A novel technique to build constitutive matrices for generalized FDTD algorithms

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Abstract

By means of some recent approaches it is possible to develop generalized FDTD algorithms working in an explicit way on unstructured grids. The critical point of these algorithms is the difficulty in the construction of the constitutive matrices, better known as discrete hodge operators. In these paper we propose a novel technique for the construction of the constitutive matrices in order to have some features that can guarantee the stability and the consistency of the generalized FDTD algorithms.

1 Introduction

The study of the mathematical structure common to many physical theories [1] provides a new discrete mathematical model of the electromagnetic field theory. This new model is based on the followings tools:
1)Two oriented space-time cell complexes and a relationship of duality between them. A space cell complex, synonymous of three dimensional grid, is a structured collection of points, lines, surfaces and volumes whereas a time cell complex, synonymous of one dimensional grid, is a structured collection of instants and intervals [2].
2)The global (integral) variables (Electric voltage $\mathbf{V}$, Magnetic voltage $\mathbf{F}$, Electric flux $\mathbf{\Psi}$, Magnetic flux $\mathbf{\Phi}$, Electric current $\mathbf{I}$, Electric charge content $\mathbf{Q_c}$), in order to represent physical variables, and their physically coherent association with the oriented space and time cells [1][2].
3)A discrete formulation of the electromagnetic laws by the global variables on the cell complexes. In particular the discrete laws can be divided into two classes:
Field equations (topological equations). They can be enforced in a discrete form by using appropriate incidence matrices. If we denote with $\mathbf{G}$, $\mathbf{C}$, $\mathbf{D}$ and $\tilde{\mathbf{G}} = \mathbf{D^T}$, $\tilde{\mathbf{C}} = \mathbf{C^T}$, $\tilde{\mathbf{D}} = -\mathbf{G^T}$, the incidence matrices [1][3][5] related to the primal and dual cell complexes respectively, which are the discrete counterparts of the differential operators $gradient$, $curl$ and $divergence$, the topological equations can be expressed as follows:
-*Faraday-Neumann law*: $\mathbf{C}\mathbf{V}^{n+1/2} = -(\mathbf{\Phi}^{n+1} - \mathbf{\Phi}^{n})/\tau$
-*Magnetic Gauss law*: $\mathbf{D}\mathbf{\Phi}^{n} = 0$
-*Ampère-Maxwell law*: $\tilde{\mathbf{C}}\mathbf{F}^{n} = (\mathbf{\Psi}^{n+1/2} - \mathbf{\Psi}^{n-1/2})/\tau + \mathbf{I}^{n}$
-*Electric Gauss law*: $\tilde{\mathbf{D}}\mathbf{\Psi}^{n+1/2} = \mathbf{Q_c}^{n+1/2}$
where $\mathbf{V}^{n+1/2}$, $\mathbf{\Phi}^{n}$, $\mathbf{F}^{n}$, $\mathbf{\Psi}^{n+1/2}$, $\mathbf{I}^{n}$, $\mathbf{Q_c}^{n+1/2}$ are scalar arrays, τ is the time step and the primes n e $n+1/2$ indicate the primal and the dual time instants respectively.
Constitutive relations. They can be enforced in a discrete form by using suitable constitutive matrices. Let us denote with $\mathbf{M}_{\varepsilon}$, $\mathbf{M}_{\varepsilon i}$, $\mathbf{M}_{\mu}$,$\mathbf{M}_{\nu}$ the constitutive matrices that enter in the following algebraic constitutive relations:
Electric constitutive relations $\mathbf{\Psi}^{n+1/2} = \mathbf{M}_{\varepsilon}\mathbf{V}^{n+1/2}$, $\mathbf{V}^{n+1/2} = \mathbf{M}_{\varepsilon i}\mathbf{\Psi}^{n+1/2}$
Magnetic constitutive relations $\mathbf{\Phi}^{n} = \mathbf{M}_{\mu}\mathbf{F}^{n}$, $\mathbf{F}^{n} = \mathbf{M}_{\nu}\mathbf{\Phi}^{n}$

The applications of the previous tools give rise to a new method (Cell Method CM) for solving electromagnetic static and dynamic problems both in frequency [3][4] and in

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time domain [2] on unstructured grids. In particular from the field equations and the constitutive relations we can set up a generalized FDTD explicit algorithm as follows:

$$\begin{cases} \mathbf{F}^n = \mathbf{F}^{n-1} - \tau \mathbf{M}_\nu \mathbf{C} \mathbf{V}^{n-1/2} \\ \mathbf{V}^{n+1/2} = \mathbf{V}^{n-1/2} + \tau \mathbf{M}_{\varepsilon i} (\mathbf{C}^T \mathbf{F}^n + \mathbf{I}^n) \end{cases} \tag{1}$$

