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CONSERVATION OF DISCRETE ENERGY AND RELATED LAWS IN THE FINITE INTEGRATION TECHNIQUE

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Abstract—We report some properties of the Finite Integration Technique (FIT), which are related to the definition of a discrete energy quantity. Starting with the well-known identities for the operator matrices of the FIT, not only the conservation of discrete energy in time and frequency domain simulations is derived, but also some important orthogonality properties for eigenmodes in cavities and waveguides. Algebraic proofs are presented, which follow the vector-analytical proofs of the related theorems of the classical (continuous) theory. Thus, the discretization approach of the FIT can be considered as the framework for a consistent discrete electromagnetic field theory.

1. INTRODUCTION

One of the key points of the Finite Integration Technique [1, 2] is the use of a system of two computational grids, the primary grid G and the dual grid $\widetilde{G}$. In the simplest case these are Cartesian-type coordinate grids (sometimes referred to as Yee-type grids [3]), but a large variety of more general grids are allowed, such as cylindrical or spherical coordinate grids, triangular [4] or non-orthogonal grids [5].

As state variables of the FIT we introduce electric and magnetic grid voltages and fluxes, which are defined as the integrals of the electric and magnetic field vectors over elementary objects of the computational grid: Grid voltages

$$\widehat{e}_i = \int_{L_i} \vec{E}(\vec{r},t) \cdot d\vec{s}, \quad \widehat{H}_j = \int_{\widetilde{L}_j} \vec{H}(\vec{r},t) \cdot d\vec{s}, \tag{1}$$

and grid fluxes

$$\widehat{\widehat{\mathbf{d}}}_i = \int_{\widetilde{A}_i} \vec{D}(\vec{r},t) \cdot d\vec{A}, \quad \widehat{\widehat{b}}_j = \int_{A_j} \vec{B}(\vec{r},t) \cdot d\vec{A}, \quad \widehat{\widehat{\mathbf{j}}}_i = \int_{\widetilde{A}_i} \vec{J}(\vec{r},t) \cdot d\vec{A}, \tag{2}$$

where L_i, A_j are the edges and facets of the primary grid G, and $\widetilde{L}_j$, $\widetilde{A}_i$ denote the edges and facets of the dual grid $\widetilde{G}$. The indices are chosen such, that the primary facet A_j has the same index as the intersecting edge $\widetilde{L}_j$ of the dual grid (same to $\widetilde{A}_i$ and L_i).

Using these definitions, Maxwell's equations can be transformed into a set of matrix-vector-equations for the algebraic vectors $\widehat{\mathbf{e}}$, $\widehat{\widehat{\mathbf{d}}}$, $\widehat{\mathbf{h}}$, $\widehat{\widehat{\mathbf{b}}}$, and $\widehat{\widehat{\mathbf{j}}}$

$$\mathbf{C}\,\widehat{\mathbf{e}} = -\frac{d}{dt}\widehat{\widehat{\mathbf{b}}}, \qquad \widetilde{\mathbf{C}}\,\widehat{\mathbf{h}} = \frac{d}{dt}\widehat{\widehat{\mathbf{d}}} + \widehat{\widehat{\mathbf{j}}}, \tag{3}$$

$$\mathbf{S}\,\widehat{\widehat{\mathbf{b}}} = \mathbf{0}, \qquad \widetilde{\mathbf{S}}\,\widehat{\widehat{\mathbf{d}}} = \mathbf{q}, \tag{4}$$

which are referred to as *Maxwell's Grid Equations.*

The matrix $\mathbf{C}$ is the discrete curl-operator of the grid G: Its entries C_{ji} are ± 1, only if edge L_i is contained in the boundary of facet A_j, and zero otherwise (incidence relation). Analogously, the matrix $\mathbf{S}$ is the discrete div-operator[1] of the primary grid: Its entries S_{kj} are ± 1, only if facet A_j is contained in the boundary of cell k. The same applies to the matrices $\widetilde{\mathbf{S}}$ and $\widetilde{\mathbf{C}}$ and the dual grid $\widetilde{G}$.

From grid topology we find the relations

$$\mathbf{SC} = \mathbf{0} \qquad \text{and} \qquad \widetilde{\mathbf{S}}\widetilde{\mathbf{C}} = \mathbf{0}, \tag{5}$$

which in the light of the FIT have some important consequences: As direct analogs to the vector-analytical identity 'div rot=0' they ensure,

[1] For historical reasons the div-operators are denoted with $\mathbf{S}$ and $\widetilde{\mathbf{S}}$ ('source'), and symbols beginning with $\mathbf{D}$ are used for diagonal matrices.

that also in the discrete regime we can identify curl-free (solenoidal) and divergence-free fields, and a curl-field is always free of sources. This property holds exactly (up to numerical round-off) for all discrete field vectors of the FI-approach (and not only for vanishing grid step sizes $\Delta \to 0$).

Another topological result is the duality of the curl-operators

$$\widetilde{\mathbf{C}} = \mathbf{C}^T, \tag{6}$$

which plays an important role in the following analysis of the discrete eigenvalue problem of the FIT. Furthermore, the transposed matrix of the div-operator $\mathbf{S}^T$ can be identified to be the negative dual gradient:

$$\widetilde{\mathbf{G}} = -\mathbf{S}^T \qquad \text{and} \qquad \mathbf{G} = -\widetilde{\mathbf{S}}^T. \tag{7}$$

In the case of a Cartesian grid system with N_P primary nodes we can choose the indexing of the edges and facets such, that in the discrete vectors the $x-$, $y-$ and $z-$components are separated,

$$\widehat{\mathbf{e}} = \begin{pmatrix} \widehat{\mathbf{e}}_x \\ \widehat{\mathbf{e}}_y \\ \widehat{\mathbf{e}}_z \end{pmatrix}, \quad \widehat{\mathbf{h}} = \begin{pmatrix} \widehat{\mathbf{h}}_x \\ \widehat{\mathbf{h}}_y \\ \widehat{\mathbf{h}}_z \end{pmatrix}. \tag{8}$$

