(6): Some questions and answers

Summing up—provisionally

As this Series, if not its subject matter, approaches its closure, it seems appropriate to summarize our observations so far, and to address some questions that were asked at various occasions, over e-mail or in recent meetings. To most of these questions, I have only partial answers, at best. But unanswered questions are not so bad a thing in science: they may foster further progress.

What we have described so far can be characterized as *a discretization toolkit.* Faced with the task of solving electromagnetic equations in some definite physical configuration, the modeller will proceed as follows:

• Partition the region of interest into small volumes, or "3-cells", hence an algebraic structure called "the primal mesh".

This is described by sets $\mathcal{N}$, $\mathcal{E}$, $\mathcal{F}$, $\mathcal{V}$, of nodes, edges, etc., and by incidence matrices, **G**, **R**, **D**, which say how oriented p-dimensional faces, with $p \leq 3$, of said volumes, relate. (Some boundary conditions, one will recall, are taken into account by deletion of some p-cells.) We have seen repeatedly how a "dual mesh" can, conceptually at least, be associated with the primal one. (*Practical* aspects of this association are among questions to be answered.)

• Take as unknowns, or "degrees of freedom" (DoF), for the problem at hand, cell-based quantities.

As we described several times, such DoFs are the emf's along primal edges, the induction fluxes relative to primal facets, mmf's along dual edges, etc. Hence DoF arrays, **e**, **b**, $\tilde{\mathbf{h}}$, **d**, $\tilde{\mathbf{j}}$, which relate in definite ways to either the primal or the dual mesh. Some of these quantities may be imposed by the physical situation, which turns them into data. In particular, as we always assumed up to now, intensities $\tilde{\mathbf{j}}_f$ through dual facets can all be data, which one gets by (approximate) integration of the given current density $\tilde{\jmath}$ over the dual facet $\tilde{f}$. But arranging for some of them to be unknowns, linked with emf's via Ohm's law, is not difficult, as we shall see presently. Other data may come from the rest of the boundary conditions.

• Form the so-called "discrete Hodge operators".

These are square symmetric matrices, $\tilde{\star}_\mu$ and $\tilde{\star}_\varepsilon$, and their inverses. (This, for wave propagation problems. It's easy to imagine how a $\tilde{\star}_\sigma$ would intervene in an eddy-current problem, although we didn't yet address this issue: It's precisely by an equation of the form $\tilde{\mathbf{j}} = \tilde{\star}_\sigma \mathbf{e} + \tilde{\mathbf{j}}^{\mathrm{s}}$, where $\tilde{\mathbf{j}}^{\mathrm{s}}$ stands for the known "source"-current intensities, that one might account for Ohm's law.) In contrast to incidence matrices, discrete hodges require a knowledge of the metric of the mesh (lengths of edges, areas of facets, etc.), which one usually derives from a database containing nodal positions, and material properties of each elementary volume. (Such properties *are* part of the metric structure, in our view.) We return in a moment to the two main methods by which hodges can be constructed.

• Substitute **e**, **b**, $\tilde{\mathbf{h}}$, etc., for the fields e, b, $\tilde{h}$, etc., in the equations. Substitute **R** or $\mathbf{R}^t$ for rot, depending on whether the field to which this applies is on the primal side or on the dual side.

If things evolve in time, replace time-derivatives by appropriate finite differences. It may happen, in some modellings, that operators grad or div also appear in the equations. If so, substitute **G** and **D**, or $-\mathbf{D}^t$ and $-\mathbf{G}^t$, to grad and div, according to which side the DoF-array belongs in.

• Solve the algebraic equations thus obtained.

• Display the results, and discuss accuracy.

Both operations, we saw, require *interpolants*, by which one can climb back from DoF arrays to fields, and perform some error analysis that will justify the choice of Hodge operators, and hence, tell to which extent the results can be trusted. *Whitney forms*, including the well known "edge element", provide these, at least for simplicial primal meshes.

For definiteness, we'll refer to this line of attack as *Generalized Finite Differences* (GFD). Indeed, it reduces to finite differences in their basic and best known form, Yee's FDTD method, when the 3-cells are regular bricks (which are

of course, even in GFD, the recommended volume shape wherever possible; the point is that you don't easily model real objects, like a cellular phone near a human head, say, by laying only bricks).

6.1 Where is the beef?

Now, the questions.

