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TOPOLOGICAL APPROACH TO COMPUTATIONAL ELECTROMAGNETISM

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Abstract—Software systems designed to solve Maxwell's equations need abstractions that accurately explain what different kinds of electromagnetic problems really do have in common. Computational electromagnetics calls for higher level abstractions than what is typically needed in ordinary engineering problems. In this paper Maxwell's equations are described by exploiting basic concepts of set theory. Although our approach unavoidably increases the level of abstraction, it also simplifies the overall view making it easier to recognize a topological problem behind all boundary value problems modeling the electromagnetic phenomena. This enables us also to construct an algorithm which tackles the topological problem with basic tools of linear algebra.

1. INTRODUCTION

Electromagnetic phenomena is fully described by the Maxwell equations, which are typically described in terms of vector algebra. Although seldom mentioned, in the background such an approach relies on an *Euclidean space*, which is what enables one to talk of distances and angles, or of magnitudes of vectors. Since the notions of distances and angles are everyday routines, one may arrive at a conclusion that physics (i.e., modeling of nature) somehow did require Euclidean spaces. But to recognize the nature of Euclidean spaces, let us call them with another name: "Euclidean" is a synonym to *pre-Hilbertian* with finitude of dimension usually implied. Here, there is no need to go to the details of pre-Hilbertian spaces [1], it is just enough to realize that they are something which are made of several layers of structures: An Euclidean space is not a simple structure.

As is argued in [2] science is about trying to understand and see what complicated and diverse events really do have in common and to explain or to describe the behaviour accurately, simply and elegantly. When it comes to electromagnetism, vector fields and Euclidean spaces are a heavier structure than needed [3, 4, 5, 6], and they may block from seeing the principal information of Maxwell's equations. The irony is that Euclidean spaces and vector fields are rather intuitive. As soon as *simpler* –and thus, in principle, easier– structures are employed, unavoidably the level of abstraction has to increase. This is perhaps why the more powerful, accurate, and elegant models are easily considered less physical. Some may even questioned whether they are needed at all.

The nature of software design is very close to that of science. The fundamental problem in developing software is to find the right, i.e., simple, accurate, and elegant abstractions [7]. Computational electromagnetism makes no difference, and thus, there is a *practical* call to find better abstractions describing Maxwell's equations in a precise and elegant way, and such that they become easily convertible into pieces of software.

The software systems developed for electromagnetic design are typically inflexible requiring the user to input certain data (sometimes even in a certain order) to generate the result the user needs. Furthermore, such systems may also suffer for the problem that they are not able to recognize missing, incorrect, or conflicting data until it gets to the point when the solution process of a system of equations fails. But even then, there are little tools to recognize what really went wrong. One reason for this inflexibility is perhaps the *method driven* approach commonly employed in generating software. In other words, the software is a realization of some methods and algorithms, and the user is required to insert data which fits into this model. Of course, the software may try to list out all cases that are not solvable, but this is an extensive and unreliable approach.

The motivation for this paper comes from the opposite direction. The idea is to develop a *data driven* approach which by an abstract representation of the category of problems generates by top-down development an orderly (code) structure, which then enables to recognize what can or cannot be done with the data inserted by the user. The very idea is that the software system is driven by the inserted data instead of trying to fit data into a priori selected approach.

It is plain that in a single paper there is not enough room to thoroughly discuss such a topic. (There are books, such as [8], published in this kind of questions). In this paper we shall focus on the topological issues behind Maxwell's equations. In the first part of the paper we introduce a topological problem behind electromagnetic problems. By employing the language of *differential geometry* [9, 10, 11, 12, 3, 4, 5, 6] and *algebraic topology* [13], and especially of *homology* [13, 14, 15], we shall express Maxwell's equations using some simple concepts of set theory. In the second part we introduce an algorithm exploiting the basic tools of linear algebra to tackle the topological problem introduced in the first part. In addition, an example and some practical hints are presented.

