The FEMAX finite-element package for computing three-dimensional time-domain electromagnetic fields in inhomogeneous media

G. Mur

Laboratory of Electromagnetic Research, Faculty of Electrical Engineering, Delft University of Technology, PO Box 5031, 2600GA, Delft, The Netherlands

ABSTRACT

An efficient and accurate finite-element package is described for computing transient as well as time-harmonic three-dimensional electromagnetic fields in inhomogeneous media. For the expansion of the field in an inhomogeneous configuration, edge elements are used along the interfaces between media with different medium properties to allow for the continuity conditions of the field across these interfaces, nodal elements are used in the remaining homogeneous subdomains. In the domain of computation the package decides locally what type of element has to be used for obtaining the user-specified accuracy of modeling the field. In this way optimum results are obtained both in regard to computational efficiency and in regard to desired accuracy. The electromagnetic compatibility relations are implemented for avoiding spurious solutions.

INTRODUCTION

In view of its flexibility, the finite-element method seems to be the most suitable one to compute electromagnetic fields in inhomogeneous media. When computing three-dimensional electromagnetic fields in inhomogeneous media in terms of the electric field strength, it is necessary to use a computational technique that accounts for the continuity of the tangential components of the electric field strength across interfaces where the constitutive coefficients jump, and that allows for a jump in the normal component of the electric field strength. For time-harmonic electromagnetic fields a code using such a technique was described earlier in [1]. In the present paper we shall discuss a code for solving transient electromagnetic field problems that was designed using the same basic approach as the one used in [1], i.e. the electric field strength is modeled using a combination of consistently linear edge and nodal expansion functions such that all continuity conditions can be satisfied and that the computational efficiency is optimized.

Computing the electric field strength directly yields highly accurate results as compared with the formulations using potentials. The latter methods have the disadvantage that the electric field strength can only be ob-
tained from the potential solution by performing a numerical differentiation which causes a large loss of accuracy. Potential methods have the additional disadvantages of requiring the use of a gauge to make them unique, and that they may fail, or cause difficulties, in multiply connected regions [2].

In our approach, the problem of modeling discontinuous electromagnetic fields in inhomogeneous media is solved at the element level by using finite elements, edge elements, that account for the continuity of the tangential components of the fields across interfaces where the constitutive coefficients jump, and that allow for a jump in the normal components of the field strength [3]. The disadvantage of edge elements is that they are computationally more expensive than the commonly employed nodal elements that make all field components continuous across interfaces. In [4] an improved method is described that virtually eliminates this disadvantage of edge elements by using them only for modeling the field along discontinuities and by using nodal elements elsewhere. In the domain of computation, it lets the program, for each combination of two adjacent subdomains, decide which type of element will be used. For "weak" discontinuities (i.e. discontinuities along which ignoring the jump in the normal component of the field strength would not yield unacceptably large errors) in electromagnetic properties between subdomains it will use nodal elements, for "large" differences it will use edge elements. The degree of inhomogeneity (discontinuity) above which edge elements are used is user-defined and has to be chosen in accordance with the final accuracy the user aims at. In the present paper the formulation given in [5] is summarized and slightly extended by putting more emphasis on the compatibility relations, and the FEMAX finite-element package, developed on the basis of the latter formulation is described.

THE EXPANSION FUNCTIONS

For topological reasons, the geometrical domain in which the finite-element method is applied, is subdivided into tetrahedra. To specify a position in space, we employ the coordinates \( \{x, y, z\} \) with respect to the Cartesian reference frame with origin \( O \) and three mutually perpendicular base vectors \( \{i_1, i_2, i_3\} \) each of unit length. The linear functions \( \phi_i(r) \) (the barycentric coordinates) that equal unity at the vertex \( r = r_i \) \( i = 0, 1, 2, 3 \) and are zero at the remaining three vertices of a tetrahedron \( T \) can be written as

\[
\phi_i(r) = \frac{1}{4} - (r - r_i) \cdot A_i / 3V, \quad i = 0, 1, 2, 3, \quad (1)
\]

where \( A_i \) denote the vectorial areas of the faces of \( T \) and \( V \) its volume. The local nodal expansion functions \( W_{i,j}^{(N)}(r) \) in \( T \) are taken as

\[
W_{i,j}^{(N)}(r) = \phi_i(r)i_j, \quad i = 0, 1, 2, 3 \text{ and } j = 1, 2, 3. \quad (2)
\]

The local edge expansion functions \( W_{i,j}^{(E)}(r) \) in \( T \) are taken as [3]

\[
W_{i,j}^{(E)}(r) = \phi_i(r)a_{i,j} \nabla \phi_j(r), \quad i, j = 0, 1, 2, 3, \quad i \neq j. \quad (3)
\]

