sense, thus minimizing total boundary error. The solution of (2) is equivalent to the solution of the system of equations

$$Ac_i = b_i \tag{3}$$

where $A = \tilde{A}^*\tilde{A}$ is a square, dense, Hermitian matrix and $b_i = \tilde{A}^*\tilde{b}_i$. Throughout the rest of this paper the MMP problem will be referred to as the system (3), although in practice its solution will be directly obtained from (2) with a QR-factorization, which is numerically considerably better.

Because the fundamental quantity in MMP is the electromagnetic field (both $\vec{E}$ and $\vec{H}$), the method is very versatile. Apart from ordinary boundary conditions one can also use surface impedance boundary conditions, periodic boundary conditions, or, in the context of this work, boundary conditions involving predefined values.

The fact that singularities of the expansion functions are far from the surface and that the error is distributed smoothly over the surface leads to results that are quite accurate in the nearfield. This is advantageous for the purpose of successfully coupling it with other methods over domain boundaries.

3. FINITE ELEMENT CODE

The basic equation is the vector wave equation for the electric field $\vec{E}$,

$$\operatorname{curl}\left(\frac{1}{i\omega\mu}\operatorname{curl}\vec{E}\right) + i\omega\varepsilon'\vec{E} = 0 \tag{4}$$

which is solved in a weak sense with a weighted residual method

$$\left\langle \mathrm{curl}(\frac{1}{i\omega\mu}\,\mathrm{curl}\,\underline{\vec{E}})\vec{\Phi}_j \right\rangle_V + \left\langle i\omega\epsilon'\underline{\vec{E}}\vec{\Phi}_j \right\rangle_V = 0. \qquad (5)$$

The $\vec{\Phi}_j$ are the testing functions; the $\langle\cdot\rangle_V$ denotes an integration over the domain V. After some transformations, one arrives at the system of equations

$$\left\langle (\frac{1}{i\omega\mu}\,\mathrm{curl}\,\underline{\vec{E}})\,\mathrm{curl}\,\vec{\Phi}_j \right\rangle_V + \left\langle i\omega\epsilon'\underline{\vec{E}}\vec{\Phi}_j \right\rangle_V = -\left\langle \vec{n}\times\underline{\vec{H}}\vec{\Phi}_j \right\rangle_{\partial V} \qquad (6)$$

$\langle\cdot\rangle_{\partial V}$ is an integration over the boundary of the domain V. Thus, the electric field in a domain can be obtained from the tangential components of the magnetic field on the boundary of that domain. It should be noted that one could use a dual version, in which the magnetic field would be calculated from the tangential electric field; for our purposes, however, the electric field is more interesting.

For the 3D case a tetrahedral grid with Whitney edge-elements $\vec{W}^{ij}$ is used [5, 6]. The electric field within the domain is expanded as

$$\underline{\vec{f}} = \sum c_{ij}\vec{W}^{ij} \qquad (7)$$

where the c_{ij} are complex unknowns associated with the components of the field along the edges between nodes i and j. Inserting the expansion (7) into (6) and using the same functions $\vec{W}^{ij}$ as testing functions $\vec{\Phi}$ (Galerkin's choice) leads to a linear system of equations with a square, sparse, symmetric matrix. The derived FE system of equations is equivalent to one derived with the Rayleigh-Ritz variational method from a functional.

The 2-dimensional analogs to the tetrahedral edge elements are the triangular edge elements. The vector functions related to each of the edges are shown in Figure 1.

Edge elements have several advantages over nodal elements. They are divergence-free and eliminate the problem of spurious solutions. They also avoid the problem of

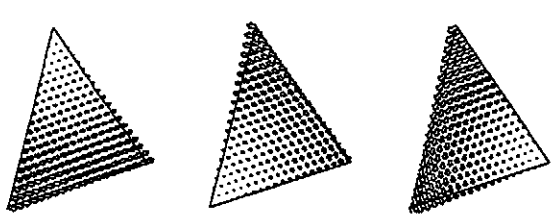

Figure 1: Vector basis functions $\vec{W}^{12}$, $\vec{W}^{23}$, and $\vec{W}^{31}$ for a triangular element, which are associated with the tangential value of the field along the corresponding edge.