2. MAXWELL EQUATIONS AS RELATIONS

Electromagnetic fields are characterized by Maxwell's equations. Their main information is in how the integral of a field over the *boundary* of any *chain* [16] matches with the integral of some other field over that chain. In more formal terms, the boundary operator ∂_p is a map from the *module* C_p of all p-chains into the module C_{p-1} containing all $(p-1)$-chains. Thus, a chain and its boundary are linked by (the graph of) a *relation* $R(\partial_p) \subset C_p \times C_{p-1}$, and evidently for all pairs $(c, c') \in R(\partial_p)$ one has

$$(c, c') \in R(\partial_p) \Leftrightarrow \partial_p c = c' .$$

Maxwell's equations involve integration, which is a bilinear operator from the cartesian product of C_p and the space F^p of p-cochains to the *field* of reals $\mathbb{R}$ (or to some other field $\mathbb{F}$):

$$\int^p : C_p \times F^p \to \mathbb{R} .$$

In general, if one has bilinear operators $f_1 : A_1 \times B_1 \to \mathbb{F}$ and $f_2 : A_2 \times B_2 \to \mathbb{F}$, and $R(A)$ is a linear relation in (i.e., a linear subspace of) the cartesian product $A_1 \times A_2$, then relation $R(A)$ and operators f_1, f_2 induce a linear relation $R(A, f) \subset B_1 \times B_2$ such that $(b_1, b_2) \in R(A, f)$ if and only if for all $(a_1, a_2) \in R(A)$ hold $f_1(a_1, b_1) = f_2(a_2, b_2)$.

Relation $R(\partial_p)$ is linear –i.e., the boundary operator is linear– and thus, $R(\partial_p)$ and the integral operators

$$\int^p : C_p \times F^p \to \mathbb{R}$$
$$\int^{p-1} : C_{p-1} \times F^{p-1} \to \mathbb{R},$$

induce relation $R(\partial_p, \int^p) \subset F^p \times F^{p-1}$ such that, if $(f, g) \in R(\partial_p, \int^p)$ then

$$\int_c^p f = \int_{c'}^{p-1} g$$

has to hold for all $(c, c') \in R(\partial_p)$.

Maxwell's equations may be considered as this kind of induced relations. For instance, Ampère's law

$$\int_{\partial c} h = \int_c (j + \partial_t d)\,, \tag{1}$$

expressing the relationship between magnetic field h and current j and the time derivative of electric flux d can be interpreted as a relation $(j + \partial_t d, h) \in R(\partial_2, \int^2)$. Correspondingly, Gauss's law

$$\int_{\partial c} b = \int_c q_m \tag{2}$$

saying the magnetic flux b over all bounding 2-chains should equal to the magnetic charge q_m that chain bounds can be viewed as a relation $(q_m, b) \in R(\partial_3, \int^3)$.

A relation $R(A) \subset A_1 \times A_2$ is said to be *one-to-one* if there is a 1-to-1 correspondence between the elements a_1 and a_2 of pair $(a_1, a_2) \in R(A)$. The constitutive laws can also be interpreted as relations. We assume that permeability μ belongs to the set M of "admissible" permeabilities, and that n is the dimension of the ambient space. Then, the constitutive law corresponds with a one-to-one relation $R_{1-1}(\mu) \in F^2 \times F^1$ defined with aid of the *Hodge operator* $*$ mapping p-cochains into $(n-p)$-cochains [10] such that

$$(b, h) \; = \; R_{1-1}(\mu) \; \Leftrightarrow \; b = \mu * h \, .$$

Besides the emphasis shifted towards the principal information of Maxwell's equations, the motivation for the use of relations is that such notions of *naive set theory* [17] can easily be transformed into pieces of software.

3. TOPOLOGICAL PROBLEM

The tools we have enable us to formulate electromagnetic problems in an alternative way. Let us assume that $\mu \in M$, $i = j + \partial_t d \in F^2$, and $q_m \in F^3$ are known in all space. Then the magnetic field is the solution of problem:

Problem 1: *Find* $(b, h) \in F^2 \times F^1$ *such that*

$$\begin{aligned} &(b, h) \in R_{1-1}(\mu)\, , \\ &(j + \partial_t d, h) \in R(\partial_2, \textstyle\int^2)\, , \\ &(q_m, b) \in R(\partial_3, \textstyle\int^3) \end{aligned}$$

hold.

Problem 1 is not, however, *well posed.* The conditions for the solution are *sufficient* in the sense that *if* there is a solution, then the solution is also *unique*. But the *existence* of the solution depends on whether i is solenoidal[1] or not.

In practical software design such problems are typically avoided by testing whether the inserted data fits into the model. However, since our goal was to develop a data driven approach to computational electromagnetism, we shall tackle the problem in another way.