As a consequence, we obtain $N_P \times N_P$-blocks $\mathbf{P}_x$, $\mathbf{P}_y$ and $\mathbf{P}_z$ in the operator matrices

$$\mathbf{C} = \begin{pmatrix} \mathbf{0} & -\mathbf{P}_z & \mathbf{P}_y \\ \mathbf{P}_z & \mathbf{0} & -\mathbf{P}_x \\ -\mathbf{P}_y & \mathbf{P}_x & \mathbf{0} \end{pmatrix}, \qquad \widetilde{\mathbf{C}} = \begin{pmatrix} \mathbf{0} & \mathbf{P}_z^T & -\mathbf{P}_y^T \\ -\mathbf{P}_z^T & \mathbf{0} & \mathbf{P}_x^T \\ \mathbf{P}_y^T & -\mathbf{P}_x^T & \mathbf{0} \end{pmatrix}, \tag{9}$$

and

$$\mathbf{S} = \begin{pmatrix} \mathbf{P}_x & \mathbf{P}_y & \mathbf{P}_z \end{pmatrix}, \qquad \widetilde{\mathbf{S}} = \begin{pmatrix} -\mathbf{P}_x^T & -\mathbf{P}_y^T & -\mathbf{P}_z^T \end{pmatrix}, \tag{10}$$

which can be identified as discrete partial differentiation operators [1, 2].

To complete the discretization approach we introduce so-called material matrices as an analog of the constitutive relations of continuous fields (without polarization vectors):

$$\widehat{\widehat{\mathbf{d}}} = \mathbf{M}_\varepsilon \,\widehat{\mathbf{e}} \qquad \widehat{\widehat{\mathbf{j}}} = \mathbf{M}_\kappa \,\widehat{\mathbf{e}} \qquad \widehat{\mathbf{h}} = \mathbf{M}_{\mu^{-1}} \,\widehat{\widehat{\mathbf{b}}} \tag{11}$$

If we assume a dual-*orthogonal* grid system, where primary edges and dual facets (or dual edges and primary facets) intersect with an angle of 90 degrees, the material matrices (11) can be defined as diagonal matrices with the entries

$$M_{\varepsilon,ii} = \frac{\overline{\varepsilon}\widetilde{A}_i}{L_i}, \qquad M_{\kappa,ii} = \frac{\overline{\kappa}\widetilde{A}_i}{L_i}, \qquad M_{\mu^{-1},jj} = \frac{\widetilde{L}_j}{\overline{\mu}A_j}, \tag{12}$$

where $\overline{\varepsilon}$, $\overline{\kappa}$ and $\overline{\mu}$ are properly averaged material coefficients. The consistency of these expressions with the continuous relations can be proven by simple Taylor expansions [2, 6].

Obviously, for positive permittivities and permeabilities the matrices $\mathbf{M}_\varepsilon$ and $\mathbf{M}_{\mu^{-1}}$ are symmetric positive definite. This property together with the duality (6) of the curl-operators can be exploited to derive a number of important theorems for the discretization approach of the FIT. This includes the conservation of energy in simulations with time-varying fields, and various orthogonality relations for the eigensolutions of the method. In the following chapters we first introduce the underlying concept of *electric and magnetic energy in the discrete system*, and then present some important consequences of this definitions and their algebraic proofs.

2. ORTHOGONALITY PROPERTIES AND DISCRETE ENERGY

For the rest of this paper we restrict our analysis to Cartesian grids, as they allow a simple but important definition of a discrete energy quantity. To motivate the following derivation, we regard the eigenvalue equation for the electric field in a lossless system (no currents)

$$\varepsilon^{-1}\text{curl}\ \mu^{-1}\text{curl}\ \vec{E} = \omega^2\vec{E} \qquad \text{(continuous)}, \tag{13}$$

$$\mathbf{M}_\varepsilon^{-1}\mathbf{C}^T\mathbf{M}_{\mu^{-1}}\mathbf{C}\ \widehat{\mathbf{e}} = \omega^2\,\widehat{\mathbf{e}} \qquad \text{(discrete)}, \tag{14}$$

where the dual curl operator in the discrete formulation was replaced by $\widetilde{\mathbf{C}} = \mathbf{C}^T$ according to (6). As the material matrices are diagonal and positive definite, we can define their real-valued 'roots'

$$\mathbf{M}_\varepsilon = \mathbf{M}_\varepsilon^{1/2}\,\mathbf{M}_\varepsilon^{1/2} \qquad\qquad \mathbf{M}_{\mu^{-1}} = \mathbf{M}_{\mu^{-1}}^{1/2}\,\mathbf{M}_{\mu^{-1}}^{1/2} \tag{15}$$

by taking the square root of each entry. The system matrix $\mathbf{A} = \mathbf{M}_\varepsilon^{-1}\mathbf{C}^T\mathbf{M}_{\mu^{-1}}\mathbf{C}$ of the algebraic eigenvalue problem can then be symmetrized by the transformation

$$\widehat{\mathbf{e}}' = \mathbf{M}_\varepsilon^{1/2}\ \widehat{\mathbf{e}}, \tag{16}$$

leading to

$$\mathbf{M}_\varepsilon^{-1/2}\mathbf{C}^T\mathbf{M}_{\mu^{-1}}\mathbf{C}\mathbf{M}_\varepsilon^{-1/2}\ \widehat{\mathbf{e}}' = \omega^2\,\widehat{\mathbf{e}}', \tag{17}$$

with the symmetric positive semidefinite system matrix

$$\mathbf{A}' = \mathbf{M}_\varepsilon^{-1/2}\mathbf{C}^T\mathbf{M}_{\mu^{-1}}\mathbf{C}\mathbf{M}_\varepsilon^{-1/2} = (\mathbf{M}_{\mu^{-1}}^{1/2}\mathbf{C}\mathbf{M}_\varepsilon^{-1/2})^T\ (\mathbf{M}_{\mu^{-1}}^{1/2}\mathbf{C}\mathbf{M}_\varepsilon^{-1/2}). \tag{18}$$

Thus all eigenvalues $\lambda = \omega^2$ of equations (14) and (17) are real-valued and non-negative numbers, and all eigensolutions represent either static solutions (with $\omega = 0$) or undamped oscillations with real eigenfrequencies $\omega > 0$. This is discussed in more detail in [2, 6].

