A Symbolic Procedure for the Diagonalization of Linear PDEs in Accelerated Computational Engineering

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1 Abstract

In this contribution we conjecture that systems of linearized Partial Differential Equations, viewed as consistent models for physically realizable systems, are diagonalizable. While this property is interesting for its own sake, our discussion will focus on technicalities and implications for advanced accelerated computing. We will demonstrate that diagonalization with respect to a chosen spatial coordinate systematically "reshuffles" the original PDEs and creates equivalent differential forms. It turns out that diagonalization automatically distinguishes the variables in the interface- and boundary conditions defined on surfaces normal to the diagonalization direction.

2 Introduction

Since early 90's in the past century we have been focusing on the acceleration of computer simulations of Partial Differential Equations and accuracy enhancement of the numerical solutions. We have devised a symbolic procedure for systematically and automatically diagonalizing the linear PDEs commonly encountered in mathematical physics and computational engineering applications.

This presentation provides a detailed account of the ideas behind diagonalization, and briefly discusses its implications for designing robust, accurate and accelerated algorithms for solving Boundary Value Problems in both integral- and differential form. We start with a conjecture stating that *all linearized PDEs, viewed as consistent models for physically realizable systems, diagonalizable.* D-forms are equivalent to the parent PDEs. However, they explicitly distinguish the space coordinate with respect to which the diagonalization has been performed. D-forms allow several useful interpretations which are generally deeply hidden in the originating PDEs. We demonstrate the technical details by converting two systems of PDEs into their equivalent D-forms: (i) the electromagnetic wave equations for vector fields in fully bianisotropic and transversally inhomogeneous media, and (ii) magnetostatic equations. For the diagonalization of several other PDEs we refer to [1], [2]. We propose a symbolic notation, which can easily be automated, and replaces tedious calculations by a *simply-by-inspection* manipulatory procedure. In this respect, the present work is a continuation of the work in [1] and [2]. For reasons to be made clear soon we refer to D-representations as the Huygens' Principle in Differential Form. This interpretation can favorably be used for (i) generating novel stencils in the finite difference method, (ii) constructing functionals in the finite element method, and most importantly, (iii) formulating and regularizing singular surface integrals in the Boundary Element Method applications [1], [2]. D-forms in spectral domain are algebraic eigenvalue equations. Using the associated eigenpairs, Green's functions in question can easily be constructed [1], [2]. Furthermore, D-forms facilitate the investigation of the asymptotic properties of the eigenpairs in the far- and near-field in the spectral domain [1], [2]. In accordance with Heisenberg's uncertainty principle these asymptotic expansions correspond to the near- and far-fields in the spatial domain, respectively. In particular, utilizing the far-field expansions in the spectral domain an easy-to-implement recipe for the regularization of singular surface integrals emerges.

3 Diagonalization and its Interpretation

Consider a differentiable 3-manifold $\mathbf{M^3}$. Let $\mathcal{A}\boldsymbol{u} = 0$ represent a system of linear homogeneous PDEs in $\mathbf{\Omega}$ with given conditions on the boundary $\partial\mathbf{\Omega}$, with $\mathbf{\Omega}$ and $\partial\mathbf{\Omega} \subset \mathbf{M^3}$. At a point $p \in \mathbf{\Omega}$ consider the local coordiante system (ξ, η, ζ). We refer to the $\zeta-$direction as the "normal" direction (N-direction), and the plane normal to ζ as the "tangent" plane (T-plane) at p.

Diagonalization with respect to the N-direction transforms $\mathcal{A}\boldsymbol{u} = 0$ into an equivalent form $\mathcal{L}\Psi = \partial_\zeta \Psi$ (D-form) with distinct properties:

1. $\mathcal{L} = \mathcal{L}(\xi, \eta)$. (For time dependent problems the list of arguments contains the time variable t, or, ω, its dual variable in the Fourier domain.)
2. The components of Ψ are *exclusively* those field variables which enter into the interface- (and boundary) conditions on the $T-$plane. Without any jump discontinuities we obtain $\Psi(\zeta^+) = \Psi(\zeta^-)$, which we preferably will write as $\Psi^< = \Psi^>$.
3. Let Ψ be known and continuously differentiable to any order required in the $\epsilon-$neighborhood $\mathcal{N}(p, \epsilon)$ ($\subset T-$plane). Construct $\mathcal{L}\Psi$ on $\mathcal{N}(p, \epsilon)$. Then, according to $\mathcal{L}\Psi = \partial_\zeta \Psi$, the rate of change of Ψ in the N-direction is uniquely determined at p.
4. The property that $\mathcal{L}$ merely depends on ξ and η allows further conclusions. Differentiate both sides of $\mathcal{L}\Psi = \partial_\zeta \Psi$ with respect to ζ, and interchange the order of ∂_ζ and $\mathcal{L}$ at the L.H.S. to obtain $\mathcal{L}\partial_\zeta \Psi = \partial_\zeta^{(2)} \Psi$. Substitute for $\partial_\zeta \Psi$ from the D-form and introduce $\mathcal{L}^{(2)} = \mathcal{L}\mathcal{L}$ to get $\mathcal{L}^{(2)}\Psi = \partial_\zeta^{(2)}\Psi$. By an induction argument $\mathcal{L}^{(n)}\Psi = \partial_\zeta^{(n)}\Psi$ for $n \in N$.
5. Therefore, in the neighborhood of p in the N-direction, we have:

$$\Psi(\xi,\eta,\zeta+h) = \sum_n \frac{h^n}{n!}\left\{\mathcal{L}^{(n)}\Psi\right\}_{(\xi,\eta,\zeta)} \tag{1}$$