Q. – *Though known as a supporter of edge elements, you advocate here an approach in which finite elements seem to play quite a modest role. Did you change your mind?*

A. Hardly. Whitney forms *are* the right finite elements for differential forms. Edge elements for e, facet-elements for b, this is the basic tenet. I sure continue to stand for that. But yes, the role of finite elements, or perhaps more accurately said, of variational formulations in numerical methods may have been exaggerated. For long, the dominant paradigm was: Give a variational form to your problem (minimize, or perhaps stationarize, this or that functional over this or that Hilbert space of a priori eligible fields). Restrict consideration to some finite-dimensional subspace, generated by a set of basis fields, called finite elements. (There is more in the notion, but let's not err.) Hence a system of equations, or an ODE system. Solve. Plot. Check. Assess accuracy.

The obvious difference there, with respect to GFD, is that one needs finite elements much earlier. They are essential. Without them, no discrete equations. Besides, the *technique* to prove that the method works, based on the variational method, forces one to adopt the variational method in the first place in order to just *describe* the numerical method. Conceptually, these two phases of the action should be distinct—as they are in GFD.

I would be the last to deny the virtues of the variational method: Among other things, it helps us to be *thorough* in the description of a problem: No way to forget some subtle constraint of topological origin, for instance, or to impose too many boundary conditions, because it would result in a flawed formulation (with either an infinity of solutions or none), something which can then (hopefully) be detected by theoretical reasoning—not discovered with embarrassment a few minutes before the client comes for the contract-clinching demo.

Yet, not being able to simply explain (to a programmer, for instance) what the method is, which recipe one should follow, without first explaining the mathematical foundations in painful detail, is a terrible burden. It faces teachers with the impossible challenge of dumping high-level mathematics into reluctant minds *as a precondition to* giving them the useful (and much easier to understand) stuff. It reduces the workforce in research groups, since only the mathematical élite seems qualified enough. And it forces users to rely on proprietary "codes", rather than using open-source software pieces that would correspond to elements of the above "toolkit".

In GFD, while the methodological advantages of the variational method are retained,[1] such obstacles are removed, because the need for finite elements is relaxed and postponed. The first thing they serve for, building a discrete Hodge operator, can be achieved without them in a different, much more transparent way, if one uses mutually orthogonal meshes. Then comes the minute of truth—did we get a convergent method of approximation? And there, finite elements are necessary. But at this late stage, the question is one for specialists. Error analysis, speed of convergence, are no less important issues in GFD. They still call for the

[1] The tools in the kit incoporate them, in some way. This point could not be explained in general without some deep forays in topology, but an example will perhaps do. Consider eddy currents induced in a conductive torus by temporal variations of the current in some exciting coil. Setting up eddy-current equations inside the torus, plus magnetostatic equations outside (of course parameterized by time), plus the obvious conditions of tangential and normal continuity at the boundary, will *not* make a well posed problem. There is something else to say, about the relation between total current and rate of change of the flux traversing the torus loop. This kind of "non-local" boundary condition is very easily overlooked, and is one of these things the variational approach helps not to forget about. In GFD, the existence of a problem is revealed by the fact that the range of **G** does not completely fill the kernel of **R**, something a software element can test for you, automatically, as soon as the mesh has been completed. Work is in progress, in some research groups [5, 12] to design such "watchdog" software tools.

attention of professionals (and much is left there to do), but don't stand in the way of teaching and training. Which is as it should be: Driving instructors don't teach you thermodynamics, do they?

Q. – *How effective is all this, in practice? Have you done numerical experiments?*

A. This question has been asked a couple of times in a way that seemed to imply that GFD was a novel proposal I would be making. Not so. GFD is an approach common to several groups of researchers, loosely connected if at all, who discovered its main elements independently. (See e.g., in addition to alrady cited work, [10] on Tonti's method, Shashkov et al. [8] on "mimetic discretization", Chew et al. [13] on "lattice" approaches.) One should turn to their publications, especially those of the Darmstadt group, which has the largest accumulated experience [2], for evidence about the effectiveness of the method.

Q. – *Well, then, so nothing new under the sun. But if so, what's the purpose of all this differential geometric apparatus? After all, this is not elementary mathematics either.*

A. No, the geometric approach by itself does not generate new *algorithms*. Even the fact that it brings in a new *understanding* of existing algorithms is not so compelling a reason to decide on seriously studying it. After all, as a friend recently observed, when people in good command of an efficient method understand what they are doing in their own way, they tend to care little for explanations of the, allegedly, "real nature" of what they do. Which benefit they may expect in getting acquainted with a new perspective, when the effort involved is not negligible, is then a legitimate prior question.