Another important property of eigenvalue problems with a positive definite system matrix is the orthogonality of the modes: For each pair of eigenvectors with different eigenvalues we have

$$(\,\widehat{\mathbf{e}}'_\xi)^H\ \widehat{\mathbf{e}}'_\eta = 0 \qquad (\lambda_\xi \neq \lambda_\eta). \tag{19}$$

Re-substituting the original vectors applying (16), we can normalize the eigenmodes to get

$$\widehat{\mathbf{e}}_\xi^H\,\mathbf{M}_\varepsilon\ \widehat{\mathbf{e}}_\eta =\ \widehat{\mathbf{e}}_\xi^H\ \widehat{\widehat{\mathbf{d}}}_\eta = \begin{cases} 0 & (\xi \neq \eta) \\ 1\ \text{Watt} & (\xi = \eta). \end{cases} \tag{20}$$

From the physical dimension of the scalar product $[\,\widehat{\mathbf{e}}_\xi^H\ \widehat{\widehat{\mathbf{d}}}_\xi] = 1$ Watt it can be identified as an energy-related form, and this motivates the definitions of the (time-averaged) total stored electric and magnetic *discrete energy*:

$$\overline{W}_e = \frac{1}{4}\,\widehat{\mathbf{e}}^H\ \widehat{\widehat{\mathbf{d}}}, \qquad\qquad \overline{W}_m = \frac{1}{4}\,\widehat{\mathbf{h}}^H\ \widehat{\widehat{\mathbf{b}}}. \tag{21}$$

For an interpretation of these formulas we consider two (real-valued) components $\widehat{e}_i$ and $\widehat{\widehat{D}}_i$, which refer to a primary grid edge L_i in x-direction, and to the corresponding dual facet $\widetilde{A}_i$. According to Fig. 1 this facet consists of four parts $\Delta\widetilde{A}_k$ ($k = 1 \ldots 4$) with eventually different permittivities ε_k.

Based on the (continuous) E_x-component of the electric field at the intersection point, the first order approximations

$$\widehat{e}_i \approx E_x \cdot L_i, \qquad\qquad \widehat{\widehat{\mathbf{d}}}_i \approx E_x \cdot \sum_{k=1}^{4} \varepsilon_k\,\Delta\widetilde{A}_k, \tag{22}$$

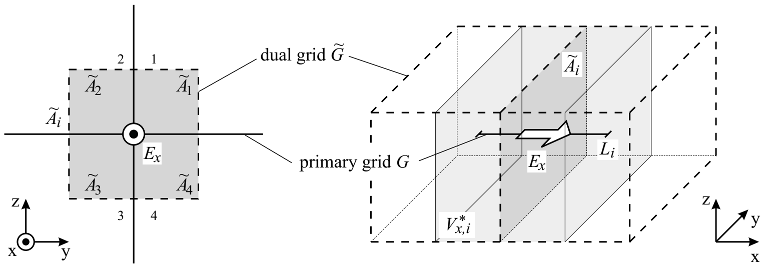

Figure 1. Calculation of the discrete electric energy referring to one pair of components $\widehat{e}_i$ and $\widehat{\widehat{D}}_i$. The integration volume $V^*_{x,i}$ consists of one half of two neighboring dual cells and may contain up to four different materials.

(which are also the basis of the discrete material relations) yield

$$\begin{aligned} \frac{1}{4}\,\widehat{e}_i \cdot \widehat{\widehat{\mathbf{d}}}_i &\approx \frac{1}{4}\sum_{k=1}^{4} \varepsilon_k E_x^2 \cdot L_i\,\Delta\widetilde{A}_k \\ &\approx \frac{1}{4}\int\limits_{V^*_{x,i}} \varepsilon E_x^2\, dV = \overline{W}^*_{x,i}. \end{aligned} \tag{23}$$

This expression can be considered as an approximation of the stored energy of the x-component of the discrete electric field in the 'mixed' cell

$$V^*_{x,i} = L_i\,\widetilde{A}_i, \tag{24}$$

which is a combination of two half dual cells (cf. Fig. 1). The consistency of this discrete energy quantity can be easily proven by a Taylor expansion of $E_x(x, y, z)$ — the same argumentation as for the consistency of the material relations.

For all x-components in $\widehat{\mathbf{e}}$ and $\widehat{\widehat{\mathbf{d}}}$ we have

$$\bigcup_i V^*_{x,i} = \Omega \quad \text{(problem domain)}, \tag{25}$$

and obviously this is also true for the y- and z-components (yielding three different segmentations of Ω). Thus, the scalar product in (21) as the summation of all cell energies

$$\frac{1}{4}\,\widehat{\mathbf{e}}^H\,\widehat{\widehat{\mathbf{d}}} = \sum_i \overline{W}^*_{x,i} + \sum_i \overline{W}^*_{y,i} + \sum_i \overline{W}^*_{z,i} \tag{26}$$

is the *total stored discrete electric energy* in the grid. The derivation of the magnetic energy is completely analogous.

For static or transient fields, where no time-averaging has to be performed, the corresponding definitions are

$$W_e = \frac{1}{2}\,\widehat{\mathbf{e}}^T\,\widehat{\widehat{\mathbf{d}}}, \qquad\qquad W_m = \frac{1}{2}\,\widehat{\mathbf{h}}^T\,\widehat{\widehat{\mathbf{b}}}. \tag{27}$$

3. ENERGY CONSERVATION IN THE DISCRETE SYSTEM

Based on this definition of the discrete energy we will now consider its transient characteristics for time-varying fields [2, 7].

In a first step the time derivatives in (3) are left untouched, and thus the conservation of discrete energy is only analyzed for the spatial discretization scheme itself. This is sufficient, for example, for time-harmonic fields, if the time-dependence is implicitly (and without approximations) introduced by a complex exponential expression. For the general case of transient fields, however, the time axis has to be discretized too, and thus also the time integration scheme applied to Maxwell's Grid Equations has to be taken into account.

