

THE GEOMETRY OF TIME-STEPPING

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Abstract—The space-time geometric structure of Maxwell's equations is examined and a subset of them is found to define a pair of exact discrete time-stepping relations. The desirability of adopting an approach to the discretization of electromagnetic problems which exploits this fact is advocated, and the name *topological time-stepping* for numerical schemes complying with it is suggested. The analysis of the equations leading to this kind of time-stepping reveals that these equations are naturally written in terms of integrated field quantities associated with space-time domains. It is therefore suggested that these quantities be adopted as state variables within numerical methods. A list of supplementary prescriptions for a discretization of electromagnetic problems suiting this philosophy is given, with particular emphasis on the necessity to adopt a space-time approach in each discretization step. It is shown that some existing methods already comply with these tenets, but that this fact is not explicitly recognized and exploited. The role of the constitutive equations in this discretization philosophy is briefly analyzed. The extension of this approach to more general kinds of space-time meshes, to other sets of basic time-stepping equations and to other field theories is finally considered.

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- 2 The Founding Equations
- 3 The FDTD Time-Stepping Reconsidered
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1. INTRODUCTION

Time-domain methods for the full-wave analysis of three-dimensional electromagnetic problems, which include methods such as the Finite-Difference Time-Domain method (FDTD) and the Finite Integration Theory (FIT) method, are enjoying great popularity within the Computational Electromagnetics community. This is witnessed not only by the amount of literature devoted to these methods but also by the appearance of several professional simulation packages whose calculation engines are based on them, in addition to the more established ones based on methods such as the Finite Element method and the Method of Moments. A variety of reasons contribute to the diffusion of time-domain methods, for example the possibility to obtain broadband data from a single simulation run, the favorable rate of growth of the required computational resources with the problem size and complexity (provided a minimal critical mass of resources is available), and the existence of convincing implementations for many kinds of material models and boundary conditions. These favorable properties seem able to balance the fact that the struggle to overcome the limitations of the geometrical modeling capabilities traditionally associated with these methods does not appear to have fully succeeded yet.

The present paper focuses on one aspect of time-domain methods, namely, time-stepping formulas, and shows that, with respect to the traditional time-domain approaches, a fundamental improvement derived for time-domain methods from the adoption of a new time-stepping philosophy, which appears to be intrinsically built into the physical laws of electromagnetism. This is made apparent by examining the geometrical backcloth on which these laws are founded, an analysis which reveals the fundamental role played in this improvement by the adoption of a space-time approach (as opposed to one which discretizes separately the space and time variables).

A note of warning is in order about the approach and the terminology adopted within the present work. The concepts that are going to be presented can be given an elegant formulation using the language of algebraic topology. However, since the adoption of this language tends to obscure the simplicity and direct physical meaning of the concepts, that option is not pursued here. The interested reader can find in [5] a reformulation of most of the concepts treated in this

paper in the more abstract and precise language of algebraic topology.

2. THE FOUNDING EQUATIONS

Faraday's law of induction says that for any surface S bounded by the curve ∂S the following relation holds

$$\int_{\partial S} \mathbf{E} + \frac{d}{dt} \int_S \mathbf{B} = 0 \quad (1)$$

where \mathbf{E} is the electric field intensity and \mathbf{B} is the magnetic flux density. Integrating Equation (1) for a time interval $[t_1, t_2]$, we obtain

$$\int_{t_1}^{t_2} \int_{\partial S} \mathbf{E} + \int_S \mathbf{B} \Big|_{t_2} - \int_S \mathbf{B} \Big|_{t_1} = 0 \quad (2)$$

Rearranging the terms appearing in Equation (2) we can write it as follows

$$\int_S \mathbf{B} \Big|_{t_2} = \int_S \mathbf{B} \Big|_{t_1} - \int_{t_1}^{t_2} \int_{\partial S} \mathbf{E} \quad (3)$$

Equation (3) enjoys a number of interesting properties from the point of view of a time-domain numerical method. First, it applies to surfaces and time intervals which are not required to be infinitesimal in extension. This means that within a numerical method the surface S can be one of the faces of the cells which form the mesh and the interval $[t_1, t_2]$ can be a discrete time-step. Moreover, Equation (3) expresses the quantity on the left side, which is defined at the time instant t_2 , in terms of quantities defined (except for the negligible contribution of the line ∂S considered at the time instant t_2) at time instants which precede t_2 . Consequently, Faraday's induction law written in the space-time integral form of Equation (3) defines an explicit time-stepping relation which applies exactly (i.e., without approximations) to discrete space-time domains.

A relevant feature of Equation (3) that will be discussed in more detail later is the fact that it is an algebraic relation between integrals of field quantities evaluated on space-time domains. A bit of reflection reveals that the physical quantities that correspond to these integrals enjoy a logical (and historical) primacy over the corresponding field quantities \mathbf{E} and \mathbf{B} . The latter are actually physical-mathematical abstractions derived by means of a limit process performed on the integral quantities by letting the integration domain shrink to zero, whereas the integral quantities can be thought of as representing the results of actual measurements. To simplify the formulas and

to emphasize their priority over field quantities, let us associate a symbol to the integral quantities appearing in Equation (3). A simple check reveals that all these quantities have the physical dimension of a magnetic flux. Moreover, all are obtained from an integral evaluated on a two-dimensional space-time domain. This entitles us to consider both kinds of integral quantities as manifestations of the same physical quantity: magnetic flux [5]. We shall therefore write

$$\phi_{S \times t}^b \stackrel{\text{def}}{=} \int_S \mathbf{B} \Big|_t \quad (4)$$

$$\phi_{\gamma \times [t_1, t_2]}^e \stackrel{\text{def}}{=} \int_{t_1}^{t_2} \int_{\gamma} \mathbf{E} \quad (5)$$

where the symbol \times denotes the cartesian product. Note that for the sake of generality we have substituted in Equation (5) the generic regular curve γ to the closed curve ∂S appearing in Faraday's law. Let us call ϕ^b the magnetic part of the magnetic flux and ϕ^e the electric part of it. Thanks to these definitions we can rewrite Faraday's induction law as follows

$$\phi_{S \times t_2}^b = \phi_{S \times t_1}^b - \phi_{\partial S \times [t_1, t_2]}^e \quad (6)$$

and give it the following simple geometrical illustration [1, 6]. The curve ∂S considered during the time interval $[t_1, t_2]$ forms a two-dimensional space-time cylinder $\partial S \times [t_1, t_2]$. The surface S considered at the time instant t_1 (i.e., the cartesian product $S \times t_1$) forms the bottom of that cylinder, whereas the surface $S \times t_2$ constitutes its top (Figure 1).

Faraday's law then asserts that the algebraic sum of the electric and magnetic parts of the magnetic flux associated with a surface of this kind is always zero. Correspondingly, Equation (6) shows that we can exploit this property to determine the value of the magnetic flux ϕ^b associated with the cylinder's top, provided we know the values of ϕ^e and ϕ^b associated with the cylinder's surface and bottom, respectively (Figure 2).

Remark: The terms appearing in Equation (6) are endowed with signs that are a consequence of the orientation of the surfaces with which these terms appear to be associated. The orientation of geometric objects plays a fundamental role in the establishment of a coherent set of equations for a physical theory. This appears clearly provided the concept of orientation is unfolded in all its complexity, taking into account in particular the existence of two kinds of orientation. There is no room here for a complete treatment of this fascinating subject. The reader is referred to [5] for an analysis which includes the issue of orientation.