6. Consider a closed surface $\gamma \subset \mathbf{\Omega}$. At each point (ξ,η,ζ) of γ proceed as sketched above and construct the field Ψ' at all points $(\xi,\eta,\zeta+h)$, such that the entirety of these points build the surface γ', with $\gamma' \subset \mathbf{\Omega}$. This interpretation suggests referring to the diagonalization as the Huygence principle in differential form. These considerations allow the construction of useful and fast algorithms for the BEM [3]-[9], Finite Difference Method [10], and the Finite Element Method applications.
7. Consider the Fourier transform of $\mathcal{L}\Psi = \partial_\zeta\Psi$ with respect to the spatial coordinates in the T-plane:

$$\overline{L}(k_\xi,k_\eta)\overline{\Psi} = \lambda\overline{\Psi}, \tag{2}$$

   where the bar indicates variables in the $(k_\xi,k_\eta)-$ spectral domain.
8. In view of (2) consider the eigenvalues $\lambda(k_\xi,k_\eta)$ and the associated eigenvectors $\overline{\Psi}(k_\xi,k_\eta)$ for asymptotically large k_ξ and k_η. According to the Heisenberg uncertainty principle the far field in the spectral domain corresponds to the near field in the spatial domain. Therefore, it can be postulated that the $(k_\xi,k_\eta \to \infty)$ asymptotics of the eigenpairs provide the ingredients for expanding the near fields in the spatial domain. Indeed we have shown [1], [2] that this is valid. Furthermore, the asymptotic eigenpairs can be used to regularize surface integrals, with (weak-, strong-, or hyper-) singular kernels [11]: A major source for numerical difficulties in the BEM applications originate in the inadequate treatment of the kernel singularities in surface integrals. This may lead to inaccurate near field distributions and thus divergent or near-divergent numerical results. Regularization techniques using spectral domain asymptotics allow us, however, to "zoom" into these difficulties and "temper" their behavior to any degree we desire.
9. Consider $\mathcal{A}\boldsymbol{u} = \boldsymbol{s}$ with the source function $\boldsymbol{s} = \boldsymbol{J}\delta(\zeta-\zeta_0)$. Here, $\delta(\cdot)$ stands for the Dirac delta function. Diagonalization applied to this equation automatically generates the interface equations. Thereby, in contrast to the expositions in standard text books, there is no need for introducing a thin pillbox, and the subsequent limiting process.

4 Procedural Details of the Diagonalization

We choose a cartesian coordinate system (x,y,z), and perform the diagonalization with respect to the $z-$coordiante. A few comments and preparatory calculations are in place.

4.1 Domain Decomposition

Adopt the following representation for the field[1] $\Psi(x,y,z)$.

$$\Psi(x,y,z) = \Psi^{<}(x,y,z)\mathcal{H}(z_0 - z) + \Psi^{>}(x,y,z)\mathcal{H}(z - z_0), \tag{3}$$

$\Psi(.)$ may be scalar or a vector. $\mathcal{H}(\cdot)$ is the Heaviside's step function: $\mathcal{H}(z)$ is 0 for $z < 0$, and 1 for $z > 0$. Obviously we have

$$\partial_a \Psi(x,y,z) = \left\{\partial_a \Psi^{<}(x,y,z)\right\}\mathcal{H}(z_0 - z) + \left\{\partial_a \Psi^{>}(x,y,z)\right\}\mathcal{H}(z - z_0), \tag{4}$$

with a representing x or y. Furthermore, with $\partial_z \mathcal{H}(z_0 - z) = -\delta(z_0 - z) = -\delta(z - z_0)$ and $\partial_z \mathcal{H}(z - z_0) = \delta(z - z_0)$ we obtain

$$\begin{aligned}\partial_z \Psi(x,y,z) =& \left\{\partial_z \Psi^{<}(x,y,z)\right\}\mathcal{H}(z_0 - z) + \left\{\partial_z \Psi^{>}(x,y,z)\right\}\mathcal{H}(z - z_0) \\ &+ \left\{-\Psi^{<}(x,y,z) + \Psi^{>}(x,y,z)\right\}\delta(z - z_0).\end{aligned} \tag{5}$$

4.2 A Convenient Symbolic Representation of the Curl Operator

In order to facilitate our manipulations and to allow symbolic computations we write the curl operator in the form

$$\begin{aligned}\boldsymbol{\nabla}\times = \begin{bmatrix} 0 & -\partial_z & \partial_y \\ \partial_z & 0 & -\partial_x \\ -\partial_y & \partial_x & 0 \end{bmatrix} =& \partial_x \underbrace{\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{bmatrix}}_{N_1} + \partial_y \underbrace{\begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{bmatrix}}_{N_2} + \partial_z \underbrace{\begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}}_{N_3} \\ =& \partial_x N_1 + \partial_y N_2 + \partial_z N_3,\end{aligned} \tag{6}$$

The matrices N_i $(i = 1,2,3)$ are defined in (6). Note that

$$N_i^T N_i = \begin{bmatrix} 1-\delta_{1i} & 0 & 0 \\ 0 & 1-\delta_{2i} & 0 \\ 0 & 0 & 1-\delta_{3i} \end{bmatrix}; \quad i = 1,2,3. \tag{7}$$

(Here, δ_{mn} stands for the Kronecker symbol.) These properties motivate appropriate decompositions of the 3×3 identity matrix I, which will be used for the diagonalization, e.g. consider the decomposition induced by N_1:

[1] The differentiability of the involved functions, to any order required, has been assumed.

$$I = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} + \begin{bmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \underbrace{\begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}}_{U_1} + \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & -1 & 0 \end{bmatrix} \underbrace{\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{bmatrix}}_{N_1}$$
$$= U_1 U_1 + N_1^T N_1 \tag{8}$$

The matrix U_1 has been introduced in (8). Similarly, we obtain (9) by introducing U_2 and U_3 *mutatis mutandis*[2]:

$$I = U_i U_i + N_i^T N_i; \quad i = 2, 3. \tag{9}$$

The relationships in (10) hold true (0 stands for the 3×3 null matrix):

$$U_i N_i = N_i U_i = U_i N_i^T = N_i^T U_i = 0; \quad i = 1, 2, 3. \tag{10}$$

It is instructive to examine further properties of N_i and establish a connection between these matrices and the proper rotation matrices in R^3.