Discrete space – continuous time

The total discrete energy in the computational grid according to (27) is given by

$$W(t) = W_e(t) + W_m(t) = \frac{1}{2}\left(\,\widehat{\mathbf{e}}^T(t)\,\widehat{\widehat{\mathbf{d}}}(t) + \widehat{\mathbf{h}}^T(t)\,\widehat{\widehat{\mathbf{b}}}(t)\right). \tag{28}$$

Exploiting the symmetry of the material matrices, we obtain for the time derivative of this equation:

$$\begin{aligned}
\frac{d}{dt}W(t) &= \frac{1}{2}\left(\frac{d}{dt}\,\widehat{\mathbf{e}}^T\,\widehat{\widehat{\mathbf{d}}} + \widehat{\mathbf{e}}^T\frac{d}{dt}\,\widehat{\widehat{\mathbf{d}}} \;+\; \frac{d}{dt}\,\widehat{\mathbf{h}}^T\,\widehat{\widehat{\mathbf{b}}} + \widehat{\mathbf{h}}^T\frac{d}{dt}\,\widehat{\widehat{\mathbf{b}}}\right)\\
&= \frac{1}{2}\left((\mathbf{M}_\varepsilon\,\widehat{\mathbf{e}})^T\frac{d}{dt}\,\widehat{\mathbf{e}} + \widehat{\mathbf{e}}^T\frac{d}{dt}\,\widehat{\widehat{\mathbf{d}}} \;+\; (\mathbf{M}_\mu\,\widehat{\mathbf{h}})^T\frac{d}{dt}\,\widehat{\mathbf{h}} + \widehat{\mathbf{h}}^T\frac{d}{dt}\,\widehat{\widehat{\mathbf{b}}}\right)\\
&= \widehat{\mathbf{e}}^T\frac{d}{dt}\,\widehat{\widehat{\mathbf{d}}} \;+\; \widehat{\mathbf{h}}^T\frac{d}{dt}\,\widehat{\widehat{\mathbf{b}}}.
\end{aligned} \tag{29}$$

Putting in Maxwell's Grid Equations (3) and the duality relation (6), a discrete form of Poynting's law for the total energy in the grid can be derived:

$$\frac{d}{dt}W = \widehat{\mathbf{e}}^T(\widetilde{\mathbf{C}}\,\widehat{\mathbf{h}} - \widehat{\widehat{\mathbf{j}}}\,) - \widehat{\mathbf{h}}^T\mathbf{C}\,\widehat{\mathbf{e}} = -\,\widehat{\mathbf{e}}^T\,\widehat{\widehat{\mathbf{j}}}\,. \tag{30}$$

As the basic formulation in (3) implies closed boundary conditions, there is no radiation term in this formula. If only the energy in a sub-domain of the grid is to be considered, such a radiation term can be formulated by a proper definition of a discrete energy flow vector [8], where components of the discrete electric and magnetic voltages have to be locally interpolated.

For time harmonic processes an additional result concerning the discrete energy conservation can be found. Assuming a time harmonic problem with no external current excitation or losses, all eigenmodes $\widehat{\mathbf{e}}$ and the related fluxes $\widehat{\widehat{\mathbf{d}}}$ can be chosen to be real-valued, yielding purely imaginary magnetic vectors $\widehat{\mathbf{h}}$ and $\widehat{\widehat{\mathbf{b}}}$. Using the time-harmonic form of (3),

$$\mathbf{C}\,\widehat{\mathbf{e}} = -i\omega\,\widehat{\widehat{\mathbf{b}}}, \qquad \widetilde{\mathbf{C}}\,\widehat{\mathbf{h}} = i\omega\,\widehat{\widehat{\mathbf{d}}}, \tag{31}$$

we obtain the relation

$$\begin{aligned}\frac{1}{4}\,\widehat{\mathbf{e}}^H\,\widehat{\widehat{\mathbf{d}}} &= \frac{1}{4}\,\frac{1}{i\omega}\,\widehat{\mathbf{e}}^H\widetilde{\mathbf{C}}\,\widehat{\mathbf{h}} = \frac{1}{4}\,\frac{1}{i\omega}(\mathbf{C}\,\widehat{\mathbf{e}})^H\,\widehat{\mathbf{h}} \\ &= -\frac{1}{4}\,\frac{1}{i\omega}(i\omega\,\widehat{\widehat{\mathbf{b}}})^H\,\widehat{\mathbf{h}} = \frac{1}{4}\,\widehat{\widehat{\mathbf{b}}}^H\,\widehat{\mathbf{h}} = \frac{1}{4}\,\widehat{\mathbf{h}}^H\,\widehat{\widehat{\mathbf{b}}}.\end{aligned} \tag{32}$$

Thus for the time-averaged magnetic and electric energy the time harmonic equilibrium relation

$$W_m = W_e \tag{33}$$

holds also in the discrete sense within the FI-theory.

Discrete space – discrete time

The most common time integration algorithm in connection with the FIT is the leapfrog-scheme [2, 3], which follows from (3), if the time derivatives are substituted by central differences. Having in mind the energy definitions above, we introduce the scaled composed vector

$$\begin{aligned}\mathbf{y}(t) &= \begin{pmatrix} \mathbf{M}_\mu^{1/2}\,\widehat{\mathbf{h}}(t) \\ \mathbf{M}_\varepsilon^{1/2}\,\widehat{\mathbf{e}}(t) \end{pmatrix} \quad \text{with} \\ \left\|\mathbf{y}(t)\right\|_2^2 &= \widehat{\mathbf{h}}^T\mathbf{M}_\mu\,\widehat{\mathbf{h}} + \widehat{\mathbf{e}}^T\mathbf{M}_\varepsilon\,\widehat{\mathbf{e}} = 2\cdot W_{tot}(t).\end{aligned} \tag{34}$$

Maxwell's Grid Equations (without currents) then can be written as one system of ordinary differential equations

$$\frac{d}{dt}\mathbf{y} = \mathbf{A}_t\,\mathbf{y}, \tag{35}$$

with

$$\mathbf{A}_t = \begin{pmatrix} \mathbf{0} & -\mathbf{M}_\mu^{-1/2}\mathbf{C}\mathbf{M}_\varepsilon^{-1/2} \\ \mathbf{M}_\varepsilon^{-1/2}\mathbf{C}^T\mathbf{M}_\mu^{-1/2} & \mathbf{0} \end{pmatrix} = \begin{pmatrix} \mathbf{0} & \mathbf{A}_1 \\ -\mathbf{A}_1^T & \mathbf{0} \end{pmatrix}. \tag{36}$$