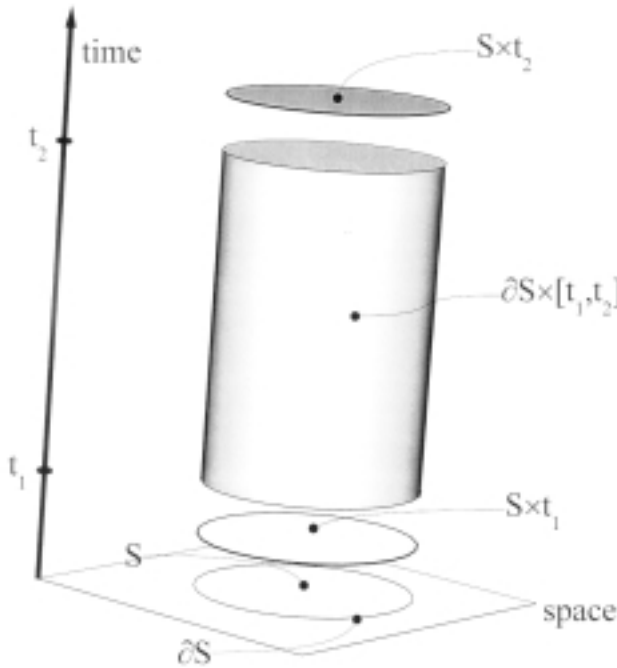


Figure 1. Exploded view of the space-time geometrical objects that enter the formulation of Faraday's induction law in integral form. The boundary ∂S of the surface S determines a two-dimensional space-time cylinder $\partial S \times [t_1, t_2]$, which has the surface S considered at the time instant t_1 (i.e., $S \times t_1$) at its bottom, and the same surface considered at the time instant t_2 (i.e., $S \times t_2$) at its top.

The same geometric approach can be applied to the interpretation of Maxwell-Ampère's law. This law says that for any surface S bounded by the curve ∂S the following relation holds

$$\int_{\partial S} \mathbf{H} - \frac{d}{dt} \int_S \mathbf{D} = \int_S \mathbf{J} \quad (7)$$

where \mathbf{H} is the magnetic field intensity and \mathbf{D} is the electric flux density. Integrating Equation (7) for a time interval $[t_1, t_2]$ we obtain

$$\int_{t_1}^{t_2} \int_{\partial S} \mathbf{H} - \int_S \mathbf{D} \Big|_{t_2} + \int_S \mathbf{D} \Big|_{t_1} = \int_{t_1}^{t_2} \int_S \mathbf{J} \quad (8)$$

All the terms appearing in Equation (8) have the physical dimension

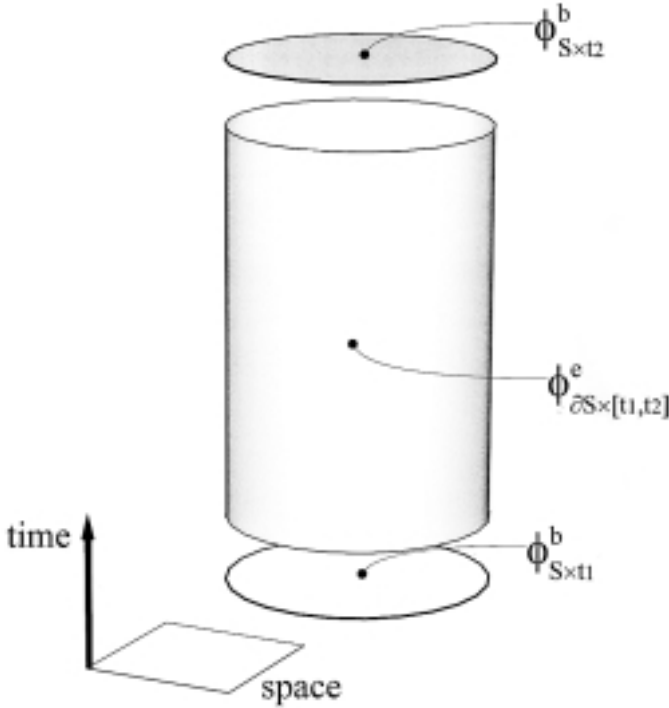


Figure 2. The physical quantities which appear in the space-time integral formulation of Faraday's induction law are the electric part of the magnetic flux ϕ^e and its magnetic part ϕ^b . The flux ϕ^e is associated with the two-dimensional space-time cylinder $\partial S \times [t_1, t_2]$, whereas ϕ^b is associated with the top and bottom surfaces $S \times t_2$ and $S \times t_1$, respectively. Faraday's law asserts that the algebraic sum of these quantities (with signs reflecting the orientation of the surfaces) is always zero. Consequently the value of ϕ^b at the final time instant t_2 can be calculated exactly from quantities defined at previous times.

of electric charge. However, the terms appearing on the left side of the equation are integrals evaluated on two-dimensional space-time domains and can therefore be considered as fluxes, whereas the integral on the right side is evaluated on a three-dimensional space-time domain and hence the corresponding quantity cannot be a flux. In fact this quantity is the charge content of the three-dimensional space-time cylinder due to the current flow through the surface S during the

time interval $[t_1, t_2]$. We shall therefore write

$$\psi_{S \times t}^d \stackrel{\text{def}}{=} \int_S \mathbf{D} \Big|_t \quad (9)$$

$$\psi_{\gamma \times [t_1, t_2]}^h \stackrel{\text{def}}{=} \int_{t_1}^{t_2} \int_{\gamma} \mathbf{H} \quad (10)$$

and

$$Q_{S \times [t_1, t_2]}^j \stackrel{\text{def}}{=} \int_{t_1}^{t_2} \int_S \mathbf{J}$$

where ψ^d is the electric part of the electric flux, ψ^h is the magnetic part of it and Q^j is the charge content described above. Thanks to these definitions, we can rewrite Maxwell-Ampère's law as follows

$$\psi_{S \times t_2}^d = \psi_{S \times t_1}^d + \psi_{\partial S \times [t_1, t_2]}^h - Q_{S \times [t_1, t_2]}^j \quad (11)$$

Note that, as we did for Faraday's law, we have rearranged the terms in order to express the quantity corresponding to the final time instant t_2 as a function of quantities defined (except for negligible contributions) at former times. The geometric interpretation proceeds along lines similar to those given to Faraday's law, except for the presence of a contribution associated with the three-dimensional space-time cylinder $S \times [t_1, t_2]$.

Hence, Equation (11) says that we can determine the value of the electric flux ψ^d associated with the cylinder's top surface, provided we know the values of ψ^h , ψ^d and Q^j associated with the two-dimensional cylinder's space-time surface, with its bottom surface and with the three-dimensional space-time volume, respectively (Figure 3).

3. THE FDTD TIME-STEPPING RECONSIDERED

Let us examine now what the geometrical analysis of Faraday's and Maxwell-Ampère's law carried out in the previous section reveals about the inner workings of the time-stepping formulas of an actual numerical method, namely, FDTD.