Matrices N_i and Proper Rotation Matrices R_i In view of

$$N_1 N_2 = \begin{bmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \qquad \text{and} \qquad N_2 N_1 = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \tag{11}$$

we obtain $[N_1, N_2] \overset{\text{Def}}{=} N_1 N_2 - N_2 N_1 = N_3$. Therefore, the constituent matrices N_1, N_2, and N_3 of the curl operator satisfy the defining commutation relations of the Lie algebra $\mathbf{so}(3)$, [12]:

$$[N_1, N_2] = N_3, \qquad [N_2, N_3] = N_1, \qquad [N_3, N_1] = N_2. \tag{12}$$

Rotation Group SO(3) Next we establish a relationship between N_i and the proper rotation matrices R_i defined in (13). It is known that every proper rotation in R^3 can be expressed in terms of a succession of three proper rotations about the $x-$, $y-$, and $z-$ axis. The corresponding one-parameter subgroups can be generated by the matrices $R_1(\alpha)$, $R_2(\beta)$, and $R_3(\gamma)$:

[2] In [1], [2] we have suggested an alternative decomposition of the identity matrix, which was devised for the diagonalization of PDEs arising in the theory of linear elasticity, and piezoelectricity.

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos\alpha & -\sin\alpha \\ 0 & \sin\alpha & \cos\alpha \end{bmatrix}, \quad \begin{bmatrix} \cos\beta & 0 & \sin\beta \\ 0 & 1 & \\ -\sin\beta & 0 & \cos\beta \end{bmatrix}, \quad \begin{bmatrix} \cos\gamma & -\sin\gamma & 0 \\ \sin\gamma & \cos\gamma & 0 \\ 0 & 0 & 1 \end{bmatrix}. \tag{13}$$

Each of these matrices satisfy the following properties: (i) They are orthonormal, meaning that $R_i^T(\theta)R_i(\theta) = I$. (ii) They are proper (special) in the sense that $\det\{R_i\} = 1$. (iii) The group multiplication is an analytic function of parameter θ. More precisely, $R_i(\theta_1)R_i(\theta_2) = R_i(\theta_1+\theta_2)$. (iv) The inverse operation is an analytic function of parameter θ: $R_i^{-1}(\theta) = R_i(-\theta) = R_i^T(\theta)$.

These matrices form a one-parameter Lie group and since they are *special* and *orthonormal* in R^3, they are called the special orthogonal group in 3 dimensions and denoted by $\mathbf{SO}(3)$. The basic vectors of the Lie algebra $\mathbf{so}(3)$ (the infinitesimal generators) are obtained by differentiating $R_i(\theta)$ with respect to the corresponding angle parameter θ and consecutively setting θ equal to zero. This establishes the relationship we have been looking for [12]:

$$\frac{dR_1(\alpha)}{d\alpha}\Big|_{\alpha=0} = N_1, \quad \frac{dR_2(\beta)}{d\beta}\Big|_{\beta=0} = N_2, \quad \frac{dR_3(\gamma)}{d\gamma}\Big|_{\gamma=0} = N_3. \tag{14}$$

A Convenient Symbolic Representation of the Nabla Operator

$$\boldsymbol{\nabla} = \begin{bmatrix} \partial_x \\ \partial_y \\ \partial_z \end{bmatrix} = \underbrace{\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix}}_{N_{12}} \begin{bmatrix} \partial_x \\ \partial_y \\ 0 \end{bmatrix} + \underbrace{\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}}_{U_3} \begin{bmatrix} 0 \\ 0 \\ \partial_z \end{bmatrix} \tag{15a}$$

$$= N_{12} \begin{bmatrix} \partial_x \\ \partial_y \\ 0 \end{bmatrix} + U_3 \begin{bmatrix} 0 \\ 0 \\ \partial_z \end{bmatrix} \tag{15b}$$

5 Maxwell's Equations in Differential Form

Consider the Maxwell's equations in differential form with $\boldsymbol{J}$ and ρ being, respectively, the electric current density and the charge density:

$$\boldsymbol{\nabla} \times \boldsymbol{H} - \frac{\partial \boldsymbol{D}}{\partial t} = \boldsymbol{J} \tag{16a}$$

$$\boldsymbol{\nabla} \times \boldsymbol{E} + \frac{\partial \boldsymbol{B}}{\partial t} = 0 \tag{16b}$$

$$\boldsymbol{\nabla} \cdot \boldsymbol{B} = 0 \tag{16c}$$

$$\boldsymbol{\nabla} \cdot \boldsymbol{D} = \rho \tag{16d}$$

Applying the dot product of $\boldsymbol{\nabla}$ to both sides of (16a) and using (16d) we obtain the continuity equation $\partial\rho/\partial t + \boldsymbol{\nabla} \cdot \boldsymbol{J} = 0$. The field variables in (16) are as follows. $\boldsymbol{E}$: electric field; $\boldsymbol{D}$: dielectric displacement; $\boldsymbol{H}$: magnetic field; $\boldsymbol{B}$: magnetic induction.

