Technical Article

A Synergetic Story of Evolving Thoughts

In the beginning of 90's at Argonne National Laboratory we had a small team with Larry Turner and with Bill Trowbridge as an external member developing integral equation approaches for magnetostatic and eddy current problems. Our first aim was to develop an error estimator for the well known GFUN approach [1] - which is perhaps the most reinvented formulation in our community - and for this reason we wanted to analyse why GFUN suffered the so called "looping problem" [2].

The basic idea behind GFUN is simple. Magnetic field h is decomposed into two components h^s and h^m due to source currents and magnetization M, respectively. Next one introduces an integral operator $H : m \to h^m$. Denoting by $H(m)$ the "value" the operator assumes at m we may write

$$h - H(\chi h) = h^s . \qquad (1)$$

The system of equations is obtained by solving (1) in the centroids of the elements in which case the problem becomes solvable in terms of h.

There had been a lot of work around this idea already in the late 60's and in the beginning of 70's especially in the group led by Bill Trowbridge at the Rutherford Appleton Laboratory in England and GFUN code was a result of these studies. Larry Turner was a leading member of the group and with others [3] they had a lot of numerical experience of GFUN. The members of the group must have been some kind of "computer nerds" of the beginning of the 70's as they had optimization and particle tracking supported with interactive graphics already at the time when pocket calculators were not yet part of every day life. However, in the second half of 1970's partial differential equations became much more appealing in nonlinear magnetostatics and the researches around integral methods were gradually diminished. Still some outstanding papers were published, such as e.g. [4] although they seem to get easily forgotten. It was a challenge to go back to this old material, read the old hand written notes and try to create something new out of it. "The uncrowded paths are on the deep unbroken fields of snow".

One of the first questions was, what did GFUN actually solve. It was not h as it was not possible to construct any kind of discrete h-field possessing proper continuity conditions. The same held good for magnetic flux density b. This question turned out to be rather difficult and to avoid it we chose the standard engineering approach: if there is a major problem take a step backwards and try another route. So, that's what we did and less than a year later we had a new integral code called GFUNET [5] which removed many of the practical problems of the old GFUN, including the "looping" problem referred to above. With John Simkin's support GFUNET was also connected to a standard pre and post processing environment. But if there been open questions before with GFUN now we had more of them. Perhaps the most amazing fact was that GFUNET yielded similar kind of results as other h-oriented formulations such as the standard magnetostatic FEM-codes based on scalar potentials - although GFUNET was very different. Basically GFUNET was built around (1), but the equations "matched" along edges instead of points. Knowing that the circulation of h vanishes around all (bounding) cycles, we were able to construct a system of equations solving the circulation's of h along the edges of the spanning tree.

It was intuitively clear that our approach was somehow complementary to Albanese and Rubinacci's eddy current formulation for nonmagnetic materials [6]. In fact, at first I had misunderstood what they did and that's how the complementary idea was picked. In their case the spanning tree was removed from the system whereas we needed the spanning tree but not the complement. Thence, it was reasonable to assume that the combination of the two would be a full integral approach for the eddy current problem including magnetic materials. But that was almost all we knew at that time. I started to wonder myself, where is the divergence condition hiding. As the code yielded similar kind of results as other h-methods, the div $b = 0$ condition had to be somehow involved in the system. Hence, the main question was to understand what really were the equations we solved.

Later on back in Tampere my colleague Kimmo Forsman implemented a "weighted version" of GFUNET following John Simkin's similar kind of approach with a later version of GFUN[1]. This means that the starting point was a weighted version of (1), i.e.

$$\int_\Omega w' \cdot h - \int_\Omega w' \cdot H(\chi h) = \int_\Omega w' \cdot h^s \;\; \forall w' \in \mathbb{L}^2(\Omega) \quad (2)$$

where $\mathbb{L}^2(\Omega)$ is the space of square integrable vector fields in domain Ω. With the new code we discovered two interesting facts. First, if $H(\chi h)$ and h^s were represented in a discrete space, we got precisely the same results as before. Secondly, if we tried to integrate terms $\int_\Omega w' \cdot H(\chi h)$ and $\int_\Omega w' \cdot h^s$ as accurately as possible[2] the results were significantly worse than what the first version of GFUNET gave. The first property of the weighted version gave some light on what was going on, but still our puzzle was not solved.