The FDTD method applies to the solution of initial-boundary value electromagnetic problems. The domain of a typical FDTD problem is therefore constituted by the cartesian product of the spatial domain of the problem and of the time interval for which the solution is sought. In its basic form the FDTD method discretizes the spatial domain by means of two uniform orthogonal cartesian grids reciprocally staggered in each direction by a half step. These grids determine therefore two sets of rectangular cells. To simplify the

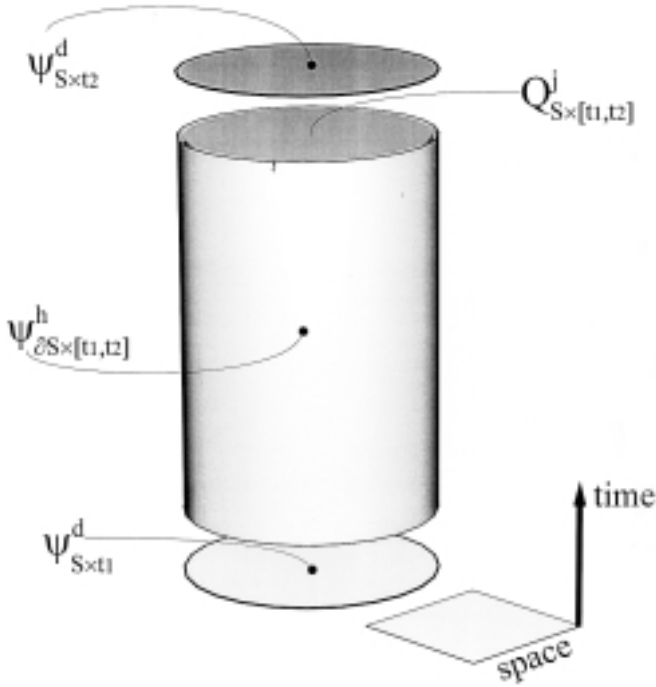


Figure 3. The physical quantities which appear in the space-time integral formulation of Maxwell-Ampère's law are the electric part ψ^d , the magnetic part ψ^h of the electric flux, and the electric charge content Q^j . The flux ψ^h is associated with the two-dimensional space-time cylinder $\partial S \times [t_1, t_2]$, whereas ψ^d is associated with the top and bottom surfaces $S \times t_2$ and $S \times t_1$, respectively. The charge Q^j is associated with the three-dimensional space-time cylinder $S \times [t_1, t_2]$. Maxwell-Ampère's law asserts that the algebraic sum of the electric flux associated with the surface of the cylinder equals the amount of charge contained within it. This permits the determination of ψ^d at the final time instant t_2 of the interval from quantities defined at previous times.

notation it is expedient to align the coordinate axes with the edges of the cells, to make the origin correspond to a node of one of the two grids and call Δx , Δy , Δz the corresponding step widths.

The fields are represented on this discretized domain by associating the field quantities with the edges of the cells. In particular, with each edge of one of the grids is associated the average value of the component of \mathbf{E} along that edge, and with each edge of the other grid

is associated the average value of the component of \mathbf{H} along that edge. The grid housing on its edges the \mathbf{E} field is usually called the *primary* grid whereas that housing \mathbf{H} is called the *secondary* grid. Each field value is usually assumed to be attached to the midpoint of the edge it refers so that the following index notation can be adopted

$$\begin{aligned} E_{x(i+\frac{1}{2},j,k)} &\stackrel{\text{def}}{=} E_x((i+\frac{1}{2})\Delta x, j\Delta y, k\Delta z) \\ H_{x(i,j+\frac{1}{2},k+\frac{1}{2})} &\stackrel{\text{def}}{=} H_x(i\Delta x, (j+\frac{1}{2})\Delta y, (k+\frac{1}{2})\Delta z) \end{aligned} \quad (12)$$

with the obvious extension to the remaining field components. All this can be represented graphically by means of the so-called Yee cell (Figure 4).

We must now consider how the FDTD method deals with the time variable. The time interval which constitutes the time domain of the problem is discretized by FDTD using two dual uniform grids, one for each spatial grid, defined on the time axis and mutually staggered by half the time step Δt . Corresponding to the primary and secondary grids in space we have therefore a primary and a secondary grid in time. By considering the product of each space grid by the corresponding time grid one obtains two space-time grids staggered in both space and time. The FDTD state variables are assumed to be the time average of the field components during a time step. For example the components of \mathbf{E} are thought of as time averages evaluated for primary time intervals and are traditionally assumed to be attached to the midpoint of those time intervals. According to this additional association and with the adoption of an index for the time variable, the notation for the field quantities becomes

$$\begin{aligned} \mathbf{E}_{x(i+\frac{1}{2},j,k,n+\frac{1}{2})} &\stackrel{\text{def}}{=} \mathbf{E}_x((i+\frac{1}{2})\Delta x, j\Delta y, k\Delta z, (n+\frac{1}{2})\Delta t) \\ \mathbf{H}_{x(i,j+\frac{1}{2},k+\frac{1}{2},n)} &\stackrel{\text{def}}{=} \mathbf{H}_x(i\Delta x, (j+\frac{1}{2})\Delta y, (k+\frac{1}{2})\Delta z, n\Delta t) \end{aligned} \quad (13)$$

with the obvious extension to the remaining field components.

Let us now consider simultaneously the space and time variables as discretized by the FDTD method. We have seen that the field quantities which constitute the state variables of this method are staggered not only in space but also in time. From this point of view the limitations of the traditional representation of Figure 4 become apparent. Albeit correct from the point of view of the disposition of the state variables in space, that representation tends to convey the misleading idea that field quantities which are actually specified by the FDTD method as existing at different time instants, be instead

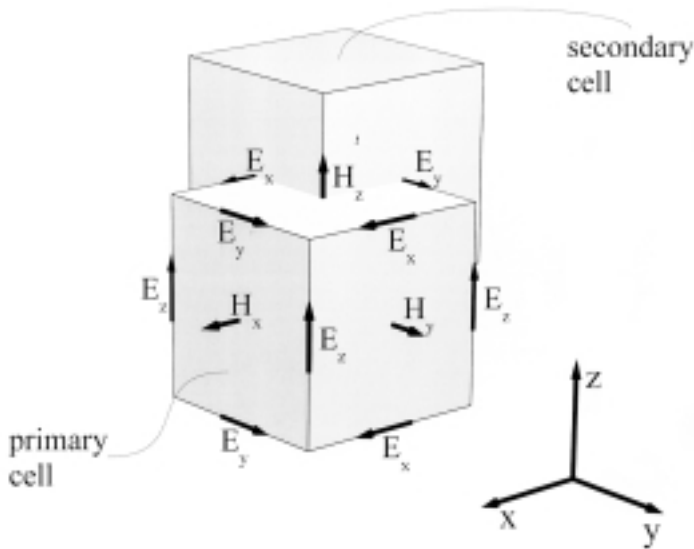


Figure 4. The primary and secondary Yee cells that are at the basis of the FDTD method. Primary cells have the average value of the components of \mathbf{E} along their edges attached to the midpoint of the corresponding edge. The components of \mathbf{H} , which are attached to the edges of secondary cells, appear therefore at the center of the faces of primary cells. We will see later that thanks to the constitutive equations, the components of \mathbf{H} can be interpreted as components of the magnetic flux density field \mathbf{B} attached to the faces of primary cells. Correspondingly, the components of \mathbf{E} are located at the center of the faces of secondary cells and can be interpreted as components of the electric flux density \mathbf{D} .

simultaneously defined at a common time instant. To circumvent this problem let us consider instead of the Yee cell, a Yee *hypercell*, i.e. the space-time object which is determined by the evolution of a Yee cell during a time step. For example, if we consider the evolution of a primary cell of the spatial grid for the duration of a primary time step, we obtain a primary hypercell (Figure 5).