5.1 Constitutive Equations

General Bianisotropic Media In fully bianisotropic media we have the relationships in (17) for the field vectors $\boldsymbol{D}$ and $\boldsymbol{B}$. The material parameters $\varepsilon_{ij}, \xi_{ij}, \zeta_{ij}$, and μ_{ij}; $i, j = 1, 2, 3$ constitute 3×3 matrices.

$$\boldsymbol{D} = \underline{\underline{\varepsilon}}\boldsymbol{E} + \underline{\underline{\xi}}, \quad \boldsymbol{B} = \underline{\underline{\zeta}}\boldsymbol{E} + \underline{\underline{\mu}}\boldsymbol{H}. \tag{17}$$

Let $\boldsymbol{x}$ represent $\boldsymbol{E}$ or $\boldsymbol{H}$, and $\underline{\underline{\kappa}}$ either of the matrices in (17). General physical properties, such as passivity and reciprocity, translate into specific constraints imposed on the involved material matrices. In present discussion we merely require the existence of these matrices. This means that for general bianisotropic media, for example, we require that $\underline{\underline{\kappa}}\boldsymbol{x} \neq 0$ for every $\boldsymbol{x} \neq 0$. The D-procedure will result in a set of necessary conditions on the material matrices.

General Anisotropic Media Fully anisotropic media are characterized by the fact that $\underline{\underline{\xi}} = \underline{\underline{\zeta}} = 0$, and that $\underline{\underline{\varepsilon}}\boldsymbol{x} \neq 0$, and $\underline{\underline{\mu}}\boldsymbol{x} \neq 0$ for $\boldsymbol{x} \neq 0$.

Isotropic Media Here we have $\underline{\underline{\xi}} = \underline{\underline{\zeta}} = 0$, in addition to $\underline{\underline{\varepsilon}}\boldsymbol{x} = \alpha I$ and $\underline{\underline{\mu}}\boldsymbol{x} = \beta I$ with $\alpha, \beta \in R^+$.

5.2 Maxwell's Equations in Static Limit ($\partial/\partial t \equiv 0$)

$$\boldsymbol{\nabla} \times \boldsymbol{H} = \boldsymbol{J}, \quad \boldsymbol{\nabla} \times \boldsymbol{E} = 0, \quad \boldsymbol{\nabla} \cdot \boldsymbol{B} = 0, \quad \boldsymbol{\nabla} \cdot \boldsymbol{D} = \rho. \tag{18}$$

Assuming $\boldsymbol{D} = \underline{\underline{\varepsilon}}\boldsymbol{E}$ and $\boldsymbol{B} = \underline{\underline{\mu}}\boldsymbol{H}$, (18) decouples into (19) and (20).

Electrostatic Equations in Anisotropic Dielectric Media

$$\boldsymbol{\nabla} \times \boldsymbol{E} = 0, \quad \boldsymbol{\nabla} \cdot \boldsymbol{D} = \rho, \quad \boldsymbol{D} = \underline{\underline{\varepsilon}}\boldsymbol{E}. \tag{19}$$

Magnetostatic Equations in Anisotropic Magnetic Media

$$\boldsymbol{\nabla} \times \boldsymbol{H} = \boldsymbol{J}, \quad \boldsymbol{\nabla} \cdot \boldsymbol{B} = 0, \quad \boldsymbol{B} = \underline{\underline{\mu}}\boldsymbol{H}. \tag{20}$$

5.3 Diagonalization of the Electrodynamic Equations

Our objective is the diagonalization of the electrodynamic equations in general bianisotropic, source-free media[3] with respect to a coordiante variable, say, z. We adopt a harmonic time-dependence of the fields according to $e^{-j\omega t}$. Then with $\partial/\partial t \Longleftrightarrow -j\omega$ and introducing $\partial/\partial(j\omega x) = \partial/\partial\tilde{x}$, $\partial/\partial(j\omega y) = \partial/\partial\tilde{y}$, and $\partial/\partial(j\omega z) = \partial/\partial\tilde{z}$, we obtain

$$[\partial_{\tilde{x}} N_1 + \partial_{\tilde{y}} N_2 + \partial_{\tilde{z}} N_3[\, \boldsymbol{H} = -\underline{\underline{\varepsilon}}\boldsymbol{E} - \underline{\underline{\zeta}}\boldsymbol{H}, \tag{21a}$$

$$[\partial_{\tilde{x}} N_1 + \partial_{\tilde{y}} N_2 + \partial_{\tilde{z}} N_3]\, \boldsymbol{E} = \underline{\underline{\xi}}\boldsymbol{E} + \underline{\underline{\mu}}\boldsymbol{H}. \tag{21b}$$

Multiply (21) by N_3^T, and U_3 from the LHS, and insert the decomposition $U_3 U_3 + N_3 N_3^T$ for the identity matrix between the material matrices and the field vectors at the RHS, to arrive at (22).