The system matrix A_t of this time domain formulation is skew-symmetric and thus has only purely imaginary eigenvalues $\lambda_{t,i} = i\omega_i$. The corresponding eigenvectors

$$\mathbf{y}_t = \begin{pmatrix} \widehat{\mathbf{h}}_i' \\ \widehat{\mathbf{e}}_i' \end{pmatrix} = \begin{pmatrix} \mathbf{M}_\mu^{1/2}\,\widehat{\mathbf{h}}_i \\ \mathbf{M}_\varepsilon^{1/2}\,\widehat{\mathbf{e}}_i \end{pmatrix} \tag{37}$$

fulfill the relations

$$\mathbf{A}_1\,\widehat{\mathbf{e}}_i' = \lambda_{t,i}\,\widehat{\mathbf{h}}_i' \qquad \text{and} \qquad -\mathbf{A}_1\,\widehat{\mathbf{h}}_i' = \lambda_{t,i}\,\widehat{\mathbf{e}}_i'. \tag{38}$$

Using this notation, the update-equations of the leapfrog-algorithm for full and half time steps $t_m = t_0 + m \cdot \Delta t$ appear as

$$\mathbf{y}^{(m+1)} = \mathbf{B}\,\mathbf{y}^{(m)} \tag{39}$$

with

$$\mathbf{y}^{(m)} = \begin{pmatrix} \mathbf{M}_\mu^{1/2}\ \widehat{\mathbf{h}}^{(m)} \\ \mathbf{M}_\varepsilon^{1/2}\ \widehat{\mathbf{e}}^{(m+1/2)} \end{pmatrix} \qquad \text{and}$$

$$\mathbf{B} = \begin{pmatrix} \mathbf{I} & \Delta t\mathbf{A}_1 \\ -\Delta t\,\mathbf{A}_1^T & \mathbf{I} + \Delta t^2\,\mathbf{A}_1^T\mathbf{A}_1 \end{pmatrix}. \tag{40}$$

Note, that despite of the staggered allocation of the electric and magnetic field vectors on the time axis, the squared Euclidean norm of $\mathbf{y}^{(m)}$ can still be considered as a discrete energy definition — not only in an algebraic sense, but also physically due to the convergence to the time-continuous formulation for $\Delta t \to 0$.

To analyze the time dependence of the discrete energy we compute the eigenvalues and eigenvectors of the iteration matrix $\mathbf{B}$ using the approach

$$\mathbf{y}_{B,i} = \begin{pmatrix} \widehat{\mathbf{h}}_i' \\ \alpha\,\widehat{\mathbf{e}}_i' \end{pmatrix} \qquad \text{with} \quad \alpha \in \mathbf{C}$$

$$\Rightarrow \quad \mathbf{B}\,\mathbf{y}_{B,i} = \begin{pmatrix} \widehat{\mathbf{h}}_i'\,(1 + \alpha\Delta t\lambda_{t,i}) \\ \alpha\,\widehat{\mathbf{e}}_i'\,(1 + \frac{1}{\alpha}\Delta t\lambda_{t,i} + \Delta t^2\lambda_{t,i}^2) \end{pmatrix}, \tag{41}$$

where the relations (38) have been applied several times. Obviously, $\mathbf{y}_{B,i}$ is an eigenvector of $\mathbf{B}$ with the corresponding eigenvalue

$$\lambda_{B,i} = 1 + \alpha \Delta t \lambda_{t,i}, \tag{42}$$

if α fulfills the equation

$$1 + \alpha \Delta t \lambda_{t,i} = 1 + \frac{1}{\alpha} \Delta t \lambda_{t,i} + \Delta t^2 \lambda_{t,i}^2. \tag{43}$$

From (42) and (43) we obtain the following relation between the eigenvalues $\lambda_{A,i} = i\omega_i$ of the system matrix $\mathbf{A}_t$ and $\lambda_{B,i}$ of the iteration matrix $\mathbf{B}$:

$$\lambda_{B,i} = \frac{2 - (\Delta t \omega_i)^2}{2} \pm \sqrt{\left(\frac{2 - (\Delta t \omega_i)^2}{2} \right)^2 - 1} \, . \tag{44}$$

Under the Courant-condition

$$|\Delta t \; \omega_i| \leq 2 \tag{45}$$

the expression under the root is always negative, leading to complex eigenvalues $\lambda_{B,i}$ with

$$|\lambda_{B,i}| = 1. \tag{46}$$

Thus the norm (the energy) of all eigenvectors of $\mathbf{B}$ remains unchanged in each iteration step. As these eigenvectors build an orthogonal basis, this is also true for an arbitrary vector $\mathbf{y}$,

$$\left\| \mathbf{y}^{(m+1)} \right\|_2 = \left\| \mathbf{B} \mathbf{y}^{(m)} \right\|_2 = \left\| \mathbf{y}^{(m)} \right\|_2, \tag{47}$$

which is the desired proof for the energy conservation of the FIT combined with the leapfrog scheme.

4. ORTHOGONALITY OF DISCRETE WAVEGUIDE MODES

In the previous chapters the orthogonality properties of the three-dimensional[2] eigenmodes of the FIT-discretization based on a energy-related inner product has been proven.

A similar theorem can also be formulated for the two-dimensional modes in waveguides, or — to be more general — in two-dimensional

[2] The dimension here refers to the number of spatial directions, not to the number of degrees of freedom.

cross-sections of a Cartesian grid. To this end we first derive the discrete eigenvalue equation for such modes [9].