In (3) the factor \( a_{i,j} = |r_i - r_j| \) is used for making \( W_{i,j}^{(E)}(r) \) dimensionless and for a scaling such that the condition of the matrices in the final system of differential equations is optimized.
It is easily shown that nodal expansion functions are computationally more efficient than edge expansion functions and that the former should be used whenever the use of the latter is not necessary because of the local degree of inhomogeneity. When \( \mathbf{r} \in \mathcal{T} \), the electric field strength \( \mathbf{E} \) is expanded as

\[
\mathbf{E}(\mathbf{r}, t) = \sum_{i=0}^{3} \sum_{j} e_{i,j}(t) \mathbf{W}^{(N,E)}_{i,j}(\mathbf{r}),
\]

where \( e_{i,j}(t) \) are the unknown time-dependent field expansion coefficients, and where \( \mathbf{W}^{(N,E)}_{i,j}(\mathbf{r}) \) may either be an edge (E) or a nodal (N) expansion function. In (4) the summation over \( j \) runs over values that depend on the type of element that is locally used. Because of the fact that both the nodal and the edge elements are consistently linear vector functions of the spatial coordinates, the local approximation error caused by using (4) is \( O(h^2) \) where \( h \) denotes the largest dimension of the tetrahedron.

THE DISCRETIZATION OF MAXWELL’S EQUATIONS

We first describe how the system of equations in the expansion coefficients is obtained by applying the method of weighted residuals to the relevant differential equations. The method will be outlined for linear, time-invariant, locally reacting, anisotropic media. Upon eliminating the magnetic field strength \( \mathbf{H}(\mathbf{r}, t) \) from Maxwell’s equations we arrive at

\[
\epsilon \cdot \partial_t^2 \mathbf{E} + \sigma \cdot \partial_t \mathbf{E} + \nabla \times (\mu^{-1} \cdot \nabla \times \mathbf{E}) = -\partial_t \mathbf{J}^e - \nabla \times (\mu^{-1} \cdot \mathbf{K}^e),
\]

where \( \epsilon, \sigma \) and \( \mu \) are tensors of rank two, \( \mathbf{J}^e = \) volume source density of external electric current and \( \mathbf{K}^e = \) volume source density of external magnetic current. Equation (5) holds in subdomains where \( \mathbf{E} \) is twice continuously differentiable. Applying the method of weighted residuals we obtain a result that can, using (4) be written as

\[
\sum_{I=1}^{N} \partial_t e(I, t) \int_{P} \mathbf{W}(\mathbf{J}, \mathbf{r}) \cdot \epsilon(\mathbf{r}) \cdot \mathbf{W}(I, \mathbf{r})dV + \sum_{I=1}^{N} \partial_t e(I, t) \int_{P} \mathbf{W}(\mathbf{J}, \mathbf{r}) \cdot \sigma(\mathbf{r}) \cdot \mathbf{W}(I, \mathbf{r})dV
\]

\[
+ \sum_{I=1}^{N} e(I, t) \int_{P} (\nabla \times \mathbf{W}(\mathbf{J}, \mathbf{r})) \cdot \mu^{-1} \cdot (\nabla \times \mathbf{W}(I, \mathbf{r}))dV
\]

\[
= \partial_t \int_{P} \mathbf{W}(\mathbf{J}, \mathbf{r}) \cdot (\nu \times \mathbf{H}(\mathbf{r}, t))dA
\]

\[
- \partial_t \int_{P} \mathbf{W}(\mathbf{J}, \mathbf{r}) \cdot \mathbf{J}^e(\mathbf{r}, t)dV
\]

\[
- \int_{P} (\nabla \times \mathbf{W}(\mathbf{J}, \mathbf{r})) \cdot \mu^{-1} \cdot \mathbf{K}^e(\mathbf{r}, t)dV, \text{ for } J = 1, \ldots, N,
\]
where $\partial D$ denotes the outer boundary of the domain of computation $D$, $\nu$ denotes the unit vector along the outward normal to $\partial D$, and where $N$ is the number of unknowns in the expansion of the electric field strength. Which type of element is used in which subdomain depends on the local degree of discontinuity in the properties of the media [4].

Additional advantages of edge expansion functions are that they do not yield conflicting conditions at parts of interfaces where the local normal to the interface is not continuous, and that they can be used along the parts of the outer boundary that are not parallel to a nodal coordinate plane. Along those parts of the outer boundary, they yield an expansion of the field that can be used directly for imposing boundary conditions.