$$\begin{aligned}
&\left[\partial_{\tilde{x}} N_3^T N_1 + \partial_{\tilde{y}} N_3^T N_2\right] \boldsymbol{H} + \partial_{\tilde{z}} N_3^T N_3 \boldsymbol{H} && \text{(22a)}\\
&= -(N_3^T \underline{\underline{\varepsilon}} N_3)(N_3^T \boldsymbol{E}) - (N_3^T \underline{\underline{\varepsilon}} U_3)(U_3 \boldsymbol{E}) - (N_3^T \underline{\underline{\zeta}} N_3)(N_3^T \boldsymbol{H}) - (N_3^T \underline{\underline{\zeta}} U_3)(U_3 \boldsymbol{H}) &&\\
&\left[\partial_{\tilde{x}} N_3^T N_1 + \partial_{\tilde{y}} N_3^T N_2\right] \boldsymbol{E} + \partial_{\tilde{z}} N_3^T N_3 \boldsymbol{E} && \text{(22b)}\\
&= (N_3^T \underline{\underline{\xi}} N_3)(N_3^T \boldsymbol{E}) + (N_3^T \underline{\underline{\xi}} U_3)(U_3 \boldsymbol{E}) + (N_3^T \underline{\underline{\mu}} N_3)(N_3^T \boldsymbol{H}) + (N_3^T \underline{\underline{\mu}} U_3)(U_3 \boldsymbol{H}) &&\\
&[\partial_{\tilde{x}} U_3 N_1 + \partial_{\tilde{y}} U_3 N_2]\, \boldsymbol{H} + \partial_{\tilde{z}} U_3 N_3 \boldsymbol{H} && \text{(22c)}\\
&= -(U_3 \underline{\underline{\varepsilon}} N_3)(N_3^T \boldsymbol{E}) - (U_3 \underline{\underline{\varepsilon}} U_3)(U_3 \boldsymbol{E}) - (U_3 \underline{\underline{\zeta}} N_3)(N_3^T \boldsymbol{H}) - (N_3^T \underline{\underline{\zeta}} U_3)(U_3 \boldsymbol{H}) &&\\
&[\partial_{\tilde{x}} U_3 N_1 + \partial_{\tilde{y}} U_3 N_2]\, \boldsymbol{E} + \partial_{\tilde{z}} U_3 N_3 \boldsymbol{E} && \text{(22d)}\\
&= (U_3 \underline{\underline{\xi}} N_3)(N_3^T \boldsymbol{E}) + (U_3 \underline{\underline{\xi}} U_3)(U_3 \boldsymbol{E}) + (U_3 \underline{\underline{\mu}} N_3)(N_3^T \boldsymbol{H}) + (U_3 \underline{\underline{\mu}} U_3)(U_3 \boldsymbol{H}) &&
\end{aligned}$$

To convey the underlying idea consider (22a) in greater detail:

$$\begin{aligned}
&\begin{bmatrix} 0 & 0 & -\partial_{\tilde{x}} \\ 0 & 0 & -\partial_{\tilde{y}} \\ 0 & 0 & 0 \end{bmatrix} \boldsymbol{H} + \partial_{\tilde{z}} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix} \boldsymbol{H} \\
&= -\begin{pmatrix} \varepsilon_{22} & -\varepsilon_{21} & 0 \\ -\varepsilon_{12} & \varepsilon_{11} & 0 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} E_2 \\ -E_1 \\ 0 \end{pmatrix} - \begin{pmatrix} 0 & 0 & \varepsilon_{23} \\ 0 & 0 & -\varepsilon_{13} \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ E_3 \end{pmatrix} \\
&\quad - \begin{pmatrix} \zeta_{22} & -\zeta_{21} & 0 \\ -\zeta_{12} & \zeta_{11} & 0 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} H_2 \\ -H_1 \\ 0 \end{pmatrix} - \begin{pmatrix} 0 & 0 & \zeta_{23} \\ 0 & 0 & -\zeta_{13} \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ H_3 \end{pmatrix}
\end{aligned} \tag{23}$$

Obviously, we have been able to achieve several goals by one stroke: (i) The (trivial) third equation $(0 = 0)$ can be discarded. (ii) The "transversal" $(x, y)-$, and the "normal" $z-$dependences have been distinctly separated. (iii) At the

[3] Details regarding the inclusion of sources will be exemplified in Sec. 5.4.

LHS the matrices are built such, that the $x-$ and $y-$ derivatives act on H_3 only. At the same time, the $z-$derivative acts on the components H_1 and H_2 only. Equation (22b) leads to similar conclusions *mutatis mutandis.*

Next consider (22c). Written explicitly we have:

$$\begin{aligned}
&\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ -\partial_{\tilde{y}} & \partial_{\tilde{x}} & 0 \end{bmatrix} \boldsymbol{H} + \partial_{\tilde{z}} \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \boldsymbol{H} \\
&= -\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ \varepsilon_{32} & -\varepsilon_{31} & 0 \end{pmatrix} \begin{pmatrix} E_2 \\ -E_1 \\ 0 \end{pmatrix} - \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & \varepsilon_{33} \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ E_3 \end{pmatrix} \\
&\quad -\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ \zeta_{32} & -\zeta_{31} & 0 \end{pmatrix} \begin{pmatrix} H_2 \\ -H_1 \\ 0 \end{pmatrix} - \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & \zeta_{33} \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ H_3 \end{pmatrix}
\end{aligned} \tag{24}$$

Several facts are noteworthy: (i) The $z-$ variation has been eliminated. (ii) The (trivial) first two equations ($0 = 0$) can be discarded. (iii) The remaining equation allows us to express the "normal" field components E_3 and H_3 in terms of the "transversal" field components and their derivatives with respect to the "transversal" variables. Equation (22d) leads to similar conclusions *mutatis mutandis*. In summary we obtain

$$\begin{aligned}
\partial_{\tilde{z}} \begin{pmatrix} E_1 \\ E_2 \\ H_1 \\ H_2 \end{pmatrix} &= \begin{pmatrix} \xi_{21} & \xi_{22} & \mu_{21} & \mu_{22} \\ -\xi_{11} & -\xi_{12} & -\mu_{11} & -\mu_{12} \\ -\varepsilon_{21} & -\varepsilon_{22} & -\zeta_{21} & -\zeta_{22} \\ \varepsilon_{11} & \varepsilon_{12} & \zeta_{11} & \zeta_{12} \end{pmatrix} \begin{pmatrix} E_1 \\ E_2 \\ H_1 \\ H_2 \end{pmatrix} \\
&\quad + \begin{pmatrix} \xi_{23} & \mu_{23} \\ -\xi_{13} & -\mu_{13} \\ -\varepsilon_{23} & -\zeta_{23} \\ \varepsilon_{13} & \zeta_{13} \end{pmatrix} \begin{pmatrix} E_3 \\ H_3 \end{pmatrix} + \begin{bmatrix} \partial_{\tilde{x}} & 0 \\ \partial_{\tilde{y}} & 0 \\ 0 & \partial_{\tilde{x}} \\ 0 & \partial_{\tilde{y}} \end{bmatrix} \begin{pmatrix} E_3 \\ H_3 \end{pmatrix}
\end{aligned} \tag{25}$$