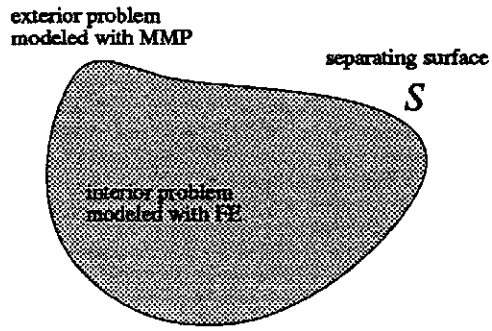

Figure 2: Separation of a problem into an interior and an exterior problem.

singularities in the field at edges and corners on the domain surface and allow easy treatment of boundary conditions and inhomogeneous domains. Furthermore, the degree of fulfillment of the continuity conditions for the normal components between the elements can be used to estimate the quality of the solution. The disadvantage of edge elements is a larger number of unknowns, which is to some extent compensated by higher sparsity of the system matrix.

4. COUPLING

A FE domain is separated from "MMP-space" with a boundary S (Figure 2). In each domain, the electromagnetic field is uniquely determined by either the tangential electric field or the tangential magnetic field on S. In our case the tangential magnetic field on S is used for the interior domain and the tangential electric field for the exterior domain. As the tangential components of an electromagnetic field are continuous across domain boundaries, a combined problem can be formulated, in which the interior and exterior problems mutually provide boundary values. The solution to the total problem therefore fulfills the continuity conditions for both the tangential electric and magnetic fields. A dual version, where the roles of the surface tangential electric and magnetic fields are reversed, is also possible. It should also be noted that instead of a single surface, two different surfaces may be used for the separation between MMP and FE and the reverse. In that case, the region enclosed by the surfaces would be part of both models.

The system of equations describing the total problem can be represented as a block system of equations

$$\begin{bmatrix} A & B \\ C & D \end{bmatrix}\begin{bmatrix} c_e \\ c_i \end{bmatrix} = \begin{bmatrix} b_e \\ b_i \end{bmatrix}. \qquad (8)$$

The components of this system of equations are the following:

- A is the MMP matrix $\tilde{A}^* \tilde{A}$.
- c_e are the unknowns for the (exterior) MMP problem.
- B translates a finite element "solution" c_i into the MMP context.
- b_e is the inhomogeneity for the (exterior) MMP problem.
- D is the sparse FE matrix.
- c_i are the unknowns for the (interior) FE problem.
- C translates a MMP "solution" c_e into the FE context.
- b_i is the inhomogeneity for the (interior) FE problem.

A simple iterative approach, similar to the one used for complex MMP-problems [1], is to alternately

1. Solve the MMP problem $Ac_e^{n+1} = b_e - Bc_i^n$
2. Solve the FE problem $Dc_i^{n+1} = b_i - Cc_e^n$

and hope for convergence of the parameters c_e^{n+1} and c_i^{n+1} to the correct solution. This approach is in essence a block Gauss-Seidel iteration in system (8); convergence is therefore only obtained if the matrix in (8) is block-diagonally dominant, i.e., the effects of the coupling are comparatively small. As a consequence, this method is limited to scatterers with high permittivity or conductivity.