The hypercell representation shows that during a primary time step, each edge of the primary spatial cell spans a space-time surface (which appears as a oblique surface in Figure 5). We saw that the FDTD state variables are assumed as associated with the midpoints of the edges of the cells and of the time-step intervals; hence, in the space-time perspective they appear to be attached to the center of the corresponding space-time surfaces. Therefore each of the quantities

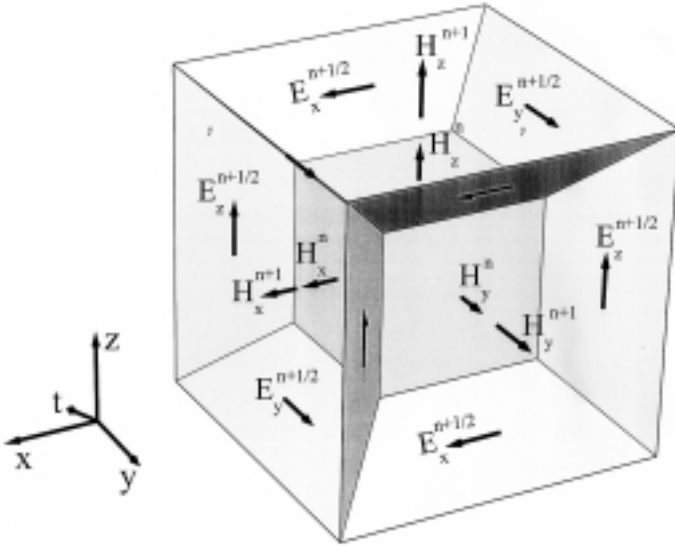


Figure 5. The primary Yee hypercell determined by the evolution of a primary Yee cell during the primary time step Δt going from the time instant $n\Delta t$ to $(n+1)\Delta t$. The components of \mathbf{E} appear attached to the centers of the space-time surfaces formed by the primary edges during their evolution in time. The components of \mathbf{H} appear instead attached to the centers of spatial surfaces considered at the initial and final time instants. Hence all components appear associated with surfaces, either in space or in space-time.

appearing in Figure 5 — which from a purely spatial point of view we considered as associated with edges - is actually attached to the center of a surface, either in space or in space-time, and is thought of as the average value of the field component for that surface.

The hypercell representation of Figure 5 shows also that for each face of the traditional Yee cell there is a space-time parallelepiped analogous to the space-time cylinder we used to interpret geometrically Faraday's law (these space-time parallelepipeds appear in Figure 5 as truncated pyramids). The edges which form the boundary of the face of the Yee cell are the analogous of the boundary ∂S shown in Figure 1 and span a two-dimensional space-time “cylinder” which has the spatial face considered at the beginning of the time step as its bottom, and the same face considered at the end of the time step as its top. The only difference between the space-time parallelepipeds of Figure 5 and the space-time cylinder of Figure 2 is therefore the presence

of the components of the fields \mathbf{E} and \mathbf{H} in place of integrated field quantities ϕ^e and ϕ^b . However, since each field quantity is considered as the average value of the field component for the surface it corresponds to, the product of each component by the extension of its face gives the value of the integrated field quantity for that face. In other words, we can write

$$\Delta y \Delta z \mu_{(i,j+\frac{1}{2},k+\frac{1}{2})} H_{x(i,j+\frac{1}{2},k+\frac{1}{2},n)} = \phi_{(i,j+\frac{1}{2},k+\frac{1}{2},n)}^{b_x} \quad (14)$$

$$\Delta y \Delta t E_{y(i,j+\frac{1}{2},k,n+\frac{1}{2})} = \phi_{(i,j+\frac{1}{2},k,n+\frac{1}{2})}^{e_y} \quad (15)$$

$$\Delta z \Delta t E_{z(i,j,k+\frac{1}{2},n+\frac{1}{2})} = \phi_{(i,j,k+\frac{1}{2},n+\frac{1}{2})}^{e_z} \quad (16)$$

where we have exploited the constitutive relation

$$B_{x(i,j+\frac{1}{2},k+\frac{1}{2},n)} = \mu_{(i,j+\frac{1}{2},k+\frac{1}{2})} H_{x(i,j+\frac{1}{2},k+\frac{1}{2},n)} \quad (17)$$

(the meaning of which will be considered in detail later). Equations (14) to (16) transform the Yee hypercell into a hypercell which has associated with its faces integrated field quantities instead of field components (Figure 6).

We will show now that, thanks to this reinterpretation of the FDTD state variables, the FDTD time-stepping formula for each component of \mathbf{H} appearing in Figure 5 is analogous to Faraday's time-stepping formula given in Equation (6). One such time-stepping formula is, for example [8]

$$\begin{aligned} \Delta y \Delta z \mu_{(i,j+\frac{1}{2},k+\frac{1}{2})} H_{x(i,j+\frac{1}{2},k+\frac{1}{2},n+1)} = \\ \Delta y \Delta z \mu_{(i,j+\frac{1}{2},k+\frac{1}{2})} H_{x(i,j+\frac{1}{2},k+\frac{1}{2},n)} + \end{aligned} \quad (18)$$

$$\begin{aligned} \Delta y \Delta t \left(E_{y(i,j+\frac{1}{2},k+1,n+\frac{1}{2})} - E_{y(i,j+\frac{1}{2},k,n+\frac{1}{2})} \right) - \\ \Delta z \Delta t \left(E_{z(i,j+1,k+\frac{1}{2},n+\frac{1}{2})} - E_{z(i,j,k+\frac{1}{2},n+\frac{1}{2})} \right) \end{aligned} \quad (19)$$

and involves the components appearing in the truncated pyramids (which are actually space-time parallelepipeds) shown in Figure 5, one of which is isolated for ease of reference in Figure 7. Exploiting Equations (14), (15) and (16) the FDTD time-stepping formula of Equation (19) can be rewritten in terms of integrated field quantities,

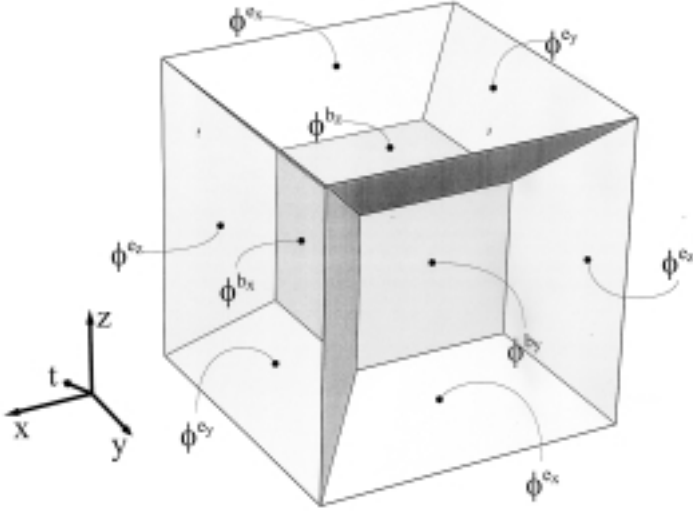


Figure 6. In a Yee hypercell each cell face considered during a time step spans a space-time cell. The field components of \mathbf{E} and \mathbf{H} of primary hypercell appear attached to the center of these space-time cells and, being average values, can be interpreted as integrated field quantities ϕ^e and ϕ^b associated with them. Note that the transition from the components of \mathbf{H} to the magnetic fluxes ϕ^b implies the constitutive equation which links the field quantities \mathbf{H} and \mathbf{B} . On this basis the FDTD time-stepping formulas for the field components of \mathbf{H} can be interpreted as the time advancement of ϕ^b dictated by Faraday's induction law.

as follows

$$\begin{aligned} \phi_{(i,j+\frac{1}{2},k+\frac{1}{2},n+1)}^{b_x} &= \phi_{(i,j+\frac{1}{2},k+\frac{1}{2},n)}^{b_x} + \\ &\phi_{(i,j+\frac{1}{2},k+1,n+\frac{1}{2})}^{e_y} - \phi_{(i,j+\frac{1}{2},k,n+\frac{1}{2})}^{e_y} - \\ &\phi_{(i,j+1,k+\frac{1}{2},n+\frac{1}{2})}^{e_z} + \phi_{(i,j,k+\frac{1}{2},n+\frac{1}{2})}^{e_z} \end{aligned} \quad (20)$$

A simple comparison reveals that Equation (20) is a particular case of the time-stepping relation (Equation (6)) which we deduced from Faraday's induction law. The same process can be obviously applied to the FDTD time-stepping formulas for the other components of the \mathbf{H} field.