$$\begin{aligned}
\begin{pmatrix} E_3 \\ H_3 \end{pmatrix} &= \begin{pmatrix} \varepsilon_{33} & \zeta_{33} \\ -\xi_{33} & -\mu_{33} \end{pmatrix}^{-1} \begin{pmatrix} -\varepsilon_{31} & -\varepsilon_{32} & -\zeta_{31} & -\zeta_{32} \\ \xi_{31} & \xi_{32} & \mu_{31} & \mu_{32} \end{pmatrix} \begin{pmatrix} E_1 \\ E_2 \\ H_1 \\ H_2 \end{pmatrix} \\
&\quad + \begin{pmatrix} \varepsilon_{33} & \zeta_{33} \\ -\xi_{33} & -\mu_{33} \end{pmatrix}^{-1} \begin{bmatrix} 0 & 0 & \partial_{\tilde{y}} & -\partial_{\tilde{x}} \\ \partial_{\tilde{y}} & -\partial_{\tilde{x}} & 0 & 0 \end{bmatrix} \begin{pmatrix} E_1 \\ E_2 \\ H_1 \\ H_2 \end{pmatrix}
\end{aligned} \tag{26}$$

Substituting[4] (26) into (25) and introducing $\Psi=(E_1,E_2,H_1,H_2)^T$ lead to

$$\mathcal{L}(\varepsilon_{ij},\xi_{ij},\zeta_{ij},\mu_{ij},\partial_{\tilde{x}},\partial_{\tilde{y}})\Psi=\partial_{\tilde{z}}\Psi. \tag{27}$$

5.4 Diagonalization of the Magnetostatic Equations

Our starting point are the equations in (20), [13]. We first assume a source free medium ($\boldsymbol{J}\equiv 0$), and then consider fields which are driven by a source function. Equation (20) implies that $\boldsymbol{B}$ can be expressed as the curl of a vector potential $\boldsymbol{A}$. Under these conditions (20) implies

$$\nabla\times\boldsymbol{H}=0, \tag{28a}$$
$$\nabla\times\boldsymbol{A}=\underline{\underline{\mu}}\boldsymbol{H}. \tag{28b}$$

Our goal is to investigate the diagonalization of (28) with respect to the $z-$coordiante. The occurance of the curl operator in both equations suggests a procedure similar to that we developed in the previous section. We insert $N_3N_3^T+U_3U_3$ for the indentity matrix I between $\underline{\underline{\mu}}$ and $\boldsymbol{H}$ at the RHS of (28b), and multiply both equations, first by N_3^T, and then by U_3, from the LHS. The resulting equations collapse in

$$\partial_z\begin{pmatrix}H_1\\H_2\end{pmatrix}=\begin{bmatrix}\partial_x\\\partial_y\end{bmatrix}H_3, \tag{29a}$$
$$\partial_z\begin{pmatrix}A_1\\A_2\end{pmatrix}=\begin{bmatrix}\partial_x\\\partial_y\end{bmatrix}A_3+\begin{pmatrix}\mu_{21}&\mu_{22}\\-\mu_{11}&-\mu_{12}\end{pmatrix}\begin{pmatrix}H_1\\H_2\end{pmatrix}+\begin{pmatrix}\mu_{23}\\-\mu_{13}\end{pmatrix}H_3, \tag{29b}$$
$$\left[-\partial_y\ \partial_x\right]\begin{pmatrix}H_1\\H_2\end{pmatrix}=0, \tag{29c}$$
$$\left[-\tfrac{1}{\mu_{33}}\partial_y\ \tfrac{1}{\mu_{33}}\partial_x\right]\begin{pmatrix}A_1\\A_2\end{pmatrix}-\left(\tfrac{\mu_{31}}{\mu_{33}}\ \tfrac{\mu_{32}}{\mu_{33}}\right)\begin{pmatrix}H_1\\H_2\end{pmatrix}=H_3. \tag{29d}$$

The appearance of the $z-$ derivatives of H_1, H_2, A_1, and A_2 in (29a) and (29b) suggest that these are the only field components which will enter into the D-form (permissible, reduced variables). Therefore, H_3 and A_3 must be eliminated by using (29c) and (29d). However, we realize that this is not possible: While (29d) is an expression for H_3 in terms of the admissible field variables[5],

[4] Note that the existence of the above inverse matrix is necessary to perform our manipulations. In particular its determinant should nonzero: $\varepsilon_{33}\mu_{33}-\zeta_{33}\xi_{33}\neq 0$. Note that diagonalization with respect to the $x-$, and $y-$ coordinates results in similar inequalities. Therfeore, we conclude that for physically realizable systems the necessary conditions $\varepsilon_{ii}\mu_{ii}-\zeta_{ii}\xi_{ii}\neq 0$, $(i=1,2,3)$ have to be satisfied.

[5] In view of (29d) $\mu_{33}\neq 0$. Analogeously, diagonalization with respect to $x-$, and $y-$ coordinates require that $\mu_{11}\neq 0$, and $\mu_{22}\neq 0$, respectively.

there is no equation available which would allow the elimination of A_3. (Equations (29c) and (29d) do not involve A_3.) *Therefore, according to our conjecture, (28) does not model a physically realizable system.* Alternatively, it can be stated that: *Assuming a general* 3×3 *matrix* $\underline{\underline{\mu}}$ *and allowing spatial variation with respect to all the three spatial coordiantes, the equations (28) are not consistent.*

Therefore, the primary objective is now to create conditions under which A_3 disappears from our equations. We can achieve this goal by assuming that there is no variation in one of the transversal directions, and/or specializing the structure of $\underline{\underline{\mu}}$. Thus, assume $\partial/\partial y \equiv 0$. Then (29) reduces to (30).