To go on, we need next to introduce the concept of an *isomorphic relation.* A relation is isomorphic if it is one-to-one and linear. Let us now denote by $\mathrm{cod}(\partial_p)$ the *codomain* (*range*) of operator ∂_p. If the linear relation $R(\partial_p) \subset C_p \times C_{p-1}$ is restricted such that the map

$$\partial_p : \, C'_p \to \mathrm{cod}(\partial_p)$$

is an isomorphism from C'_p onto $\mathrm{cod}(\partial_p)$, then the relation $R(\partial_p) \subset C'_p \times \mathrm{cod}(\partial_p)$ in the restricted space is obviously also isomorphic.

[1] A field $f \in F^2$ is *solenoidal* if its integral over all bounding 2-chains (of the form $c = \partial_3 c'$) vanish.

When the relation $R(\partial_p)$ is isomorphic, symbol $R_i(\partial_p)$ is employed to emphasize this property.

The key point is that existence of the solution of problem 1 can be guaranteed if relations $R(\partial_2, \int^2)$ and $R(\partial_3, \int^3)$ are induced by isomorphic relations $R_i(\partial_2)$ and $R_i(\partial_3)$. In such cases we shall use symbols $R_i(\partial_2, \int^2)$ and $R_i(\partial_3, \int^3)$ to denote this property.

Now, the *topological problem* of "conflicting" data is resolved. With the same assumptions as above the magnetic field can be characterized as the solution of problem:

Problem 2: *Find* $(b, h) \in F^2 \times F^1$ *such that*

$$\begin{aligned}
&(b, h) \in R_{1-1}(\mu)\,, \\
&(j + \partial_t d, h) \in R_i(\partial_2, \textstyle\int^2)\,, \\
&(q_m, b) \in R_i(\partial_3, \textstyle\int^3)
\end{aligned}$$

hold. This is a well posed problem meaning there exists a unique solution[2] for it.

When it comes to numerical computation there still remains an *algebraic* problem of finding a linearly independent basis for $R_i(\partial_2)$ and $R_i(\partial_3)$. In practice this means that Ampère's and Gauss's laws need not to be imposed over all pairs $(c, \partial c)$ in $R_i(\partial_2)$ and $R_i(\partial_3)$, but instead only over sets which form linearly independent bases of these relations.

Obviously, the electric field makes no difference with respect to the magnetic field, so as an immediate generalization we may state:

In computational electromagnetics there is a problem of **algebraic topology** *to find isomorphic relations $R_i(\partial_p)$ and a problem of* **linear algebra** *constructing linearly independent bases for these spaces.*

4. EXACT SEQUENCES AND DECOMPOSITIONS

The isomorphic relation $R_i(\partial_p)$ is related to so called *exact sequences*, which are sequences of abelian groups in the following way: A mapping α from abelian group U to another abelian group V is a *homomorphism* preserving the structure if α satisfies $\alpha(a_i + a_j) = \alpha(a_i) + \alpha(a_j)$. A sequence of abelian groups and homomorphisms

$$\cdots \longrightarrow U_{n+1} \xrightarrow{\alpha_{n+1}} U_n \xrightarrow{\alpha_n} U_{n-1} \longrightarrow \ldots$$

[2] All the solutions of problem 1 are also solutions of problem 2, but not vice versa. Furthermore, if the first problem has a solution, it is also a solution of the second one.

is *exact* if the kernel of α_n is the codomain, i.e. the image of α_{n+1} for all n. Now, an exact sequence enables one to decompose the underlying groups in the following way [15]:

Theorem 1: If $0 \to U \xrightarrow{\alpha} V \xrightarrow{\beta} W \to 0$ is an exact sequence, then there is a *direct decomposition* of V such that

$$V = \alpha(U) \oplus V',$$

where V' is a subgroup of V such that the restriction of β onto V' is an isomorphism from V' onto W. □

Now, to see what this theorem has to do with problem 2, notice first that $\mathrm{cod}(\partial_{p+1}) \subset C_p$. Thus, there is a natural injection ι from the group $B_p = \mathrm{cod}(\partial_{p+1})$ onto C_p. Second, as the boundary operator ∂_p is a map from C_p onto B_{p-1}, and since in all space the kernel Z_p of ∂_p (consisting of all p-chains whose boundary is null) coincides with B_p, we have an exact sequence

$$0 \longrightarrow Z_p \xrightarrow{\iota} C_p \xrightarrow{\partial_p} B_{p-1} \longrightarrow 0. \tag{3}$$

And now, according to theorem 1, module C_p can immediately be decomposed such that

$$C_p = Z_p \oplus C'_p = B_p \oplus C'_p, \tag{4}$$

where ∂_p is an isomorphism from C'_p onto B_{p-1}. (Notice, that C'_p is what we needed in introducing $R_i(\partial_p)$.) So, the topological problem reduces to developing an algorithm decomposing C_p into Z_p and C'_p, and it is a problem of linear algebra to find a basis for these subgroups and B_{p-1}.