Secondary Yee hypercells, i.e., hypercells obtained by considering the evolution of a secondary Yee cell during a secondary time step, can

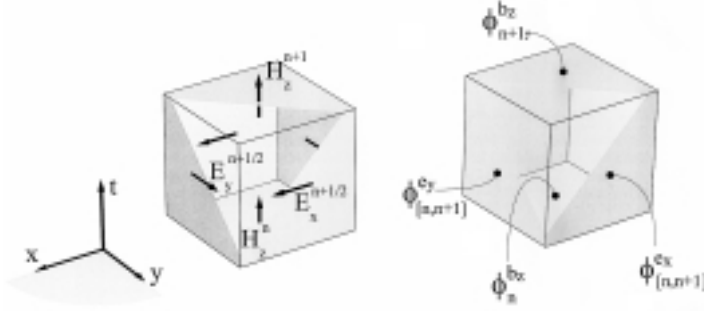


Figure 7. Each FDTD time-stepping formula for the components of \mathbf{H} involves the components of field quantities located on primary space-time parallelepipeds. On the faces of these parallelepipeds the field components appearing in the FDTD formula correspond to integrated field quantities ϕ^e and ϕ^b , and the formula itself corresponds to the time advancement of these integrated field quantities dictated by Faraday's induction law written in space-time integral form. The same can be shown to apply for the FDTD time-stepping formulas for the components of \mathbf{E} , which turn out to implement Maxwell-Ampère's law on the integrated field quantities ψ^h and ψ^d defined on the secondary space-time grid.

be obviously subjected to an analogous process leading to hypercells housing fluxes ψ^h and ψ^d and charges Q^j . Repeating the considerations above for a secondary Yee hypercell, the FDTD time stepping formula for the components of the \mathbf{E} field can be shown to be actually a case of the time-stepping relation of the kind represented by Equation (11) deduced from Maxwell-Ampère's law (Figure 8). For example, starting from the FDTD time-stepping formula for E_x [8]

$$\begin{aligned}
 & \Delta y \Delta z \varepsilon_{(i+\frac{1}{2},j,k)} E_{x(i+\frac{1}{2},j,k,n+\frac{1}{2})} = \\
 & \Delta y \Delta z \varepsilon_{(i+\frac{1}{2},j,k)} E_{x(i+\frac{1}{2},j,k,n-\frac{1}{2})} + \\
 & -\Delta y \Delta t \left(H_{y(i+\frac{1}{2},j,k+\frac{1}{2},n)} - H_{y(i,j+\frac{1}{2},k-\frac{1}{2},n)} \right) + \\
 & \Delta z \Delta t \left(H_{z(i+\frac{1}{2},j+\frac{1}{2},k,n)} - H_{z(i+\frac{1}{2},j-\frac{1}{2},k,n)} \right) \\
 & \Delta y \Delta z \Delta t \sigma_{(i+\frac{1}{2},j,k)} \left(\frac{E_{x(i+\frac{1}{2},j,k,n+\frac{1}{2})} + E_{x(i+\frac{1}{2},j,k,n-\frac{1}{2})}}{2} \right)
 \end{aligned} \tag{21}$$

and considering the field components as representatives of integrated field quantities, according to

$$\Delta y \Delta z \varepsilon_{(i+\frac{1}{2},j,k)} E_{x(i+\frac{1}{2},j,k,n+\frac{1}{2})} = \psi_{(i+\frac{1}{2},j,k,n+\frac{1}{2})}^{d_x} \tag{22}$$

$$\Delta y \Delta t H_{y(i+\frac{1}{2},j,k+\frac{1}{2},n)} = \psi_{(i+\frac{1}{2},j,k+\frac{1}{2},n)}^{h_y} \quad (23)$$

$$\Delta z \Delta t H_{z(i+\frac{1}{2},j+\frac{1}{2},k,n)} = \psi_{(i+\frac{1}{2},j+\frac{1}{2},k,n)}^{h_z} \quad (24)$$

$$\Delta y \Delta z \Delta t \sigma_{(i+\frac{1}{2},j,k)} \cdot \left(\frac{E_{x(i+\frac{1}{2},j,k,n+\frac{1}{2})} + E_{x(i+\frac{1}{2},j,k,n-\frac{1}{2})}}{2} \right) = Q_{(i+\frac{1}{2},j,k,n)}^{j_x} \quad (25)$$

(where we have used the constitutive relations linking \mathbf{E} to \mathbf{D} and to \mathbf{J}) we obtain the time-stepping formula

$$\begin{aligned} \psi_{(i+\frac{1}{2},j,k,n+\frac{1}{2})}^{d_x} &= \psi_{(i+\frac{1}{2},j,k,n-\frac{1}{2})}^{d_x} - \\ &\psi_{(i+\frac{1}{2},j,k+\frac{1}{2},n)}^{h_y} + \psi_{(i+\frac{1}{2},j,k-\frac{1}{2},n)}^{h_y} + \\ &\psi_{(i+\frac{1}{2},j+\frac{1}{2},k,n)}^{h_z} - \psi_{(i+\frac{1}{2},j-\frac{1}{2},k,n)}^{h_z} + \\ &Q_{(i+\frac{1}{2},j,k,n)}^{j_x} \end{aligned} \quad (26)$$

which corresponds to the time-stepping relation (Equation (11)) derived from Maxwell-Ampère's law.

4. TOPOLOGICAL TIME-STEPPING

Let us summarize the main points revealed by the analysis carried out in the previous sections.

- a.** *Time-stepping based on intrinsical discrete statements:* We have seen that within the equations of electromagnetism there is a set of relations which link discrete quantities defined at different time instants. These relations are intrinsically discrete in the sense that they apply not only as differential relations within infinitesimal domains, but hold exactly for macroscopical domains as well. They are consequently natural candidates for the setup of time-stepping procedures within numerical methods. The first step in the discretization of a field problem should therefore be the individuation within the equations of the problem of this special set of statements

REMARK I: Observing more closely the nature of this set of equations, one discovers that they are actually conservation or balance statements. In other words, they relate a physical quantity associated with a given domain, with another physical quantity associated with the boundary of that domain. This is apparent in

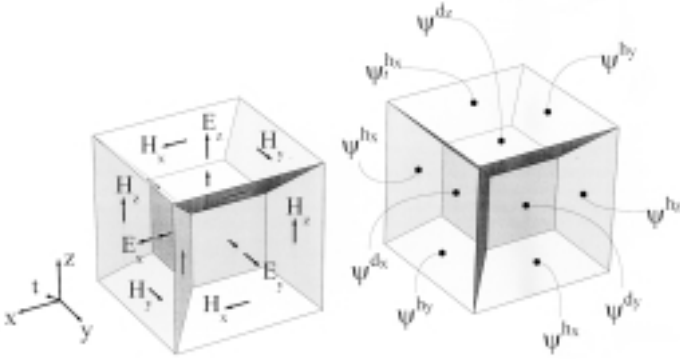


Figure 8. The secondary Yee hypercell (left) determined by the evolution of a secondary Yee cell during a secondary time step. The components of \mathbf{H} appear attached to the centers of the space-time faces, whereas the components of \mathbf{E} appear attached to the centers of spatial surfaces considered at the initial and final time instants. These field components can be considered as representatives of the integrated field quantities ψ^h , ψ^d and Q^j (this last quantity is not represented in the figure), with the constitutive relations linking \mathbf{E} to \mathbf{D} and \mathbf{J} being invoked to obtain ψ^d and Q^j . On each space-time three-dimensional cell of the hypercell, the integrated field quantities thus assigned, determine an exact time-stepping relation.