$$\partial_z H_1 = \partial_x H_3 \tag{30a}$$

$$\partial_z H_2 = 0 \tag{30b}$$

$$\partial_z A_1 = \partial_x A_3 + \mu_{21} H_1 + \mu_{22} H_2 + \mu_{23} H_3 \tag{30c}$$

$$\partial_z A_2 = -\mu_{11} H_1 - \mu_{12} H_2 - \mu_{13} H_3 \tag{30d}$$

$$\partial_x H_2 = 0 \tag{30e}$$

$$H_3 = \frac{1}{\mu_{33}} \partial_x A_2 - \frac{\mu_{31}}{\mu_{33}} H_1 - \frac{\mu_{32}}{\mu_{33}} H_2 \tag{30f}$$

Interpretation

1. Equations (30b) and (30e) imply that H_2 is a trivial solution.
2. In (30d) the undesirable field component A_3 does not appear. In order to eliminate the trivial solution H_2 from (30d) we have to set $\mu_{12} = 0$.
3. Equation (30f) is needed to eliminate H_3. To eliminate the trivial solution H_2 from this equation the condition $\mu_{32} = 0$ is necessary.
4. Setting $\mu_{21} = 0$, H_1 disappears from (30c). However, H_1 enters this equation over H_3(see (30f))! Therfeore, $\mu_{23} = 0$.

In summary it can be stated that under the conditions that

$$\underline{\underline{\mu}} = \begin{pmatrix} \mu_{11} & 0 & \mu_{13} \\ 0 & \mu_{22} & 0 \\ \mu_{31} & 0 & \mu_{33} \end{pmatrix} \qquad \text{and} \qquad \partial_y \equiv 0 \tag{31}$$

(30) decouples into (32) and (33).

$$\partial_z H_1 = \partial_x H_3 \tag{32a}$$
$$\partial_z A_2 = -\mu_{11} H_1 - \mu_{13} H_3 \tag{32b}$$
$$H_3 = \frac{1}{\mu_{33}} \partial_x A_2 - \frac{\mu_{31}}{\mu_{33}} H_1 \tag{32c}$$

$$\partial_z H_2 = 0 \tag{33a}$$
$$\partial_z A_1 = \partial_x A_3 + \mu_{22} H_2 \tag{33b}$$
$$\partial_x H_2 = 0 \tag{33c}$$

Focus on the latter system first: (33a) and (33c) imply that $H_2 = \text{const}$ in the entire space. Considering finite energy functions we have $H_2 = 0$. Therefore, from (33b) we obtain $\partial_z A_1 = \partial_x A_3$, which cannot be diagonalized, unless A_1 and A_3 vanish simultaneously. Therefore: $A_1 = A_3 = H_2 = 0$.

Consider (32) next: Substitute (32c) into (32a) and (32b), and rearrange to obtain the desired D-form:

$$\partial_z \begin{pmatrix} A_2 \\ H_1 \end{pmatrix} = \begin{pmatrix} -(\mu_{13}/\mu_{33})\partial_x & -(\mu_{11}\mu_{33} - \mu_{13}\mu_{31})/\mu_{33} \\ \partial_x (1/\mu_{33}) \partial_x & -\partial_x (\mu_{31}/\mu_{33}) \end{pmatrix} \begin{pmatrix} A_2 \\ H_1 \end{pmatrix} . \tag{34}$$

It should be pointed out that the coefficients in our PDEs may vary as functions of x, which is the independent variable on the T-plane[6].

Inclusion of Idealized Sources Consider in (20) a uniform ($J_2 = \text{const}$) electric current line:

$$\boldsymbol{J} = J_2 \boldsymbol{e}_2 \delta(x - x_0)\delta(z - z_0) \tag{35}$$

($\boldsymbol{e}_2$: unit vector in y-direction) Note that since this "source distribution" satisfies the condition $\partial/\partial_y \equiv 0$, the consistency requirement is satisfied.

Repeating the D-procedure in this Section along with our formulation in terms of the Heaviside's function in (5) we obtain

[6] A condition for obtaining meaningful results is that $\mu_{11}\mu_{33} - \mu_{13}\mu_{31} \neq 0$. Similarly, diagonalization with respect to the $x-$ and $y-$ directions results in the conditions $\mu_{22}\mu_{33} - \mu_{23}\mu_{32} \neq 0$ and $\mu_{11}\mu_{22} - \mu_{12}\mu_{21} \neq 0$.

$$
\begin{aligned}
&\left\{\begin{pmatrix} -(\mu_{13}/\mu_{33})\partial_x & -(\mu_{11}\mu_{33}-\mu_{13}\mu_{31}/\mu_{33}) \\ \partial_x(1/\mu_{33})\partial_x & -\partial_x(\mu_{31}/\mu_{33}) \end{pmatrix}\begin{pmatrix} A_2 \\ H_1 \end{pmatrix}\right\}^{<} \mathcal{H}(z_0-z) \\
+&\left\{\begin{pmatrix} -(\mu_{13}/\mu_{33})\partial_x & -(\mu_{11}\mu_{33}-\mu_{13}\mu_{31}/\mu_{33}) \\ \partial_x(1/\mu_{33})\partial_x & -\partial_x(\mu_{31}/\mu_{33}) \end{pmatrix}\begin{pmatrix} A_2 \\ H_1 \end{pmatrix}\right\}^{>} \mathcal{H}(z-z_0) \\
=&\left\{\partial_z\begin{pmatrix} A_2 \\ H_1 \end{pmatrix}\right\}^{<}\mathcal{H}(z_0-z)+\left\{\partial_z\begin{pmatrix} A_2 \\ H_1 \end{pmatrix}\right\}^{>}\mathcal{H}(z-z_0) \\
+&\left\{-\begin{pmatrix} A_2 \\ H_1 \end{pmatrix}^{<}+\begin{pmatrix} A_2 \\ H_1 \end{pmatrix}^{>}\right\}\delta(z-z_0)+\begin{pmatrix} 0 \\ -J_2\delta(x-x_0) \end{pmatrix}\delta(z-z_0)
\end{aligned}
\tag{36}
$$

Note that the definition range of $\mathcal{H}(z_0-z)$, $\mathcal{H}(z-z_0)$, and $\delta(z-z_0)$ are mutually exclusive and their union spans the entire $z-$axis. Using this property and individually equating to zero terms which are associated with $\mathcal{H}(z_0-z)$, $\mathcal{H}(z-z_0)$, and $\delta(z-z_0)$, we obtain the governing equations in $z < z_0$, and $z > z_0$, and the interface condition at $z = z_0$, respectively.