Before introducing an algorithm which tackles this problem, we shall first generalize the approach to boundary value problems supported in bounded domains with various kinds of boundary conditions and non-local conditions. (The non-local conditions correspond with things like imposed currents or voltages.)

5. BOUNDED DOMAINS

The case of a bounded domain with different kinds of boundary conditions seems to make the problem setup far more complex. This additional complexity is, however, superficial, as the problem is still built out of same kind of layers. Compared to a problem supported in the whole space, in case of a bounded domain there are, so to speak, more layers but they all are still of the same level. Let us next work this out step by step to see what it means.

The topology of all space is trivial, which means that the sequence

$$\cdots \longrightarrow C_{p+1} \xrightarrow{\partial_{p+1}} C_p \xrightarrow{\partial_p} C_{p-1} \xrightarrow{\partial_{p-1}} \ldots\,, \tag{5}$$

is exact. In other words the codomain of the boundary operator is the kernel of the next one, and thus, all chains whose boundary vanish –that is, *cycles*– are themselves boundaries of some other chains. But in a bounded domain this property of exactness is lost: A cycle is not necessary a boundary of another chain. So, in a bounded domain one can't rely on the exactness property of sequence (5). To recover from this problem another exact sequence is needed.

Let $B_p = \mathrm{cod}(\partial_{p+1})$ and $Z_p = \ker(\partial_p)$ denote the groups of bounding p-chains and p-cycles, respectively. We shall name H_p the *quotient group* Z_p/B_p whose elements are *cosets* of the form $z + B_p$ where $z \in Z_p$. This means that two cycles $z_1, z_2 \in Z_p$ belong to the same coset of H_p if $z_1 - z_2 \in B_p$. As all bounding chains are also cycles, again there is a natural injection $\iota : B_p \to Z_p$. By introducing operator κ_p taking a cycle $z \in Z_p$ into the corresponding coset of H_p, a new exact sequence [16]

$$B_p \xrightarrow{\iota} Z_p \xrightarrow{\kappa_p} H_p\,, \tag{6}$$

is obtained. Now, a combination of the exact sequences (3) and (6) yields a diagram

$$\begin{array}{l} B_p \\ \downarrow \iota \\ Z_p \xrightarrow{\iota} C_p \xrightarrow{\partial_p} B_{p-1} \\ \downarrow \kappa_p \\ H_p\,, \end{array}$$

and instead of (4) theorem 1 implies now that

$$C_p = Z_p \oplus C'_p = B_p \oplus Z'_p \oplus C'_p\,, \tag{7}$$

where ∂_p is an isomorphism from C'_p onto B_{p-1} and κ_p from Z'_p onto H_p. In other words, in bounded domains the decomposition of C_p is threefolded, whereas in all space it is always twofolded.

To complete with bounded domains we still need to take into account the effect of boundary conditions. Let us name Γ the boundary of the bounded domain Ω. The boundary itself is split into two parts $\Gamma = \Gamma^t \cup \Gamma^c$, where Γ^t represents the part of the boundary on which the *tangential trace*[3] of a field is known, and Γ^c is the complement of Γ^t on Γ. For example, in case of b, Γ^t is the part of the boundary on which the magnetic flux is locally known, and in case of h, Γ^t is the part on which the magnetomotive force is locally imposed by the boundary conditions. (Of course, one may well have $\Gamma^t = \Gamma$ or $\Gamma^t = \emptyset$.)