It is an interesting fact of life that one may be close to a solution without recognizing it. Since 1988 I had been carrying in my briefcase a paper by Bossavit about Hodge decompositions and about the so called Bihovskij-Smirnov's fivefold decomposition of the space of square integrable vector fields [7]. I had been reading the paper every now and then, but really did not get into it until Alain Bossavit inspired me and Kimmo Forsman to look at it closely while we were writing reference [8]. The mathematical tools of [7]

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[1] ref: private communication with John Simkin.

[2] $H(\chi h)$ and h^s were integrated within the elements, and the second integration was carried out numerically with a high number of Gaussian integration points.

turned out to be the key to get forward. Bihovskij-Smirnov's decomposition is a generalization of the classical Helmholtz de-composition and it is a useful tool in examining the mathematical structure involved in Maxwell's equations.

Let us assume that and that domain Ω is embedded in a three dimensional Euclidean space. A good technique to illustrate the structure behind Maxwell's equations is to display a de Rham's complex, Fig. 1.

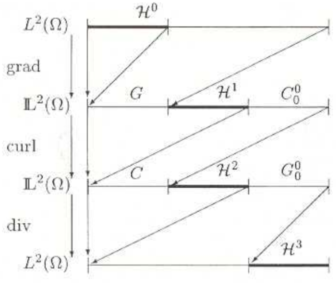

Figure 1: A de Rham's complex showing the structure behind Maxwell's equations

The horizontal lines of Fig. 1 represent the spaces of square integrable scalar and vector fields in domain Ω, i.e. $L^2(\Omega)$ and $\mathbf{IL}^2(\Omega)$, respectively. On each level non-intersecting segments of these lines represent mutually *orthogonal* subspaces[3]. The vertical arrows show how the grad, curl and div operators map these subspaces to each other. The subspace of gradients is denoted by G and C is the subspace consisting of curl fields. Subspaces H^p, $p = 0,..., 3$ are the so called pth de Rham cohomology groups. In this case H^1 and H^2 are of special interest because they are related to "loops" and "cavities". We'll get back to this point later on. C^0_0 and G^0_0 are the orthogonal complements of ker(curl) and ker(div). They consist of curls and gradients, respectively, but this time with some additional conditions, and hence the sub- and superscripts.

The classical result by Helmholtz says that any square integrable vector field in three dimensional Euclidean space can be divided uniquely into div-free and curl-free components. Equivalently one may state that, if the sources and vortices of a vector field are known and if the field vanishes at infinity, then the vector field is uniquely defined. The classical result holds for the whole space and Bihovskij-Smirnov's decomposition - which follows when levels p = 1 and p = 2 of Fig. 1 overlap - is a generalization onto bounded domains. Bounded domains are essential for us since that is typically the case in numerical computation[4].

[3] Two spaces U and V are orthogonal, if for every $u \in U$ and $v \in V$ their scalar product $\int_\Omega uv$ (scalar fields) or $\int_\Omega u \cdot v$ (vector fields) is null.

[4] Be aware, that this is typically the case also with approaches based on integral operators. The problem is solved in a bounded domain although in the post processing stage fields can be integrated on points of the exterior space.

Otherwise, the spirit of the numerical solution process is well aligned with the classical Helmholtz result. What we solve are "div-free" and "curl-free" components but this time, due to boundedness, they correspond with curl and grad components equipped with some additional conditions.

The simple example of magnetostatics will enlighten how orthogonality and the decompositions plug into our numerical approaches. In the magnetostatic case we want to find vector fields b and h such that

$$\operatorname{div} b = 0, \tag{3}$$

$$\operatorname{curl} h = j, \tag{4}$$

$$b = \mu h, \tag{5}$$

hold withinΩ, and such that the b and/or h fulfill appropriate boundary conditions.