Maxwell-Ampère's law as expressed by Equation (8), which asserts the equivalence between the electric charge content of a three-dimensional space-time cylinder and the electric flux associated with the surface of that cylinder. The same can be said to hold in the case of Faraday's law expressed by Equation (2), with the only difference that the quantity associated with the three-dimensional space-time cylinder (a magnetic charge) is always zero. When this happens the balance equation is said to be a conservation statement (in the case of Faraday's law, the conservation of magnetic flux)¹

REMARK II: Given their intrinsic discrete nature, balance and conservation statements are naturally expressed as algebraic relations between integrated field quantities from which the corresponding differential statements can be derived. We see therefore that to the distinction between algebraic and differential statements corresponds a distinction between discrete and non-discrete representations of physical quantities. One can find in the literature various name pairs used to label this latter distinction. A nonexhaustive list includes the mathematically

oriented distinction of *discrete* and *continuous* quantities, the more physically related distinction between *integrated fields* and *fields*, that between *global* and *local* quantities, that between *macroscopic* and *microscopic* quantities, and the more engineering oriented distinction between *circuit* and *field* quantities. Another good suggestion to convey the spirit of this distinction was put forth in the context of integration theory by Henri Lebesgue [3]. Lebesgue observed that the fundamental difference is that between physical quantities thought of as associated with points and quantities thought of as associated with domains of non-infinitesimal extension. He suggested therefore to call the former *point functions* (“fonctions de point”) and the latter *domain functions* (“fonctions de domaine”). Adopting the spirit of that observation we will call from now on *domain quantities* those that we have formerly called integrated fields, and *point quantities* those that are derived from domain quantities by means of a limit process.

- b. *Adoption of domain quantities as state variables:* Balance and conservation statements are naturally written in terms of domain quantities, which are directly associated with the cells of the discretization meshes, hence it is desirable to use domain quantities instead of point quantities (and, in particular, of field components) as state variables within a numerical method.
- c. *Adoption of a space-time approach:* The balance and conservation laws which determine the intrinsically discrete time-stepping equations are space-time statements written in terms of quantities associated with space-time domains, not merely with spatial domains. Therefore it is fundamental to adopt a truly space-time approach both in establishing the association of physical quantities with domains (which are therefore *space-time domain quantities*), in writing the corresponding discrete statements and in setting up the meshes which discretize the problem's domain.
- d. *Availability of suitable cells in the discretization meshes :* For each domain quantity appearing in the equations of the problem to be numerically solved, there must be available in the discretization meshes the kind of cell required to house that domain quantity. For example, to house the quantities (fluxes and charge contents) appearing in Faraday's and in Maxwell-Ampère's law we need space-time surfaces and space-time volumes, which must therefore appear in the discretization meshes of a discretized electromagnetic problem. Conversely, the mere collection of nodes of the classical Finite Difference methods does not appear sufficient for this task.

- e. *Adoption of multiple meshes:* Faraday's law and Maxwell-Ampère's law determine two distinct balance laws, each with its own set of domain quantities. We need therefore two logically distinct ensembles of space-time cells to perform the time-stepping related to these two laws. This calls for the adoption of two discretization grids or meshes, as exemplified by the pair of dual primary and secondary grids of the FDTD and FIT method². Note, however, that the two meshes might well be geometrically coincident and only logically distinct.

Keeping in mind the points enumerated above while setting up a numerical method, opens the way to the possibility to build into the method the intrinsically discrete balance laws which institute an exact link between quantities defined at different time instants. Since the validity of these balance laws do not depend on the size and the shape of the domain to which they refer, nor on the material the domain is filled with, they are endowed with a kind of “topological significance” [6], which suggests for them the name of *topological equations*. Correspondingly, for a time-stepping relation based on the exploitation of the intrinsic space-time discreteness of topological equations we suggest the name of *topological time-stepping*.

Note that, given a field problem, once the space-time domain quantities involved in it are correctly recognized and the space-time domain has been suitably discretized, the form of the topological time-stepping relations is uniquely determined. This is to be contrasted with the traditional approaches, which discretize first separately the domain in space and determine thus from the original set of partial differential equations a set of ordinary differential equations in the time variable, which are then discretized using one of the many of techniques developed for the numerical integration of ordinary differential equations.

The awareness of the existence of the topological time-stepping approach reveals the pitfalls hidden in this classical approach, namely, the possibility to obtain — by combining an arbitrary discretization

¹ Conservation statements have a deeper meaning with respect to generic balance statements. The latter can be made usually to descend from the former under mild hypotheses on the topology of the domain in which they hold. For example, in the case of electromagnetism, Maxwell-Ampère's law is a consequence, in a topologically trivial space, of the law of conservation of electric charge, and can be considered merely the relation which defines the physical quantity electric flux.

² The question of the orientation of the domains with which physical quantities are associated, the analysis of which is not dealt with in the present work, is another strong argument for the distinction of the grid on which the time stepping of electric flux and that of the magnetic flux are performed. See [5] for details.

scheme in space with an equally arbitrary one in time — a non-topological time-stepping scheme, i.e. one which does not adhere to the time advancement scheme for physical quantities dictated by the physics of the problem. Of course it is still possible that such a combination yields a topological time-stepping scheme, as testified by the FDTD equations, which - although constructed taking as a starting point Maxwell's equations written in differential form [8] - turn out to be actually interpretable as a topological time-stepping scheme. However, without the guide constituted by the topological time-stepping principle the attainment of a topological time-stepping scheme appears problematic, considering for example that in the case of FDTD that result might have been missed, had the discretization of the differential operators been performed differently, for example using some higher order approximation scheme.

As a final aside, which does not follow directly from the necessarily cursory analysis of the electromagnetic equations presented above but can be easily proved adopting a suitable formal approach, there is a further point which deserves to be included in the list of those leading to a correct approach to numerical discretization, namely the importance of a

- f. *Suitable global structure of the meshes:* To complement Faraday's and Maxwell-Ampère's law, which express a conservation and a balance statement for arbitrary space-time cylinders (i.e., particular space-time volumes of the kind $S \times [t_1, t_2]$ enclosed by space-time closed surfaces), there are Gauss' magnetic and Gauss' electric law that express the same statements for the case of arbitrary volumes in space bounded by closed surfaces in space. In terms of domain quantities these laws can be written as follows

$$\phi_{V \times t}^b = 0 \quad (27)$$

$$\psi_{\partial V \times t}^d = Q_{V \times t}^\rho \quad (28)$$

where $Q_{V \times t}^\rho$ is the electric charge content of the volume V at the time instant t . In setting up a numerical technique for an initial-value field problem we must assure that these relations, if satisfied by the domain quantities as initially assigned to the cells of the mesh, continue to be so during the time stepping. It can be proved [5, 7] that when the guidelines enumerated above are followed (and, therefore, a topological time-stepping is used), a sufficient condition for this to happen is the adoption of discretization meshes which have a suitable global structure. It is required in particular that the cells are properly joined, in such a way that the amount of change of the domain quantity

associated with each cell of the mesh following the execution of a time step be due only to the effects of a source appearing explicitly in the time-stepping formula or to a redistribution of that quantity among adjacent cells. The fact that the compliance with Gauss' laws follows only from a topological constraint on the structure of the mesh might seem trivial at first but its relevance can be appreciated considering that it assures that no additional constraints need to be imposed on the state variables to comply with these laws. This topological constraint makes of the mesh a so-called cell-complex [5]; as might be expected, both the FDTD and the FIT grids comply with it.