For the simulation of waveguide modes propagating in a coordinate-direction (here: z) of the grid,

$$\vec{E}, \vec{H} \sim e^{-i\,k_z z}, \tag{48}$$

(with the propagation constant k_z), this spatial direction can be treated by continuous rather than discrete analysis. From

$$\begin{aligned} \mathbf{P}_z\,\mathbf{f} &= \mathbf{f}\big|_{z_0+\Delta z} - \mathbf{f}\big|_{z_0} = \mathbf{f}\big|_{z_0}(e^{-i\,k_z\Delta z} - 1) \\ &\approx \mathbf{f}\big|_{z_0}(-i\,k_z\Delta z). \end{aligned} \tag{49}$$

we can substitute the differentiation operator $\mathbf{P}_z$ in the block-wise notation (9) and (10) of the operator matrices by[7]

$$\mathbf{P}_z = -i\,k_z\Delta z\,\mathbf{I}. \tag{50}$$

(Here for sake of a simplified notation the indexing system of the components has to be further specified: Pairs of transverse components $(\widehat{e}_{x,i}, \widehat{H}_{y,j})$ or $(\widehat{e}_{y,i}, \widehat{H}_{x,j})$ referring to intersecting primary and dual edges in the 2D-projection of the grid, are assumed to have the same index $i = j$; cf. Fig. 2, right.)
Note, that applying (50) to (9) and (10) results in complex-valued matrices, which are only valid for one distinct k_z. Besides, the transposed sub-matrices in $\widetilde{\mathbf{C}}$ and $\widetilde{\mathbf{S}}$ have to be replaced by the Hermitian expression $\mathbf{P}_z^H = +i\,k_z\Delta z\,\mathbf{I}$.

In the next step, we use the divergence-free condition for the electric flux to eliminate the longitudinal components from the eigenvalue equation. As the expression (50) can be easily inverted, we get

$$\widetilde{\mathbf{S}}\,\widehat{\widehat{\mathbf{d}}} = \mathbf{0} \quad \Rightarrow \quad \widehat{\widehat{\mathbf{d}}}_z = \frac{1}{i\,k_z\Delta z}(-\mathbf{P}_x^T\,\widehat{\widehat{\mathbf{d}}}_x - \mathbf{P}_y^T\,\widehat{\widehat{\mathbf{d}}}_y). \tag{51}$$

Finally a $2N_P \times 2N_P$-eigenvalue problem can be derived from (14) for the transverse components of the waveguide modes [9]:

$$(\mathbf{A}_{2D} - \omega^2\,\mathbf{I} - k_z^2\,\mathbf{B}_{2D})\ \widehat{\mathbf{e}}_t = \mathbf{0}. \tag{52}$$

In this paper we are mainly interested in the orthogonality properties of the solutions of this eigenvalue problem. Similar to the

[7] This corresponds to a first order approximation for small longitudinal grid step sizes Δz. It can be shown, however, that Δz can be shortened from all formulas based on this approximation, and thus (49) can be considered as an exact representation of the longitudinal differentiation operator in waveguides.

3D-case, from the algebraic properties of the 2D-system matrix we get the relation for the 2D-modes (index 't' for only transverse x- and y-components):

$$\widehat{\mathbf{e}}_{t,\xi}^T \,\widehat{\widehat{\mathbf{d}}}_{t,\eta} = \begin{pmatrix} \widehat{\mathbf{e}}_{x,\xi}^T & \widehat{\mathbf{e}}_{y,\xi}^T \end{pmatrix} \begin{pmatrix} \widehat{\widehat{\mathbf{d}}}_{x,\eta} \\ \widehat{\widehat{\mathbf{d}}}_{y,\eta} \end{pmatrix} = 0 \qquad (k_\xi \neq k_\eta). \tag{53}$$

If we assume a homogeneous material distribution (e.g. vacuum), a single component of this sum can be written as

$$\widehat{e}_{x,i}\,\widehat{\widehat{\mathbf{d}}}_{x,i} \approx (E_x\ \Delta x_i) \cdot (\varepsilon_0 E_x\ \Delta\widetilde{y}_i \Delta\widetilde{z}) = \varepsilon_0 \Delta\widetilde{z}\ (E_x^2\, A_{x,i}^*) \tag{54}$$

with the lengths and area as in Fig. 2 (left). Thus, for all components the discrete orthogonality relation corresponds to the dot-product based orthogonality of continuous modes in hollow waveguides [10]

$$\int_A \vec{E}_\xi \cdot \vec{E}_\eta\ dA = 0 \qquad (k_\xi \neq k_\eta). \tag{55}$$

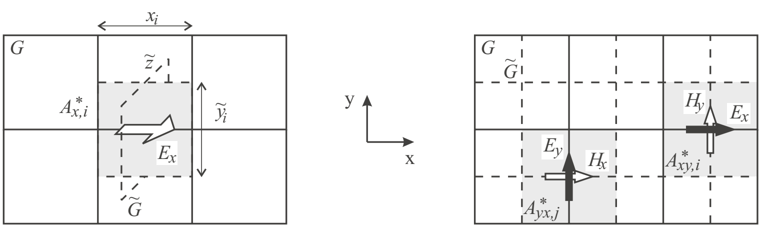

Figure 2. Orthogonality of discrete waveguide modes. Left: Energy-related orthogonality $\widehat{\mathbf{e}}_{t,\xi}^T \,\widehat{\widehat{\mathbf{d}}}_{t,\eta} = 0$ corresponding to the dot-product $\vec{E}_\xi \cdot \vec{E}_\eta$ for the continuous fields in hollow guides. Right: Energy-flow related orthogonality relation $\widehat{\mathbf{e}}_{t,\xi}^T \,\mathbf{K}\,\widehat{\mathbf{h}}_{t,\eta} = 0$ corresponding to the vector product $\vec{E}_\xi \times \vec{H}_\eta$ (with a topological matrix operator $\mathbf{K}$ according to (67)). The integration areas are implicitly defined by the integral-based state variables of the FIT.

An alternative formulation for the orthogonality of waveguide modes is based on the vector product of the electric and magnetic fields (similar to the definition of Poynting's vector):

$$\int_A (\vec{E}_\xi \times \vec{H}_\eta) \cdot d\vec{A} = 0 \qquad (|k_\xi| \neq |k_\eta|). \tag{56}$$

A corresponding theorem can be found for the discrete fields, too, and we again only use Maxwell's Grid Equations, the duality property (6), and the symmetry of the material matrices for its derivation. It is remarkable, that the algebraic proof is in close analogy to the classical proof for continuous fields (cf. [10]).