As there is an apparent problem that the curl and div operators are not defined (in the classical sense) e.g. on the material interfaces we switch to weak forms. Going through the process[5] we end up with weak forms of (3) and (4) and the idea is now to find vector fields b and h such that

$$\int_\Omega \varphi' \operatorname{div} b = 0 \quad \forall \varphi' \ L^2(\Omega) \tag{6}$$

$$\int_\Omega w' \cdot \operatorname{curl} h = \int_\Omega w' \cdot j \quad \forall w' \in \mathbf{IL}^2(\Omega) \tag{7}$$

and such that (5) and the boundary conditions are fulfilled.

There are now several choices to make. The main one is to decide whether to solve the problem in terms of b or h. Let's choose first b. Assuming the domain is topologically trivial enough and by integration by parts the magnetostatic problem becomes find the vector field b in $\mathbf{IL}^2(\Omega)$ such that

$$\int_\Omega \varphi' \operatorname{div} b = 0 \quad \forall \varphi' \ L^2(\Omega) \tag{8}$$

$$\int_\Omega b' \cdot \frac{1}{\mu} b = \int_\Gamma w' \times h \cdot n + \int_\Omega w' \cdot j \quad \forall w' \in \boldsymbol{C}, \tag{9}$$

where $\boldsymbol{C}$ is the graph of the mapping of curl from $\mathbf{IL}^2(\Omega)$ onto C (i.e. the set of all pairs $\{w',b'\}, w' \in \mathbf{IL}^2_{curl}(\Omega)$ and $b' \in$ C such that $b' = \operatorname{curl} w'$. This problem lends itself to be solved directly in terms of b using Whitney (facet) elements[6]. However, there are alternative techniques to impose (8) as well. Using an analogue of the idea of spanning trees, but now for facets, one can construct subspace C by extracting a maximal set of facets that does not generate closed (bounding) surfaces. If b is sought from C then (8) yields no information, as if $b \in$ C, then div $b = 0$, see Fig. 1. The situation is precisely the same, if we want to solve a magnetostatic problem in terms of magnetic vector potential a. If $b = \operatorname{curl} a$, this

[5] In fact, it is not simple in all its details. See reference [9].

[6] Notice that in this case $\varphi \in W^3$ which is the space spanned by "volume elements"

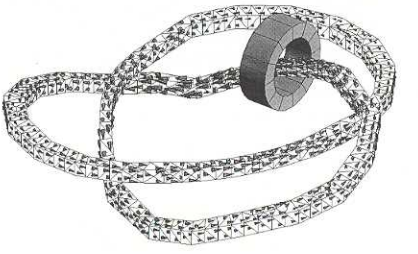

Figure 2: A coil around a magnetic knot. The cones show magnetic flux density within the knot.

implies that $b \in C$ and hence, again, there is no need for (8). In this case the problem is to find a in $\mathbf{IL}^2(\Omega)$ such that (some boundary conditions and a gauge for a are obviously needed to find a unique solution)

$$\int_\Omega \mathrm{curl}\, w' \cdot \frac{1}{\mu} \mathrm{curl}\, a = \int_\Gamma w' \times h \cdot n + \int_\Omega w' \cdot j \quad \forall w' \in \mathbf{IL}^2_{curl}(\Omega), \qquad (10)$$

But now, (10) is the same as what is obtained when one starts with a PDE in terms of a. Hence, assuming exact arithmetic it does not make a difference whether the magnetostatic problem is solved terms of b or a. Of course, some approaches are numerically more efficient than others, but that's another issue.

Going the other way around and choosing h instead of b the roles of (6) and (7) swap. Exploiting the spanning tree extraction technique or by introducing a scalar potential (or the so called "reduced scalar potential") for h, we get rid of (7) as the information of it is already included in the system. Thus the same solution is found independently whether we solve directly for h or if PDEs and potentials are employed.