The Galerkin method of weighted residuals is used, i.e. the weighting functions are taken the same as the expansion functions. Assuming the medium properties either to be constant or to vary linearly in the interior of each tetrahedron, all integrations implied in (6) can be carried out analytically and we obtain a system of coupled ordinary differential equations from which the evolution in time of the field expansion coefficients can be solved.

THE COMPATIBILITY RELATIONS

In general compatibility relations are properties of the exact Maxwell’s equations that may be lost in a discretized form of these equations. Failing to include them in the formulation may cause the type of highly inaccurate results that are commonly referred to as spurious solutions, or vector parasites. The following compatibility relations [6] were included in the formulation to overcome the consequences of the discretization.

*Interior compatibility:* Interior compatibility refers to the divergence properties of the field. In its simplest form, when the solution is known to be free of divergence, this freedom of divergence is imposed upon the solution by adding the condition

$$
\sum_{I=1}^{N} e(I,t) \int_{T} (\nabla \cdot W(J,r)) \cdot (\varepsilon \mu)^{-1} (\nabla \cdot \varepsilon W(I,r)) dV = 0
$$

(7)

to (6) for all tetrahedra $T$. The use of (7) causes the system matrices to be asymmetric in case the medium properties are not constant over a tetrahedron.

*Interface compatibility:* Interface compatibility refers to the continuity of the normal fluxes at interfaces between different media. Again assuming the simple case where the solution is free of divergence (no surface charges) this condition is imposed by adding the continuity condition

$$
\int_{T} W(r)(\nu \cdot D(r,t)_{I}) dA = 0,
$$

(8)

where $W(r)$ is a suitably chosen weighting function and where $\nu$ denotes the local unit vector normal to the interface, to (6) for all triangles in the interfaces $T$ between different media. The use of equation (8) causes the system matrix to be asymmetric.
Outer boundary compatibility: Outer boundary compatibility refers to the relation of the normal fluxes at the outer boundary of the domain of computation to the prescribed values of the tangential components of the magnetic field strength along this boundary. In its simplest form, and assuming the tangential components of the magnetic field strength to be zero, this condition reduces to the condition that the normal component of the electric flux density should be zero at the relevant part of the outer boundary. This condition can be imposed by adding the condition

$$\int_{\partial D} W(r)(\mathbf{\nu} \cdot \mathbf{D}(r, t)) dA = 0,$$

where $W(r)$ is a suitably chosen weighting function, to (6).

In the above formulations for the compatibility relations we have, for simplicity, assumed isotropic media. A choice of different formulations is available in the package for each of the compatibility relations mentioned above. Which formulation is used depends on the local medium properties, in particular on the local value of the relaxation time $\frac{\varepsilon(r)}{\sigma(r)}$ in its relation to the time step $\Delta t$ that is chosen in the algorithm for the integration of the system of differential equations. Note that this implies that, for each of the compatibility relations, different formulations may be used at different locations in the domain of computation.

THE FEMAX PACKAGE

The FEMAX package consists of the FEMAXT finite-element code and the FEMAXPT and FEMAXH codes that can be used for post processing the results obtained in FEMAXT. The package was written in FORTRAN-77.

The FEMAXT finite-element code was designed on the basis of the theory given above. Among others, it has the following properties and options:

- In the interior of the domain of computation the user can specify arbitrary distributions of the properties of the media (permittivity, conductivity and permeability) that may be either isotropic or anisotropic.
- The contrast in properties of the media in two adjacent domains below which the medium is treated as having continuously varying medium properties is specified by the user.
- In the interior of the domain of computation, the user can prescribe arbitrary volume source distributions of electric and or magnetic current.
- The distributions of the medium properties and the volume source distributions can be specified either by using user-written subroutines (in FORTRAN-77) or by using members of the collection of standard subdomains with standard distributions that are provided in the package.
- At the outer boundary of the domain of computation, the user can prescribe arbitrary distributions of (in)homogeneous Dirichlet, Neumann and/or Robin (=local impedance) boundary conditions. A local impedance boundary condition for modeling radiation into the unbounded free space surrounding the domain of computation is also available.
• The system of coupled ordinary differential equations that is generated by the finite-element package is solved using implicit one- or two-step methods. Different types of preconditioning are available.

• An option is available for solving time-harmonic problems in the time domain by using a transient from zero-state to time-harmonic. In many cases this option is more efficient than a direct solution of the time-harmonic problem in the frequency domain would be.

• Field values, as well as their history in time, can be computed at arbitrary user-specified points in the configuration.

• FEMAXT uses the SEPRAN finite-element package [7] for a number of tasks like generating the mesh and assembling the system matrix from the element matrices generated in FEMAXT.