It is therefore better to use an algorithm which does not suffer from these convergence problems, e.g., an iterative algorithm from the family of Krylov subspace methods. A partially "preconditioned" system of equations equivalent to (8) would be

$$\begin{bmatrix} I & A^{-1}B \\ C & D \end{bmatrix} \begin{bmatrix} c_e \\ c_i \end{bmatrix} = \begin{bmatrix} A^{-1}b_e \\ b_i \end{bmatrix}. \qquad (9)$$

where I is an identity matrix. To further diminish the number of unknowns for our simple case where only a single MMP problem and a single FE subproblem are present, the system (8) may be reduced to

$$\left[D - CA^{-1}B\right] c_i = b_i - CA^{-1}b_e \qquad (10)$$

by eliminating c_e. This has the form of a modified FE problem in which the new components in the coupled system of equations can be interpreted as follows:

- $CA^{-1}b_e$ is the solution (scattered field only) of the MMP problem for the incident wave, translated into the FE context.
- $CA^{-1}B$ represents an operation in which a FE state vector is translated into the MMP context and serves as an inhomogeneity for an MMP problem, which is solved and translated back into the FE context.

This system is now solved using an iterative, conjugate-gradient-like algorithm minimizing the residuals of an estimate for a solution in Krylov subspaces. The combined system matrix is neither Hermitian nor symmetric and its transpose is not readily available. A GMRES (Generalized Minimum Residual) algorithm [7] is therefore a possible choice. In GMRES, the residual of the system of equations (10) is minimized in a Krylov subspace of dimension k

$$\mathcal{K}_k = \text{span}\left\{r_0, Ar_0, A^2r_0, \ldots, A^{k-1}r_0\right\}. \qquad (11)$$

For details on the algorithm References [7] and [8] are recommended. It is important to note that in this type of algorithm the system matrix of the combined problem (10) is not used directly, but only as an operator in matrix vector products. Therefore it need not be directly available.

The evaluation of the matrix vector product

$$(D - CA^{-1}B)x$$

involves the following steps:

1. Evaluate Dx as a sparse matrix vector product.
2. Translate x into the MMP context (Bx).
3. Solve the MMP problem $Az = Bx$ and obtain $A^{-1}Bx$.
4. Translate the MMP solution into the FE context, get $CA^{-1}Bx$.
5. Add contributions from steps 1 and 4 to get the complete matrix vector product.

There is a potential for parallel execution of Step 1 and Steps 2–4.

Note that neither A^{-1}, B nor C are present in matrix form. There are not only implementational, but also numerical advantages to the case where the whole mixed matrix would actually be present: Whereas the matrix A or $CA^{-1}B$, respectively, would be very ill-conditioned, in the above presented algorithms they merely stand for an MMP problem and its solution (Step 3), which can be obtained from the original overdetermined system with numerically superior algorithms.

The convergence speed of the iterative solver can be improved by preconditioning the system (10). It is difficult to properly include the contributions of the MMP

terms in (10) into the preconditioning matrix. Therefore the preconditioner is in our case simply based on the sparse matrix D. An ILU(0) preconditioner is used [8].

5. IMPLEMENTATION

A great advantage of the presented methods are the minimal requirements for the implementation, which leaves both stand-alone versions of the involved codes practically untouched. The simple iterative algorithm does not actually require a coupled code, but can be implemented by preparing the input files containing the modifications of the right-hand sides for the subsequent problems.

The algorithm for the solution of (10) can be implemented in a FE code with an iterative solver by adding a routine for obtaining the MMP contribution to right-hand side of the FE system of equations and by modifying the matrix-vector product. Both require a call to the MMP code.

On the MMP side, matching points with an additional predefined boundary value have been added. The combined algorithm is implemented in a routine which accepts a FE state vector, converts it to a right hand side for an MMP problem, calculates the new parameters and evaluates the field values in the FE boundary points. Furthermore, a matrix-solver with Householder transformations instead of the more memory efficient, original version with Givens plane rotation [9] is used. This makes the repeated solution of MMP problems with unchanged matrix, but different right hand sides much more efficient.

The communication between the two codes is currently done with PVM [10], a message passing library for parallel processing. This allows the parallel evaluation of the two contributions in the matrix vector product on different processors. On a single machine, however, the approach has an unnecessary message-passing and synchronization overhead.