Now we can get back to where I started. The missing divergence condition of GFUNET followed from (6). As is explained thoroughly in a paper which will appear around March 1998 [10], starting from (6) one can get

$$\int_\Omega h' \cdot \mu_0 h - \int_\Omega h' \cdot \mu_0 H(\chi h) = \int_\Omega h' \cdot \mu_0 h^s \;\; \forall h' \in G. \qquad (11)$$

This is what the very first version of GFUNET did when it "matched equations along edges". Notice also the relationship between this and (2).

The real asset was, however, that de Rham complexes and Bihovskij-Smirnov's decomposition revealed the infrastructure behind the superstructures of computational electromagnetism. It was not only the connection between standard boundary value problems and approached based on integral equations which was important, but as well the systematic and consistent approach to impose well posed problems although the domain included "loops", "cavities" or even worse "knots". This is, of course, one of the main messages of Bossavit's paper [7]. The topological properties of the domain are related to the de Rham cohomology groups H^p, $p = 0,\ldots, 3$, and hence they are the key to understand when and what kind of "cuts" are needed. A grip on this makes it much easier to understand why pioneers such as Alain Bossavit, Robert Kotiuga and others encourage the use of differential forms as a native background for electromagnetism. Going in this direction leads to subjects such as homology and cohomology which are tough, but on the other hand essential. It seems that the classical training of engineers and physicists is not always precise enough in these issues. This is perhaps why one of the topics of Compumag conferences is "multiply connected regions" although simply and multiply connectedness are misleading concepts in this context (see e.g. [11] and especially [12] for a readable exposition). For these reasons I think Kotiuga's PhD thesis [13] or Bossavit's paper [7], are important milestones in our field and they both deserve more attention. In the literature one can find also many "smaller" examples of the usefulness of the mathematical background. For instance, see the effect of the right hand side to the convergence properties of an iterative solver studied in references [14] and [15]. As Ren has showed in [15] the convergence problem gets back to the properties of the discrete spaces and to the discrete operators between them. All this boils downs to the same roots of computational electromagnetism.

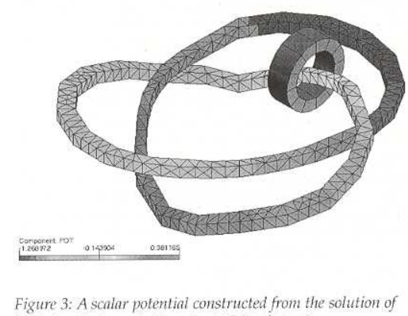

Figure 3: A scalar potential constructed from the solution of h. Notice the jump in the potential (in the top).

As a last point it is interesting to challenge the "folklore" which says that it is not possible to find a general formulation for all the problems we deal with. For instance, it is quite often said that the magnetostatic and eddy current problem require solution techniques of their own. When it comes to efficiency this may well be the case[7] but there still remains the question, could we create a methodology that generates "all" formulations, and if so, can they all be coded in a reasonable manner as one package. As can be seen from Fig. 1, there is a certain structure involved in the Maxwell's equations which repeats itself from one level

[7] It is obvious, that numerically the most efficient code is the one which is tuned for a specificproblem, because it does not carry out any extra work.

to another[8]. Recognizing the abstract structures is essential in compressing data into a compact and manageable form. This is why they are valuable. A good example is algebraic topology which changes the topological properties of a domain into algebraic ones. With no doubt that is precisely what is needed in coding. Hence, abstract theories are highly useful in developing versatile code on a very practical level. The way ahead in generating code which can tackle a large class of problems is to exploit the abstract structures involved in Maxwell's equations. I find this a rather exciting thought, especially when it is combined with the possibilities brought by modern object oriented coding.

Lauri Kettunen

PS. If nothing else, clear and unambiguous exposition seems to be related to the use of proper tools. Just compare our first paper [5] introducing the integral approach with the most recent one [10] ending into the same eddy current formulation. I think the point is much more clear in the latter one.

[8] The system is also symmetric although this is not shown in Fig. 1.

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