We start with the discrete curl-equations in (3), applied to two waveguide modes with $k_\xi \neq \pm k_\eta$. According to (50) two different $\mathbf{C}$-matrices (denoted $\mathbf{C}_\xi$ and $\mathbf{C}_\eta$) have to be used:

$$\mathbf{C}_\xi\,\widehat{\mathbf{e}}_\xi = -i\omega\,\widehat{\widehat{\mathbf{b}}}_\xi, \qquad \mathbf{C}_\eta\,\widehat{\mathbf{e}}_\eta = -i\omega\,\widehat{\widehat{\mathbf{b}}}_\eta. \tag{57}$$

Left-multiplying by $\widehat{\mathbf{h}}_\eta^T$ or $\widehat{\mathbf{h}}_\xi^T$ yields

$$\widehat{\mathbf{h}}_\eta^T\mathbf{C}_\xi\,\widehat{\mathbf{e}}_\xi = -i\omega\,\widehat{\mathbf{h}}_\eta^T\,\widehat{\widehat{\mathbf{b}}}_\xi, \qquad \widehat{\mathbf{h}}_\xi^T\mathbf{C}_\eta\,\widehat{\mathbf{e}}_\eta = -i\omega\,\widehat{\mathbf{h}}_\xi^T\,\widehat{\widehat{\mathbf{b}}}_\eta, \tag{58}$$

leading to (exploiting the symmetry of the magnetic material matrix)

$$\begin{aligned}\widehat{\mathbf{h}}_\eta^T\mathbf{C}_\xi\,\widehat{\mathbf{e}}_\xi - \widehat{\mathbf{h}}_\xi^T\mathbf{C}_\eta\,\widehat{\mathbf{e}}_\eta &= -i\omega\left((\mathbf{M}_{\mu^{-1}}\,\widehat{\widehat{\mathbf{b}}}_\eta)^T\,\widehat{\widehat{\mathbf{b}}}_\xi - (\mathbf{M}_{\mu^{-1}}\,\widehat{\widehat{\mathbf{b}}}_\xi)^T\,\widehat{\widehat{\mathbf{b}}}_\eta\right)\\ &= -i\omega\left(\widehat{\widehat{\mathbf{b}}}_\eta^T\mathbf{M}_{\mu^{-1}}^T\,\widehat{\widehat{\mathbf{b}}}_\xi - \widehat{\widehat{\mathbf{b}}}_\xi^T\mathbf{M}_{\mu^{-1}}^T\,\widehat{\widehat{\mathbf{b}}}_\eta\right) = 0.\end{aligned} \tag{59}$$

Analogously we obtain from the second curl-equation:

$$\widetilde{\mathbf{C}}_\xi\,\widehat{\mathbf{h}}_\xi = i\omega\,\widehat{\widehat{\mathbf{d}}}_\xi, \qquad \widetilde{\mathbf{C}}_\eta\,\widehat{\mathbf{h}}_\eta = i\omega\,\widehat{\widehat{\mathbf{d}}}_\eta, \tag{60}$$

$$\widehat{\mathbf{e}}_\eta^T\widetilde{\mathbf{C}}_\xi\,\widehat{\mathbf{h}}_\xi = i\omega\,\widehat{\mathbf{e}}_\eta^T\,\widehat{\widehat{\mathbf{d}}}_\xi, \qquad \widehat{\mathbf{e}}_\xi^T\widetilde{\mathbf{C}}_\eta\,\widehat{\mathbf{h}}_\eta = i\omega\,\widehat{\mathbf{e}}_\xi^T\,\widehat{\widehat{\mathbf{d}}}_\eta, \tag{61}$$

$$\begin{aligned}\widehat{\mathbf{e}}_\eta^T\widetilde{\mathbf{C}}_\xi\,\widehat{\mathbf{h}}_\xi - \widehat{\mathbf{e}}_\xi^T\widetilde{\mathbf{C}}_\eta\,\widehat{\mathbf{h}}_\eta &= i\omega\left((\mathbf{M}_\varepsilon^{-1}\,\widehat{\widehat{\mathbf{d}}}_\eta)^T\,\widehat{\widehat{\mathbf{d}}}_\xi - (\mathbf{M}_\varepsilon^{-1}\,\widehat{\widehat{\mathbf{d}}}_\xi)^T\,\widehat{\widehat{\mathbf{d}}}_\eta\right)\\ &= i\omega\left(\widehat{\widehat{\mathbf{d}}}_\eta^T(\mathbf{M}_\varepsilon^{-1})^T\,\widehat{\widehat{\mathbf{d}}}_\xi - \widehat{\widehat{\mathbf{d}}}_\xi^T(\mathbf{M}_\varepsilon^{-1})^T\,\widehat{\widehat{\mathbf{d}}}_\eta\right) = 0.\end{aligned} \tag{62}$$

Adding up (59) and (62) yields:

$$\begin{aligned}&\widehat{\mathbf{h}}_\eta^T\mathbf{C}_\xi\,\widehat{\mathbf{e}}_\xi - \widehat{\mathbf{e}}_\xi^T\widetilde{\mathbf{C}}_\eta\,\widehat{\mathbf{h}}_\eta - \widehat{\mathbf{h}}_\xi^T\mathbf{C}_\eta\,\widehat{\mathbf{e}}_\eta + \widehat{\mathbf{e}}_\eta^T\widetilde{\mathbf{C}}_\xi\,\widehat{\mathbf{h}}_\xi = 0\\ \Rightarrow\quad &\widehat{\mathbf{e}}_\xi^T(\mathbf{C}_\xi^T - \widetilde{\mathbf{C}}_\eta)\,\widehat{\mathbf{h}}_\eta - \widehat{\mathbf{e}}_\eta^T(\mathbf{C}_\eta^T - \widetilde{\mathbf{C}}_\xi)\,\widehat{\mathbf{h}}_\xi = 0.\end{aligned} \tag{63}$$