6. EXAMPLE

To illustrate the procedure, a benchmark example from a collection of canonical problems is used [11]. It is a 3-dimensional, lossy dielectric cylinder, which is terminated by spherical caps at both ends. Its radius is 0.05m, the total length 0.5m. The excitation is a plane wave with a wavelength of 1m. The electric field is parallel to the cylinder axis (see Figure 3). The material has a relative permittivity of 50 and a conductivity of $1\mathrm{Sm}^{-1}$, close to the properties of biological tissue. The internal wavelength is about 0.14m.

Three planes of symmetry are used; the total result is obtained as a superposition of results of two symmetry conforming subproblems. The FE domain in the first

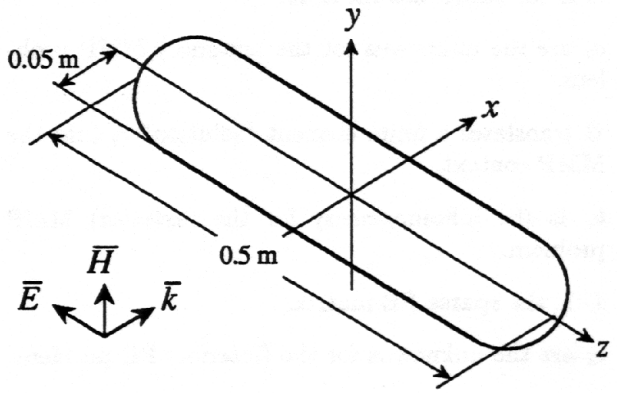

Figure 3: Geometry of the cylinder with spherical ends.

octant was discretized with a tetrahedral mesh with an average spacing of 0.01m, leading to 824 nodes, 3199 elements and 4450 edges (Figure 4).

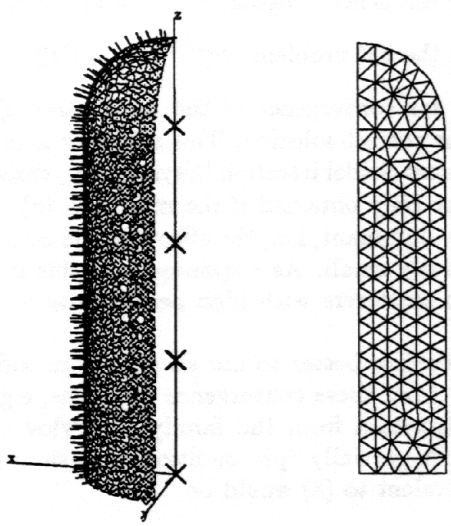

Figure 4: Surface discretization with matching points and location of the multipole expansions (left) and cut through the tetrahedral FE mesh in the z-x plane (right). Thanks to the symmetry of the problem the scatterer needs to be discretized only in the first octant.

For the MMP model, matching points that enforce the boundary conditions with the FE inhomogeneity were generated in the center of each surface triangle of the mesh on the boundary between the MMP and the FE model. The scattered field around the cylinder is expanded with 4 multipoles on the axis of the cylinder at $z = 0$, $0.0\overline{6}$, $0.1\overline{3}$ and 0.2; the even and odd models each have about 100 unknowns. For the feedback to the FE problem the electromagnetic field of the solution is eval-