However, the Computational Electromagnetism (CEM) community as a whole may find such benefits in a synthesis of the different viewpoints. The very fact that GFD, or whatever name one eventually adopts for this approach,[1] emerged in almost identical form in independent research groups, is a problem. Take for instance, [11], a work I only recently became aware of, to realize that, apart from minor variations in the definition of degrees of freedom (densities instead of integrated quantities), they propose and analyze the same network equations we dealt with here. Conceivably, the same thing might well happen again next month, with another paper from researchers outside the CEM community, and no doubt it would be the same network equations again. When parallel and independent efforts result in proving the same *theorem*, no one is surprised: there was some kind of logical necessity at work. But when it results in the same *numerical technique*, what can it mean, if not that some necessity of the same kind lies underneath?

If so, we must dig and find out. That's the real point of conceiving Maxwell's equations as relations between differential forms, i.e., between objects meant to be integrated: As soon as we have decided for one DoF per cell, the network equations follow, with inner necessity. All those making this basic choice will find the same equations.

Now, about the discrete constitutive laws, the situation is different. Not only is there this great divide between Galerkin-inspired methods and those which use a diagonal hodge, but tiny variants can be observed in the latter category. The relevant question now is, why this variety, and how much of it is allowed? The geometric approach offers an answer: in order to meet the necessary consistency property

$$(1) \qquad \tilde{\star}_\epsilon r_{\mathcal{M}} - r_{\mathcal{M}} \tilde{\star}_\epsilon \to 0 \text{ when } \mathcal{M} \to 0,$$

the discrete Hodge operator must satisfy

$$(2) \qquad \sum_{e' \in \mathcal{E}} \tilde{\star}_\epsilon^{ee'} e' = \epsilon\, \tilde{e},$$

[1] "Generalized finite volumes" has been suggested [7]. Tonti prefers "finite formulation of electromagnetism" [14], which may reveal a more ambitious agenda than simply discretizing an underlying "continuous" formulation, as we have done here. Weiland et al. [2] use "Finite Integration Technique" (FIT), which in my opinion describes well the derivation of the *network* equations, but they consider the construction of their hodges (diagonal, as a rule) as a component of FIT, as well. In contrast, I would include in GFD the Galerkin method (which they would probably consider foreign to FIT), for the reasons exposed here so far: it does generate the same network equations, and differs in the way the hodges (then, non-diagonal) are built.

where e' is the vector along edge e' and $\tilde{e}$ the vectorial area[2] of the dual facet pierced by edge e.

This is a *criterion*, the form of which explains why the hodge and the dual mesh are so closely related: A discrete Hodge operator is acceptable, as an element of the toolkit, if there is a way to devise a dual mesh that will satisfy (2). We found two examples: (1) When dual cells are orthogonal to the primal ones, and $\tilde{\star}_\epsilon^{ee}$ equals the ratio between vectors $\tilde{e}$ and e, all off-diagonal terms of $\tilde{\star}_\epsilon$ null, (2) When $\tilde{\star}_\epsilon$ equals the mass matrix of edge elements, dual cells then being those of the barycentric dual. Clearly, there are other possibilities, which remain to be explored, but we now know the rules of the game: Satisfy (2).

6.2 Technical issues

Q. – *How to construct the dual mesh?*

A. The problem, it should be stressed, is to build the *primal* mesh in such a way that a suitable dual one will exist, and "suitable" depends on which hodge one wants to use. This remark, unfortunately, is of little help. If primal 3-cells are tetrahedra with all dihedral angles acute, there is a simple solution: join the circumcenters of the primal cells, as in the Voronoi-Delaunay construction, and lo the dual orthogonal mesh. In this case, the problem is with the primal mesh, since getting the dual is a simple *local* process. But it's a tough problem, because this condition on angles is very strong.

Observe, however, that (2) is a *local* condition. It means in particular that one may well use the diagonal construction of the hodge in large homogeneous regions, where a uniform mesh is all right, and the Galerkin one at places, such as material boundaries, where the shape of the primal mesh is severely constrained. This results in a non-diagonal hodge, but with so few off-diagonal terms that it may not be a problem.

[2] Recall that the vectorial area of a triangle is its area times the normal vector. The vectorial area of a polyhedral surface is defined as the sum of vector areas of its triangular facets. When ϵ is not uniform, $\epsilon\,\tilde{e}$ is the weighted sum of vector areas of triangles that constitute the dual facet $\tilde{e}$, with the values of ϵ as weights.

Also remark that (2) is not "necessary" in that strong a sense, since its purpose is to satisfy (1), an asymptotic condition only. If (2) is violated for a small proportion of edges, and if the (virtual) refinement process makes this proportion tend to zero, (1) can still hold. So it's tolerable to cheat on some edges or facets, as Fig. 1 suggests. (Similar procedures have been tested for the MAFIA codes [1].)