The main problem in a practical use of the algorithm (1) is the difficulty in the construction of the constitutive matrices [5][6] under some constrains and desired features. As a matter of fact the constitutive matrices must be: (1)**Symmetric** and (2)**Positive definite**, in order to ensure stability of the numerical method [5][6], (3)**Sparse**, to save memory and assure fast computations. Moreover the constitutive matrices must ensure the (4)**Consistency** [6] and the (5)**Accuracy** of the numerical method.
In this paper we propose a general way to build the constitutive matrices in order to satisfy the features $(1)-(5)$. We will apply this technique here only to build the constitutive matrices for the 2D cases with triangular grids, quadrilateral grids and square grids with subgridding. The starting point will be the constitutive matrices built by the *Microcell Interpolation Scheme* (MIS) [2].

2 A consistent symmetrization of the constitutive matrices of the MIS

In the MIS a generic constitutive matrix $\mathbf{M}$, such as $\mathbf{M}_\nu$ or $\mathbf{M}_{\varepsilon i}$ i.e., is built by composition of local constitutive matrices $\mathbf{M}_a$ located along the main diagonal of $\mathbf{M}$. In the 2D cases each local constitutive matrix $\mathbf{M}_a$ links physical variables related to the geometrical elements inside and on the border of one surface S_a. Since the dimension of each $\mathbf{M}_a$ is equal to the number of edges of S_a then $\mathbf{M}$ is sparse in general. In order to meet the other features it is enough to deal with the local constitutive matrices $\mathbf{M}_a$.
Given a generic $\mathbf{M}_a$, built by the MIS, it is not symmetric in general, but it meets the feature (5) both in frequency domain [3][4] and in time domain applications [2]. Our goal is to find a new local constitutive matrix $\mathbf{M}_{aS}$ such that:
(A) $\mathbf{M}_{aS}$ is symmetric.
(B) $\mathbf{M}_{aS}$ meets the feature about the consistency [6].
(C) $\mathbf{M}_{aS}$ is as close as possible to $\mathbf{M}_a$ in a square mean.
The request (C) is formulated for two reasons based on empirical assumptions. The first is preserving the accuracy of the numerical method due to the original matrix $\mathbf{M}_a$. The second is satisfying the positive definiteness, since $\mathbf{M}_a$ has most of the larger values on the main diagonal. From the requests (A) and (B) we can set up a linear system, whose unknowns x are the entries of the difference matrix $\mathbf{M}_{aS} - \mathbf{M}_a$, that we represent in the usual form $Ax = b$. We have verified that the unknowns are more than the equations in the linear system $Ax = b$ and that at least a solution x exists in all the tested cases both in 2D and 3D. In order to satisfy the request (C) we are interested in the minimum norm solution $\|x\|_2$ that is $x = A^+b$ where $A^+$is the *Moore-Penrose pseudo inverse*[7] of A. Finally it is possible to build the symmetric local constitutive matrix $\mathbf{M}_{aS}$ from the solution x and the matrix $\mathbf{M}_a$.
In order to check if the request (C) leads to the positive definiteness of the constitutive matrices, we have performed thousands of tests on $\mathbf{M}_{aS}$ built for primal surfaces with a number of edges from 3 to 6. The percentages of the cases where $\mathbf{M}_{aS}$ has not been positive definite, due to cells with very bad shapes, have been very low (Table I).

edges	3	4	5	6
%	0.074	0.000	0.004	0.526

Table 1: Percentages of not positive definite matrices

3 Numerical results

In order to check the accuracy of CM with the new constitutive matrices it is enough to perform tests on static problems or frequency domain problems. We have performed two tests and in both of them we have compared the results using the old constitutive matrices built by MIS and the new symmetric ones (Symmetrized MIS). In the first test we have solved the Laplace equation on a square domain [0,1]x[0,1] with Dirichlet boundary condition $\varphi(x, y) = exp(x)cos(y)$. By CM the solution of the Laplace equation:

$$\mathbf{G}^T \mathbf{M}_\varepsilon \mathbf{G} \varphi = 0$$

has been calculated employing a primal triangular grid (Fig.1a) and a primal quadrilateral grid (Fig.1b). In the second test we have calculated the resonant frequencies of a $2D$ circular cavity with radius $R = 0.5$ by CM solving the following generalized eigenvalues problem for TEz modes:

$$\mathbf{C}^T \mathbf{M}_\nu \mathbf{C} \mathbf{V} = \omega^2 \mathbf{M}_\varepsilon \mathbf{V}$$

The eigenfrequencies have been calculated employing a triangular primal grid (Fig.2a), a quadrilateral primal grid (Fig.2b) and a square grid with subgridding (Fig.3a). From the results of the two tests e can verify that the new symmetric matrices ensure the accuracy of CM.