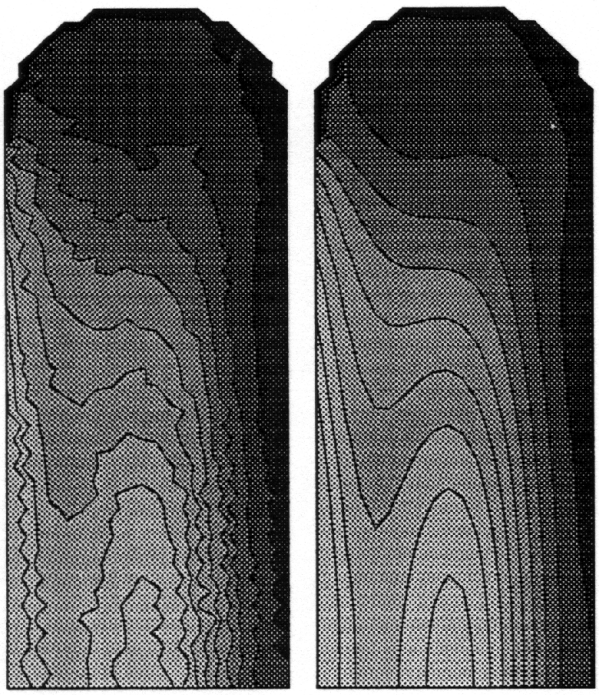

Figure 5: FE/MMP solution of the field in the cylinder (left) and the pure MMP solution (right), sampled on a regular 20 by 50 grid. The specific absorption rate is shown in the x-z plane with the same scaling for both solutions; the higher the absorption, the lighter the color. A plane wave is incident from the left.

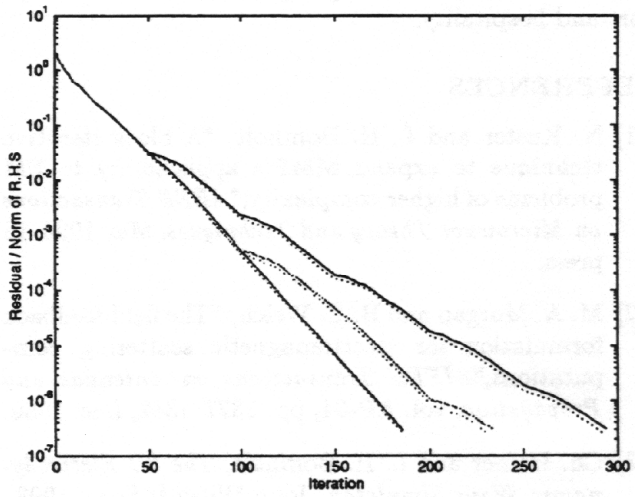

Figure 6: Residual as a function of iteration step for the pure FE problem (lines) and for the mixed FE/MMP algorithm (dotted line). Versions without restart, with a restart every 100 steps and with a restart every 50 steps are shown.

uated in the surface nodes of the FE mesh.

This benchmark problem can also be solved with high accuracy using the 3D MMP code alone [11], which gives a reference for the solutions obtained with the coupled method. In that case, the interior field is approximated by a high-order spherical expansion with Bessel functions in the center of the cylinder. Both results are shown in Figure 5. The wiggly nature of the lines in the FE solution is due to the discontinuity of the solution across element boundaries.

To indicate how much the presence of the MMP terms in the FE system of equations affects the convergence behavior, the relative residual as a function of the number of iteration steps during the solution of the even part of the problem is shown in Figure 6, once for the pure FE problem with the correct boundary conditions from the pure MMP problem, once for the mixed FE/MMP algorithm.

In the same figure the effect of restarting the GMRES algorithm can be seen. A disadvantage of GMRES is that the minimization of the residual error requires keeping all the vectors that build up the Krylov subspace. Therefore both the cost in memory and computer time increase as the algorithm proceeds. Breaking off the algorithm after a certain number of iterations and restarting it with the improved solution offers a way out, however, at the cost of slower convergence, or, if the number of iterations between restarts is too small, no convergence at all. Other transpose-free algorithms such as CGS (conjugate gradient squared), Bi-CGSTAB (biconjugate gradient stabilized) or algorithms based on the QMR (quasi-minimum residual) method [8], which all have a constant cost per iteration, could provide an alternative, but this has not yet been tried.

7. CONCLUSION

The MMP code has been successfully coupled with a FE code. The coupling has been made in a way which has minimal impact on either of the codes, so that the full modeling power of each code is preserved. This provides a useful extension to both of the involved methods and holds promise for a variety of problems which are difficult or impossible to treat with either method by itself. The iterative approach, especially when applied to systems of the form (9), can also be extended to hybrid combinations involving other or more than two participating methods or models.

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