5. THE MISSING LINK

Generalizing Equation (20) we can write the generic form of the topological time-stepping formula for the domain quantity ϕ^b as follows

$$\Phi_{n+1}^b = \Phi_n^b - \mathbf{I}_c \Phi_{n+\frac{1}{2}}^e \quad (29)$$

where Φ^b and Φ^e are vectors which collect all the instances of ϕ^b and ϕ^e appearing in the primary space-time mesh, and \mathbf{I}_c is a matrix whose nonzero entries are only 1 and -1 and which represents in discrete form the action of the curl operator on the primary mesh. For the topological time-stepping of ψ^d , generalizing Equation (26), we have correspondingly

$$\Psi_{n+\frac{1}{2}}^d = \Psi_{n-\frac{1}{2}}^d + \tilde{\mathbf{I}}_c \Psi_n^h - \mathbf{Q}_n^j \quad (30)$$

where Ψ^d , Ψ^h and \mathbf{Q}^j are vectors which collect all the instances of ψ^d , ψ^h and Q^j appearing in the secondary mesh, and $\tilde{\mathbf{I}}_c$ is a matrix whose nonzero entries are only 1 and -1 and which represents in discrete form the action of the curl operator on the secondary mesh. We emphasize once again that Equation (29) and Equation (30) are exact discrete statements which derive directly from the balance and conservation laws of electromagnetism written for a space-time mesh. In other words, only the space-time domain was discretized to obtain these equations, not some set of partial differential equations.

The topological time-stepping formulas of Equation (29) and Equation (30), however, do not determine alone a complete time-advancement strategy and consequently neither a numerical method. This can be understood by considering the number of state variables appearing in these two equations. Even supposing that the values of Φ^b and of Ψ^d at the initial time instant be assigned as problem

data, there remains the problem to determine the values of Φ^e , Ψ^d and \mathbf{Q}^j to be inserted in the time-stepping equations to advance in time Φ^b and of Ψ^d . Geometrically, with reference to Figure 2 and Figure 3, this situation corresponds to the impossibility to obtain from this equations alone the value of the quantities associated with the two-dimensional and three-dimensional space-time cylinders, the knowledge of which is however necessary to perform the transition from the quantity associated with the bottom surface to that associated with the top surface.

On the other hand, we know that Maxwell's equations (which are only balance and conservation laws, i.e. topological equations, and a subset of which Equation (29) and Equation (30) are the discretized form of) by themselves do not determine the evolution of the electromagnetic field. To obtain a set of equation able to do this, we must add to Maxwell's equations a set of equations which represent a mathematical model of the material behavior (plus, of course, suitable initial and boundary conditions). These mathematical models of materials are the so-called *constitutive* or *material equations*. A simple example of such a set for the case of electromagnetism is constituted by the following three equations

$$\mathbf{D} = \varepsilon \mathbf{E} \quad (31)$$

$$\mathbf{B} = \mu \mathbf{H} \quad (32)$$

$$\mathbf{J} = \sigma \mathbf{E} \quad (33)$$

Note that these equations are given as relations between point quantities, and there appears to be no obvious way to transform them into exact relations between the corresponding domain quantities. Once the possibility of a topological time-stepping approach is recognized, the determination of a discrete representation for the constitutive equations becomes in fact the central point in the setup of a time-domain numerical method, since the discrete rendering of the topological equations follows automatically from the discretization of the space-time domain of the problem.

The general problem of the determination of a discrete form for constitutive equations will not be treated in detail here. For this important topic the reader is referred to [5]. We will only note that this process can be carried out in general only at the cost of some approximation, and that this is indeed the phase where the approximation enters the discretization of a physical field problem. We will present only the final result of this discretization process, namely, the relations

$$\Phi^e = C_{\varepsilon-1} \left(\Psi^d \right) \quad (34)$$

$$\Psi^h = C_{\mu^{-1}} (\Phi^b) \quad (35)$$

$$\mathbf{Q}^j = C_{\sigma} (\Phi^e) \quad (36)$$

where $C_{\varepsilon^{-1}}$, $C_{\mu^{-1}}$ and C_{σ} are mathematical relations between the vectors which collect the domain quantities defined on the primary and secondary mesh, and which discretize the constitutive links between the corresponding point quantities. Usually these discrete relations are linear links represented by matrices. For example in the case of the FDTD method, combining Equations (14) to (26) it can be shown that they correspond to

$$\phi_{(i,j+\frac{1}{2},k+\frac{1}{2},n)}^{b_x} = \mu_{(i,j+\frac{1}{2},k+\frac{1}{2})} \frac{\Delta y \Delta z}{\Delta x \Delta t} \psi_{(i,j+\frac{1}{2},k+\frac{1}{2},n)}^{h_x} \quad (37)$$

$$\psi_{(i+\frac{1}{2},j,k,n+\frac{1}{2})}^{d_x} = \varepsilon_{(i+\frac{1}{2},j,k)} \frac{\Delta y \Delta z}{\Delta x \Delta t} \phi_{(i+\frac{1}{2},j,k,n+\frac{1}{2})}^{e_x} \quad (38)$$

$$Q_{(i+\frac{1}{2},j,k,n)}^{j_x} = \sigma_{(i+\frac{1}{2},j,k)} \frac{\Delta y \Delta z}{\Delta x} \cdot \left(\frac{\phi_{(i+\frac{1}{2},j,k,n+\frac{1}{2})}^{e_x} + \phi_{(i+\frac{1}{2},j,k,n-\frac{1}{2})}^{e_x}}{2} \right) \quad (39)$$

where, using Equation (38), Equation (39) can be rewritten as a direct link between \mathbf{Q}^j and Ψ^d , as follows

$$Q_{(i+\frac{1}{2},j,k,n)}^{j_x} = \Delta t \frac{\sigma_{(i+\frac{1}{2},j,k)}}{\varepsilon_{(i+\frac{1}{2},j,k)}} \left(\frac{\psi_{(i+\frac{1}{2},j,k,n+\frac{1}{2})}^{d_x} + \psi_{(i+\frac{1}{2},j,k,n-\frac{1}{2})}^{d_x}}{2} \right) \quad (40)$$

Analogous relations can be written for the remaining state variables. Note that contrary to the other discrete constitutive links, the right side of Equation (39) involves two instances of the independent domain quantity ϕ^e considered at two different time instants. This anomaly is due to the fact that the corresponding dependent quantity $Q_{(\cdot,\cdot,\cdot,n)}^j$ is defined on a space-time domain which spans a time step going from the time instant $(n - \frac{1}{2})\Delta t$ to $(n + \frac{1}{2})\Delta t$, which would be only partially covered by the information carried separately by the domain quantities $\phi_{(\cdot,\cdot,\cdot,n-\frac{1}{2})}^{e_x}$ and $\phi_{(\cdot,\cdot,\cdot,n+\frac{1}{2})}^{e_x}$.