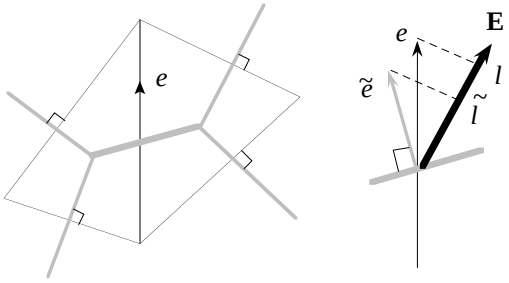

Figure 1. "Cheating", when an occasional dual facet cannot be made orthogonal to its primal edge (e here). Instead of ϵ area$(\tilde{e})$/length(e), set $\tilde{\star}_\epsilon^{ee}$ equal to $\epsilon\,(\mathbf{E}\cdot\tilde{e})/(\mathbf{E}\cdot e)$, i.e., to $\epsilon\,l'/l$, with the notations of the figure, where **E** is a guesstimate of the direction of the electric field in the vicinity. (Recall that e and $\tilde{e}$ stand for the vector along e and the vectorial area of $\tilde{e}$.) This amounts to replace length(e) by the length of its projection onto the support of **E**, and area$(\tilde{e})$ by the apparent area when looking parallel to **E**.

Q. – *Which elements for cells of general shape?*

A. We have had edge elements for hexahedra (not necessarily with plane facets) for long [15], and more recently, for shapes such as pyramids [4, 3, 6], compatible enough to ensure tangential continuity of the interpolated fields when used together. The problem is crucial if one wants the analytical form of the interpolants, in order for instance to compute the Galerkin hodge. If one uses the orthogonal construction and the diagonal hodge, it's no more a practical issue but a theoretical one: The only problem is to find *some* convergent $p_{\mathcal{M}}$, in last installment's notation. To this effect, one may rely on the convergence properties of simplicial Whitney forms, and build interpolants as weighted combinations of these.

To be specific, suppose each p-cell of the mesh $\mathcal{M}$, for all p, has been provided with a "center", in the precise sense of *JSAEM 7*, 2 (1999), p. 158, i.e., a point with respect to which the cell is star-shaped. Then, join the centers in order to obtain a simplicial re-

finement, $\overline{\mathcal{M}}$ say, where the new set $\overline{\mathcal{S}}_p$ of p-simplices contains the old one $\mathcal{S}_p$. In similar style, let $\mathbf{u}$ and $\overline{\mathbf{u}}$ stand for DoF arrays indexed over $\mathcal{S}_p$ and $\overline{\mathcal{S}}_p$ respectively, with $\overline{\mathbf{u}}_s = \mathbf{u}_s$ for all s in $\mathcal{S}_p$. Our problem is to define $p_{\mathcal{M}}\mathbf{u}$, knowing what $p_{\overline{\mathcal{M}}}\overline{\mathbf{u}}$ is. Isn't it obvious? Just take for $p_{\mathcal{M}}\mathbf{u}$ the *smallest*, in the energy norm, of the $p_{\overline{\mathcal{M}}}\overline{\mathbf{u}}$'s, with respect to all $\overline{\mathbf{u}}$'s compatible with $\mathbf{u}$.

The family of interpolants thus obtained is to our cellular mesh, for all purposes, what Whitney forms were to a simplicial mesh. Purists, however, will object against calling them "Whitney forms", because they are metric-dependent, unlike the standard Whitney forms. The same construction on the dual side will provide similar pseudo-whitneys on the dual mesh.

Q. – *What about higher-degree Whitney forms?*

A. When using the Galerkin method, finite elements of higher polynomial degree give schemes of higher accuracy, which more than compensates for the increased number of DoFs. Hence the interest for Whitney forms of higher polynomial degree. But a caveat about that: Our approach to network equations, as exposed so far, is in jeopardy if there is more than one DoF per cell, so it's not so clear what to do of higher-degree Whitney forms out of the rather restrictive context of the Galerkin method. Since the red thread in GFD has been, up to now, the duality between chains (formal sums of cells) and DoF arrays, these forms make full sense only if we can associate their DoFs with well identified geometric objects.

Thus, though this is a very promising area for future progress, it should be explored with the right equipment. A good compass, in my opinion, is this "partition of unity" property,

$$\sum\nolimits_{e\in\mathcal{E}} e\rangle\langle w^e(x) = 1,$$

in the esoteric notation of last time, or more clearly, in terms of vector proxies,

$$\sum\nolimits_{e\in\mathcal{E}} (\mathbf{W}^e(x)\cdot v)\, e = v,$$

at all points x and for all vectors v, where e, again, is the vector along edge e. From this, which generalizes the $\sum_{n\in\mathcal{N}} \lambda^n(x) = 1$ valid for nodal 0-forms,[3] and has counterparts for simplices of all degrees, we were able to prove that the mass matrix of edge elements does satisfy the criterion (2). This was, at the root, the reason why edge elements give a convergent scheme in the Galerkin approach. Therefore, this property should be taken seriously: whatever Whitney elements of higher degree are, *they must constitute a partition of unity*.