4 CONCLUSION

In this paper we have proposed a novel technique for the construction of the constitutive matrices with some features in order to guarantee the stability and the consistency of some generalized FDTD algorithms. In the 2D cases analyzed in the paper the technique can guarantee a priori the sparsity and the symmetry of the constitutive matrices and the consistency of the numerical method. Moreover some mumerical tests have shown that most of the constitutive matrices are positive definite and that they lead to accurate results. Further work is anyway necessary to check if there are some cases (2D and 3D) where the technique fails and in particular how to modify the technique for those few cases where the constitutive matrices are not definite positive.

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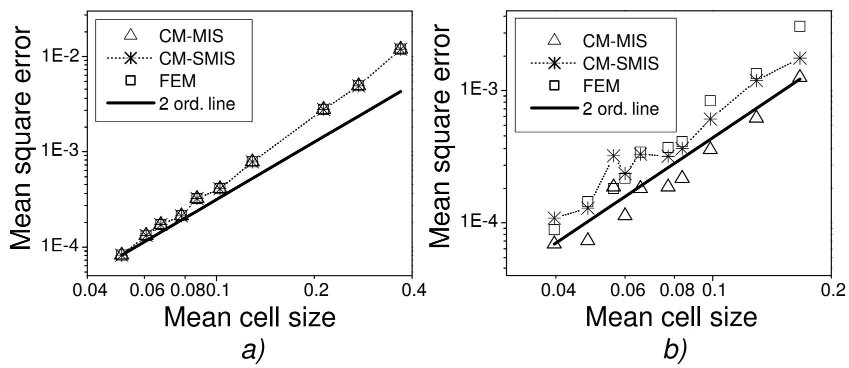

Figure 1: Mean square error vs mean cell size in the solution of the Laplace problem on a square domain (a) using a triangular grid (b) using a quadrilateral grid.

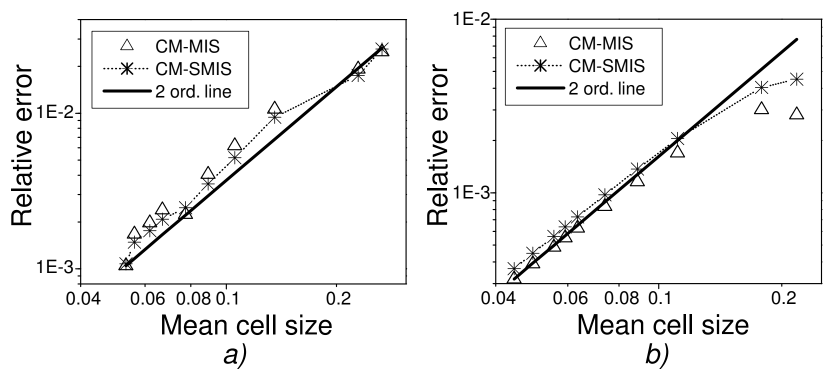

Figure 2: Relative error vs mean cell size in the calculus of the resonant frequency of a circular cavity (a) using a triangular grid (b) using a quadrilateral grid.

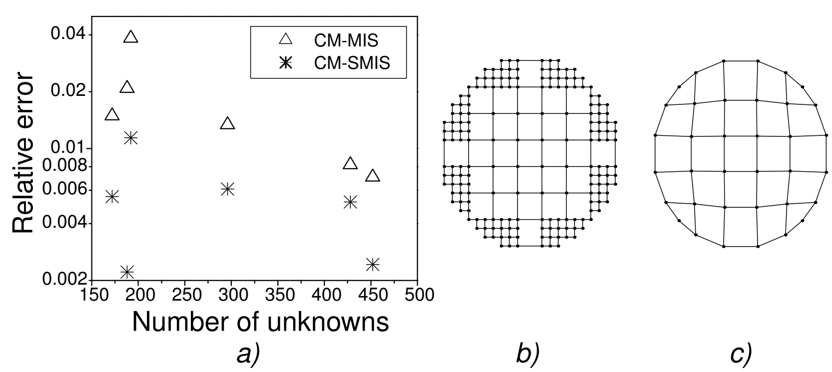

Figure 3: (a) Relative error vs number of unknowns in the calculus of the resonant frequency of a circular cavity with a square grid and subgridding. (b) Primal square grid with subgridding. (c) Primal quadrilateral grid.