The FEMAXPT and FEMAXH codes are used for post processing data prepared in FEMAXT. FEMAXPT is used for making contour plots of field values, and of quantities that can be expressed in terms of the field values. FEMAXH is used for plotting the solution as a function of time.

NUMERICAL RESULTS

As an example we consider the scattering of a time-harmonic plane wave by an inhomogeneous isotropic cubic scatterer. The scatterer consists of an inner cube covering the region \( D_1 = \left\{ -0.075 \leq x \leq 0.075m, -0.075 \leq y \leq 0.075m, -0.075 \leq z \leq 0.075m \right\} \), with medium properties \( \{ \varepsilon_1 = 70\varepsilon_0 F/m, \sigma_1 = 0.68S/m, \mu_1 = \mu_0 H/m \} \). The inner cube is imbedded in a second cube covering the region \( D_2 = \left\{ -0.15 \leq x \leq 0.15m, -0.15 \leq y \leq 0.15m, -0.15 \leq z \leq 0.15m \right\} \), with medium properties \( \{ \varepsilon_2 = 7.5\varepsilon_0 F/m, \sigma_2 = 0.05S/m, \mu_2 = \mu_0 H/m \} \). The second cube is surrounded by a vacuum.

This problem was solved under the condition that edge expansion functions are used when the relative contrast in the numerical value of \( \varepsilon \) and/or \( \sigma \) in two adjacent tetrahedra exceeds 10%, nodal expansion functions are used in regions with lower contrasts. With this choice edge elements are used along the surfaces of the two cubes, nodal elements are used elsewhere.

The electric field strength of the time-harmonic incident plane wave, having a frequency \( f = 10^8 \) Hz, can be written as

\[
E^{\text{inc}} = \cos(\omega(t - z/c_0))\hat{z},
\]

where \( \omega = 2\pi f \) denotes the angular frequency and where \( c_0 = \omega(\varepsilon_0\mu_0)^{-1/2} \) denotes the speed of light in vacuo.

Using symmetry, the domain of computation \( D_3 \) is chosen as \( D_3 = \left\{ 0 \leq x \leq 0.225m, 0 \leq y \leq 0.225m, -0.225 \leq z \leq 0.225m \right\} \). The mesh consists of 15x15x30 cubes of equal size, each being subdivided into 6 tetrahedra. For the discretization in time we have chosen a time step \( \Delta t = T/20 = 5\times10^{-10}s \).

The boundary conditions have been chosen as follows: at the plane \( x = 0 \) the tangential part of electric field strength is set to zero, at the plane \( y = 0 \) the tangential part of the magnetic field strength is set to zero and at the the remaining parts of the outer boundary an inhomogeneous absorbing boundary condition [8] is used that, while taking into account the incident field, exactly absorbs scattered waves that have a normal incidence upon the outer boundary. The initial values at \( t = -\Delta t \) and \( t = 0 \) (a
two-step method is used) are set to zero. The transient time is chosen as \( t_{tr} = 5T \), with this choice an acceptable approximation of the steady state was achieved immediately after the transient period [8]. The medium properties and the frequency chosen are typical for hyperthermia applications. With the discretization used we have a total number of 32252 degrees of freedom, 1232 of these degrees of freedom being set to zero because of the boundary conditions. An average of 11 iterations is required for solving the asymmetric system of equations each time step, each iteration requiring approximately 3.5 seconds of CPU-time at a VAXstation 4000 90.

![Contour plot](image)

**Fig. 1.** Contour plot of \( \Re(\hat{E}_x(x, y, z = 0)) \).

In Fig. 1 a contour plot is given of the real part \( \Re(\hat{E}_x) \) of the complex-valued time-harmonic solution \( \hat{E}_x \) in the plane \( z = 0 \).

About 20Mbytes are required for storing all data relevant for solving the system of coupled ordinary differential equations, about 90Mbytes are required for generating these equations. The storage of the executable requires 3.2Mbyte.
CONCLUSION

We have shown that the FEMAX package is an efficient and accurate tool for computing transient as well as time-harmonic electromagnetic fields in inhomogeneous media. Its efficiency is achieved by making an optimum choice between the use of edge elements for modeling "strong" discontinuities and nodal elements for modeling subdomains with continuously varying medium properties and "weak" discontinuities. Its accuracy is achieved by using consistently linear expansions and by carefully taking into account all relevant compatibility relations so as to avoid any spurious solutions.

The package is capable of computing fields in arbitrarily inhomogeneous and (an)isotropic configurations with arbitrary source distributions and for a wide range of boundary conditions along an arbitrarily shaped outer boundary. All sources and boundary conditions may vary arbitrarily in time.

REFERENCES