Now (a heuristic move, not a formal assertion, even less a proof), the product of two partitions of unity makes a partition of unity. Let us, therefore, take as second-degree edge elements, on a simplicial mesh, the products $\lambda^n\, w^e$, indexed over the set $\mathcal{N}\times\mathcal{E}$. Actually, let's do that for all simplicial degrees, in all dimensions: second-degree p-forms are the products $\lambda^n\, w^s$, where n spans the set of nodes, and s the set $\mathcal{S}_p$ of p-simplices.

Forms obtained in this manner have all the required properties. In particular, they constitute an exact sequence, i.e., if for instance $b = \sum_{n,f} \mathbf{b}_{nf}\lambda^n\, w^f$ has a divergence-free proxy ($\mathrm{d}b = 0$), then there are DoFs $\mathbf{a}_{ne}$ such that $b = \mathrm{d}(\sum_{n,e} \mathbf{a}_{ne}\lambda^n\, w^e)$.

The main problem with such forms is the interpretation of degrees of freedom such as $\mathbf{a}_{ne}$. With standard Whitney forms, the DoF $\mathbf{a}_e$ was the integral of the 1-form $a = \sum_{e'} \mathbf{a}_{e'} w^{e'}$ over edge e. Here, we cannot expect to find a family of simple 1-chains such that $\mathbf{a}_{ne}$ would be the integral of $a = \sum_{ne} \mathbf{a}_{ne}\lambda^n\, w^e$ over one of them, *and have a null integral over all other chains* of the family. Although such a family will exist, the emphasized condition makes it anything but simple. We must be content with less: 1-cells such that integrals of $\sum_{n,e} \mathbf{a}_{ne}\lambda^n\, w^e$ over them determine the $\mathbf{a}_{ne}$s, and in clear one-to-one correspondence with the basis forms $\lambda^n\, w^e$ (Fig. 2). Let's call such cells (introduced in [9]) "small" edges, an ad hoc terminology.

[3] I denote here by λ^n the same nodal hat functions that were called w^n last time. This is for readability only, $\lambda^n w^s$ being better than $w^n w^s$ in this respect.

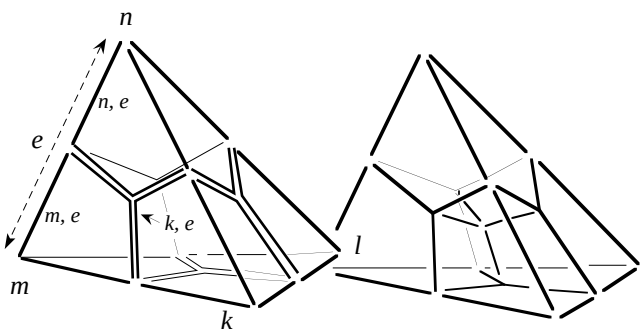

Figure 2. Left: Small edges (some of them are broken lines) associated with forms $\lambda^n\, w^e$. Right: One of the possible systems of chain elements in 1-1 correspondence with *independent* degrees of freedom.

A problem then emerges: There are 24 small edges, but the dimension of the space generated by the $\lambda^n\, w^e$, if the mesh reduces to this single tetrahedron, is only 20! This is due to the relation

$$\sum\nolimits_e \mathbf{R}_{fe} \lambda^{f-e} w^e = 0,$$

here written for edges and facets, but actually a general property of Whitney forms. (λ^{f-e} denotes, if $\mathbf{R}_{fe} \neq 0$, the hat function of the node opposite edge e in facet f.) Since each facet contributes one such constraint, the span of the forms $\lambda^n\, w^e$ has dimension $2(E+F)$.

We might just omit one small edge out of three on each facet, but this is an ugly solution. Fig. 2, right, suggests a better one. It shows 20 "chain elements" (12 half-edges, four inner segments, and the four three-pronged stars, which themselves are 1-chains formed of 3 small segments each). This time, 1-chains formed from these elements have the desired property (and no smaller set of chain elements can do): A second-order one-form whose integrals over all of them vanish must itself vanish.

The reader will easily guess about "small facets" and "small volumes", and may want to tackle the challenge of finding a nicely symmetric set of 2-chain elements (15 instead of 16; total dimension of the span $3(F+T)$).

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