5.5 Diagonalization of the Electrostatic Equations

Consider (19). Let $\underline{\underline{\varepsilon}}$ be a general 3×3 matrix. In contrast to Sec. 5.4, our analysis here is three-dimensional $(\partial/\partial y \neq 0)$.

Equation (19) implies that $\boldsymbol{E}$ can be written as a gradient of a scalar potential function $\boldsymbol{E} = -\boldsymbol{\nabla}\varphi$. Therefore, in source-free media the governing equations are $\boldsymbol{\nabla}\cdot\boldsymbol{D} = 0$, and $\boldsymbol{D} = -\underline{\underline{\varepsilon}}\boldsymbol{\nabla}\varphi$.

It can be shown [1], [2] that the following is valid[7]

$$
\begin{pmatrix} L_{11} & L_{12} \\ L_{21} & L_{22} \end{pmatrix}\begin{pmatrix} \varphi \\ D_3 \end{pmatrix} = \partial_z\begin{pmatrix} \varphi \\ D_3 \end{pmatrix}. \tag{37}
$$

Written explicitely L_{ij} $(i,j=1,2)$ are:

$$
L_{11} = -\begin{pmatrix} \varepsilon_{13}/\varepsilon_{33} & \varepsilon_{23}/\varepsilon_{33} \end{pmatrix}\begin{bmatrix} \partial_x \\ \partial_y \end{bmatrix} = L_{22}^T \tag{38a}
$$

$$
L_{12} = -1/\varepsilon_{33} \tag{38b}
$$

$$
L_{21} = \begin{bmatrix} \partial_x \\ \partial_y \end{bmatrix}\begin{pmatrix} (\varepsilon_{11}\varepsilon_{33}-\varepsilon_{13}^2)/\varepsilon_{33} & (\varepsilon_{12}\varepsilon_{33}-\varepsilon_{13}\varepsilon_{23})/\varepsilon_{33} \\ (\varepsilon_{21}\varepsilon_{33}-\varepsilon_{13}\varepsilon_{23})/\varepsilon_{33} & (\varepsilon_{22}\varepsilon_{33}-\varepsilon_{23}^2)/\varepsilon_{33} \end{pmatrix}\begin{bmatrix} \partial_x \\ \partial_y \end{bmatrix} \tag{38c}
$$

[7] Notice that we are requiring that $\varepsilon_{33} \neq 0$. The diagonalization with respect to the $x-$ and $y-$ coordinates would require that $\varepsilon_{11} \neq 0$ and $\varepsilon_{22} \neq 0$, respectively. Therefore, necessary conditions for physical realizability of the present problem are $\varepsilon_{ii} \neq 0$, with $i = 1, 2, 3$.

6 Conclusion

In this contribution we conjectured that systems of linearized Partial Differential Equations, considered as consistent models for physically realizable systems, are diagonalizable. We examined two problems in computational electromagnetics and showed that the associated PDEs are diagonalizable. We made clear that the diagonalization with respect to a given spatial coordinate is a process for systematically "reshuffling" the original PDEs, and creating equivalent reduced differential forms. Furthermore, we demosntrated that the diagonalization procedure automatically selects the variables which enter into the interface- and boundary eqautions related to surfaces normal to the diagonalization direction.

It should be pointed out that using our regularization technique moments of Green's functions associated with a given Boundary Value Problems can be written in coordinate-free, frequency-, and material independent forms, and therefore, these moments can be regarded as *universal functions* for the underlying class of problems [3]. The universal functions are generally astonishingly smooth; they can be precalculated, stored, and thus retrieved as often as required (data recycling). This capability allows us to separate the scientific computing efforts from the pre- and postprocessing steps in simulations. These considerations have been instrumental in the development of the Fast-MoM, which is an accelerated form of the conventional Method of Moments [4]-[7]. Using precalculated universal functions the computation times for the calculation of *impedance matrices* in the BEM applications reduce to the times required for retrieving data from the chosen storage medium. However, in spite of this advancement, a major drawback in the BEM still remains to be removed: the impedance matrices are dense. Several techniques have been suggested in literature for obtaining sparse matrices, each with its own limitation. We have suggested a procedure which consists of constructing problem-specific orthogonal sequences of basis functions derived from the involved Green's functions [18], [19], and [20]. The idea is to expand the unknowns in our problems in terms of basis functions which embed in their structures intrinsic features of the underlying PDEs: Using Meyer's orthogonalization technique [14]-[17], and Green's functions, we have constructed functions which are orthonormal to their integer-translates [18], [19], and [20]. In the case of Laplace operator, we have been able to prove that the resulting functions support a multiresolution analysis, and leads to *Green's-functions-based scaling functions and wavelets.*

Our present research includes the investigation of alternative *localization* techniques for generating sparse impedance matrices in the MoM applications, e.g. coherent states and Wannier fucntions. Furthermore, we are investigating the *existence* question of the diagonalized forms: Why is it possible to diagonalize a certain systems of linearized PDEs in the first place? And, viewed from a physical prospective, what are the necessary and sufficient conditions for their formulation.

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