The FIT method [7] adopts a set of discrete constitutive operators similar to those of the FDTD method, whereas some generalization of the FDTD method, such as the Discrete Surface Integral method (DSI) [4], adopt a more complex discrete representation of constitutive equations, while maintaining the topological time-stepping

of FDTD. This follows from the fact that, contrary to the case of topological equations, many possible approaches to the discretization of constitutive equations are possible. This fact opens the way to the construction of a multiplicity of methods based on the combination of the unique topological time-stepping formula (for a given choice of the mesh) with the many possible approximate discrete constitutive equations. We can write a formula which represents the generic result of this combination for the case of electromagnetism. Combining Equation (34), Equation (35) and Equation (36) we obtain

$$\Phi_{n+1}^b = \Phi_n^b - \mathbf{I}_r C_{\varepsilon^{-1}} (\Psi^d) \quad (41)$$

$$\Psi_{n+\frac{1}{2}}^d = \Psi_{n-\frac{1}{2}}^d + \mathbf{I}_d C_{\mu^{-1}} (\Phi^b) - C_{\sigma, \varepsilon^{-1}} (\Psi^d) \quad (42)$$

where we have written the operator $C_{\sigma, \varepsilon^{-1}}$ in place of the composition of $C_{\varepsilon^{-1}}$ and C_{σ} to allow for a more general approach to the discretization of the link between \mathbf{D} and \mathbf{Q} , and where the vectors Ψ^d and Φ^b operated upon by the constitutive operators lack the time index to allow for the whole space-time vector to enter the relation. The resulting variety of time-domain methods complying with the philosophy of topological time-stepping appears therefore quite large. One can indeed have the impression, when exposed for the first time to the assertion of the uniqueness of the topological time-stepping formula, that the variety of methods which comply with the topological time-stepping approach be very limited. By considering however the presence of the constitutive equations, one realizes instead that many methods belong to that ensemble, including high order methods in both space and time, and methods with implicit time-stepping.

Note, finally, that the present approach reveals the otherwise mysterious effectiveness of the leapfrog scheme in the discretization of the time variable of semidiscretized problems. By staggering by a half step in time the state variables attached to the primary and secondary grid, the leapfrog method places them exactly where an elementary discretization strategy of the constitutive equations can transform those defined on the primary grid in the domain quantities required by the topological time-stepping relations on the secondary grid (and vice versa), i.e, at the center of the space-time “cylinders” which determine the time-stepping itself.

6. GENERALIZATIONS

The case of FDTD as a method complying with the philosophy of topological time-stepping is only an example. As hinted above, other

time-domain methods for electromagnetic problems, such as the FIT and DSI methods, can be reconducted to that philosophy. All these methods consider only meshes or grids obtained as cartesian products of separate discretizations of the domain in space and in time. This is a consequence of the fact that in their classical (i.e. non four-dimensional) version, Maxwell's equations have built into them the distinction between the space and time variables. However, Faraday's law and Gauss' electric law are only particular cases of a more general law of conservation of the magnetic flux, which says that the magnetic flux associated with the boundary of any space-time three-dimensional volume is always zero. This statement can be written as follows

$$\phi_{\partial\mathcal{V}} = 0 \quad (43)$$

where we use the symbol \mathcal{V} to mean a generic three-dimensional space-time volume. When \mathcal{V} is of the form $V \times t$, Equation (45) corresponds to Gauss' electric law, whereas when \mathcal{V} is of the form $S \times [t_1, t_2]$ it corresponds to Faraday's induction law. Correspondingly, Maxwell-Ampère's law and Gauss' magnetic law are particular cases of a more general space-time balance statement, namely

$$\psi_{\partial\mathcal{V}} = Q_{\mathcal{V}} \quad (44)$$

which reduces to them when \mathcal{V} is of the form $S \times [t_1, t_2]$ and $V \times t$, respectively.

The existence of these two more general space-time topological statements implies that the topological time-stepping approach is applicable for the development of numerical methods which can use generic space-time meshes, not necessarily obtained as products of separate space and time discretizations (Figure 9). This kind of mesh is required, for example, when one or both the space meshes move in time with respect to the reference frame of the problem. The choice of a generic space-time grid might indeed seem at first very strange and in fact this route does not seem to have been actually pursued in numerical electromagnetism. However, in the field of Computational Fluid Dynamics (where it is often desirable to limit the relative displacement of the mesh with respect to the flow), the Space-Time Conservation Element and Solution Element method (CE/SE) developed by Chang and colleagues [2] proceeds exactly along this lines, advocating a true space-time approach and using cells that are not cartesian products of space and time components in the selected reference frame.

Another fact that must be considered when applying the approach advocated in the present work, is the relation that links the conservation and balance laws. Maxwell's equations are based on two

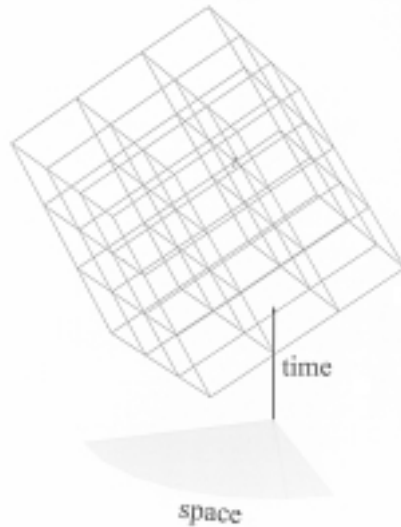


Figure 9. The topological equations which serve as the basis of the topological time-stepping statements apply in general to space-time domains which are not necessarily obtained as cartesian products of a domain in space and of a domain in time. Correspondingly there is the possibility to develop numerical methods based on the topological time-stepping principle and which make use of meshes that are not obtained as products of separate discretization of the domain in space and in time.

conservation laws: that of electric charge and that of magnetic flux [6]. The law of electric charge conservation corresponds to the statement

$$Q_{\partial\mathcal{H}} = 0 \quad (45)$$

where \mathcal{H} is any space-time hypervolume. From this statements there follows, in a topologically trivial space, Maxwell-Ampère's law and Gauss' magnetic law. The law of conservation of magnetic flux is expressed by Equation (45) and encompasses Faraday's induction law and Gauss' electric law. From it there follows, in a topologically trivial space, a space-time balance statement which defines the electromagnetic potentials. Hence we see that we have at our disposal on each mesh a pair of time-dependent topological statements (of which, one is a balance and one a conservation law) within which we can select the pair to employ for the topological time-stepping. It is the range of available constitutive equations that usually determines the subset of those statements that will be actually used to set up the actual algorithm.

Finally, it is worth noting that the example of the CE/SE method mentioned above reveals that what said here about electromagnetism applies also to other field theories. In fact it is clear that this approach applies to all field theories which have within their equations a set of space-time topological statements, i.e. of space-time balance or conservation laws. Since this is true for almost all non-static physical field theories, the scope of the topological time-stepping philosophy appears indeed very broad.

7. CONCLUSIONS

We have shown that electromagnetism has built into its equations a set of intrinsically discrete time-dependent statements which can serve as a natural basis of a numerical time-stepping strategy. When the space-time domain of a problem has been discretized, these statements translate directly into a set of time-stepping relations, provided the proper space-time meshes have been defined and the corresponding integrated field quantities have been selected as state variables. Moreover, the role of constitutive equations in the discretization process stands out very clearly once the intrinsically discrete statements have been singled out. This approach calls for the adoption of a space-time point of view in all phases of the discretization process. An analysis of some successful time-domain methods reveals however that until now the intrinsic space-time discreteness the electromagnetic equations has not been explicitly acknowledged and exploited by numerical methods (although in some cases, for example the FIT method, the intrinsic discreteness in space has been recognized). The correction of this state of affairs can bring advantages both from the point of view of the comprehension and fine tuning of existing methods and of the development of new ones. This applies not only to electromagnetism but also to generic physical field theories, and it appears desirable that in all these cases the approach presented here be built into numerical methods from the start and the favorable properties which ensue, at last fully enjoyed.

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