If we introduce now the block-wise notation of $\mathbf{C}$ and $\widetilde{\mathbf{C}}$ according to (9) and (50), we get

$$\begin{aligned}\mathbf{C}_\xi^T - \widetilde{\mathbf{C}}_\eta &= \begin{pmatrix} 0 & -ik_\xi\mathbf{I} & -\mathbf{P}_v^T\\ ik_\xi\mathbf{I} & 0 & \mathbf{P}_x^T\\ \mathbf{P}_v^T & -\mathbf{P}_x^T & 0\end{pmatrix} - \begin{pmatrix} 0 & ik_\eta\mathbf{I} & -\mathbf{P}_v^T\\ -ik_\eta\mathbf{I} & 0 & \mathbf{P}_x^T\\ \mathbf{P}_v^T & -\mathbf{P}_x^T & 0\end{pmatrix}\\ &= -i(k_\xi + k_\eta)\begin{pmatrix} 0 & \mathbf{I} & 0\\ -\mathbf{I} & 0 & 0\\ 0 & 0 & 0\end{pmatrix}.\end{aligned} \tag{64}$$

Thus, the transverse fields

$$\widehat{\mathbf{e}}_{t,\xi} = \begin{pmatrix} \widehat{\mathbf{e}}_{x,\xi} \\ \widehat{\mathbf{e}}_{y,\xi} \end{pmatrix} \qquad \widehat{\mathbf{h}}_{t,\xi} = \begin{pmatrix} \widehat{\mathbf{h}}_{x,\xi} \\ \widehat{\mathbf{h}}_{y,\xi} \end{pmatrix} \tag{65}$$

fulfill the relation

$$(k_\xi + k_\eta) \left(\widehat{\mathbf{e}}_{t,\xi}^T \mathbf{K} \widehat{\mathbf{h}}_{t,\eta} - \widehat{\mathbf{e}}_{t,\eta}^T \mathbf{K} \widehat{\mathbf{h}}_{t,\xi} \right) = 0, \tag{66}$$

with the matrix operator

$$\mathbf{K} = \begin{pmatrix} 0 & \mathbf{I} \\ -\mathbf{I} & 0 \end{pmatrix}. \tag{67}$$

For $k_\xi \neq -k_\eta$ as assumed above we finally get

$$\widehat{\mathbf{e}}_{t,\xi}^T \mathbf{K} \widehat{\mathbf{h}}_{t,\eta} - \widehat{\mathbf{e}}_{t,\eta}^T \mathbf{K} \widehat{\mathbf{h}}_{t,\xi} = 0. \tag{68}$$

If we change the sign of one of the propagation constants in this derivation (for a wave propagation in the opposite direction),

$$k'_\xi = -k_\xi, \qquad \widehat{\mathbf{e}}'_{t,\xi} = \widehat{\mathbf{e}}_{t,\xi}, \qquad \widehat{\mathbf{h}}'_{t,\xi} = -\widehat{\mathbf{h}}_{t,\xi}. \tag{69}$$

we get the relation

$$(-k_\xi + k_\eta) \left(\widehat{\mathbf{e}}_{t,\xi}^T \mathbf{K} \widehat{\mathbf{h}}_{t,\eta} + \widehat{\mathbf{e}}_{t,\eta}^T \mathbf{K} \widehat{\mathbf{h}}_{t,\xi} \right) = 0, \tag{70}$$

instead of (66), leading to (for $k_\xi \neq k_\eta$):

$$\widehat{\mathbf{e}}_{t,\xi}^T \mathbf{K} \widehat{\mathbf{h}}_{t,\eta} + \widehat{\mathbf{e}}_{t,\eta}^T \mathbf{K} \widehat{\mathbf{h}}_{t,\xi} = 0. \tag{71}$$

Adding up (68) and (71) finally yields the desired orthogonality relation for the discrete eigenmodes in waveguides:

$$\widehat{\mathbf{e}}_{t,\xi}^T \mathbf{K} \widehat{\mathbf{h}}_{t,\eta} = 0 \qquad (k_\xi \neq \pm k_\eta). \tag{72}$$

For each set of degenerated modes with $k_\xi = \pm k_\eta$ a linear combination can be found such, that (72) is fulfilled, too.

The geometrical interpretation of this orthogonality relation is shown in Fig. 2 (right). By the entries ± 1 in the topological operator $\mathbf{K}$, pairs of components $\widehat{e}_{x,i}$, $\widehat{\mathbf{h}}_{y,i}$ and $\widehat{e}_{y,j}$, $\widehat{\mathbf{h}}_{x,j}$ are coupled to each other, which are related to perpendicular edges; and each product of the corresponding field strengths can be considered as a part of the desired expression $\vec{E} \times \vec{H}$. The grid sizes implied in the discrete voltage quantities define again integration areas $A^*_{xy,i}$ and $A^*_{yx,j}$, which cover the cross section of the waveguide. Thus, (72) can be identified as a discrete analog of the integral over the vector product of $\vec{E}_\xi$ and $\vec{H}_\eta$ in (56).

5. CONCLUSION

In this paper we presented the concept of discrete energy quantities for the electric and magnetic grid voltages — the state variables of the Finite Integration Technique — in a Cartesian grid system.

A central point of the derivation is the first-order interpretation of the discrete voltages as products of a continuous field quantity and the metric of the corresponding edges and facets of the grid. This leads to the geometrical interpretation of the energy quantities as sum over all cell-energies, using different segmentations of the computation domain.

Several algebraic proofs for important properties of the FIT have been presented, including the energy conservation of the FIT both in frequency and time domain, the energy-based orthogonality of the three-dimensional eigenmodes, and two different formulations for the orthogonality of two-dimensional modes in longitudinally homogeneous waveguides.

All these proofs are based on only a few algebraic properties of the discretization scheme — namely the duality of the discrete curl-operators and the definition of symmetric and positive definite material matrices. These properties thus can be considered to be key points of the formulation, and have to be preserved for any extensions of the method (like e.g. sub-gridding techniques, non-orthogonal grids, or higher-order schemes).

Not only the presented theorems themselves but also their derivations and proofs within the discrete algebraic system are in close analogy to the vector-analytical analysis of continuous fields. The Finite Integration Technique therefore can be considered as a unique and consistent discrete electromagnetic field theory.

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