We shall denote by $C_p(\Omega)$ and $C_p(\Gamma^t)$ the modules of p-chains in domain Ω and in Γ^t, respectively. As all p-cells on Γ^t lie also in Ω, there exists a rather trivial map η_p^t from $C_p(\Gamma^t)$ onto $C_p(\Omega)$. (A superscript, here t, is employed to point to the submanifold, here to Γ^t, with respect to which the operator is relative.) The quotient group $C_p(\Omega, \Gamma^t)$ consists of cosets of the form $c + C_p(\Gamma^t)$ where c is a chain of $C_p(\Omega)$. Informally, the elements of $C_p(\Omega, \Gamma^t)$ are chains whose properties are not dictated by Γ^t. The quotient group $C_p(\Omega, \Gamma^t)$ is often called a *relative* chain group. [18]

In this case the boundary operator should also be extended to the relative case. The relative boundary operator ∂_p^t is defined as a map

$$\partial_p^t : C_p(\Omega, \Gamma^t) \to C_{p-1}(\Omega, \Gamma^t)$$

extending the meaning of ∂_p such that

$$\partial_p^t \, : \, c + C_p(\Gamma^t) \to \partial_p c + C_{p-1}(\Gamma^t) \, .$$

As an immediate consequence one can also find the relative groups of cycles and bounding cycles: If one has $z \in Z_p(\Omega)$ and $b \in B_p(\Omega)$, then

$$z' = z + C_p(\Gamma^t) \qquad \text{and} \tag{8}$$
$$b' = b + C_p(\Gamma^t) \tag{9}$$

are evidently elements of $C_p(\Omega, \Gamma^t)$. The relative groups $Z_p(\Omega, \Gamma^t)$ and $B_p(\Omega, \Gamma^t)$ are formed such that [18]

$$z' \in Z_p(\Omega, \Gamma^t) \text{ if } \partial_p^t z' = 0 \, ,$$

in other words if $\partial_p z \in \eta_p(C_p(\Gamma^t))$, and

$$b' \in B_p(\Omega, \Gamma^t) \text{ if } b' = \partial_p^t c' \text{ for some } c' \in C_{p+1}(\Omega, \Gamma^t) \, ,$$

that is, if $\partial_p c - b \in \eta_p(C_p(\Gamma^t))$ for some $c \in C_{p+1}(\Omega)$.

Intuitively, a chain belongs to $Z_p(\Omega, \Gamma^t)$, and it is called a *relative cycle mod* Γ^t if its boundary lies completely in Γ^t. Correspondingly, a p-chain c is in $B_p(\Omega, \Gamma^t)$, and it is called a *bounding cycle mod* Γ^t, if one

[3] This corresponds with Dirichlet type of boundary conditions.

can find a $(p+1)$-chain c' in $C_{p+1}(\Omega)$ such that $\partial c' - c$ lies completely on Γ^t.

Now, let us name λ_p^t the operator taking a chain $c \in C_p(\Omega)$ into the corresponding coset $C_p(\Omega, \Gamma^t)$ of relative chains. Then we have three short exact sequences:

$$Z_p(\Omega,\Gamma^t) \xrightarrow{\iota} C_p(\Omega,\Gamma^t) \xrightarrow{\partial_p^t} B_{p-1}(\Omega,\Gamma^t)\,, \tag{10}$$

$$B_p(\Omega,\Gamma^t) \xrightarrow{\iota} Z_p(\Omega,\Gamma^t) \xrightarrow{\kappa_p^t} H_p(\Omega,\Gamma^t)\,, \tag{11}$$

$$C_p(\Gamma^t) \xrightarrow{\eta_p^t} C_p(\Omega) \xrightarrow{\lambda_p^t} C_p(\Omega,\Gamma^t)\,. \tag{12}$$

and by combining them all together, the following diagram is obtained:

$$\begin{array}{ccccc}
 & & B_p(\Omega,\Gamma^t) \xrightarrow{\iota} & Z_p(\Omega,\Gamma^t) & \xrightarrow{\kappa_p^t} H_p(\Omega,\Gamma^t) \\
 & & & \downarrow \iota & \\
C_p(\Gamma^t) & \xrightarrow{\eta_p^t} & C_p(\Omega) \xrightarrow{\lambda_p^t} & C_p(\Omega,\Gamma^t) & \\
 & & & \downarrow \partial_p^t & \\
 & & & B_{p-1}(\Omega,\Gamma^t)\,. &
\end{array}$$

The corresponding decomposition is

$$C_p(\Omega) \;=\; B_p(\Omega,\Gamma^t) \,\oplus\, Z'_p \,\oplus C'_p \,\oplus\, C''_p\,, \tag{13}$$

where ∂_p^t is an isomorphism from C'_p onto $B_{p-1}(\Omega,\Gamma^t)$, κ_p^t from Z'_p onto $H_p(\Omega,\Gamma^t)$, and η_p^t from $C_p(\Gamma^t)$ onto C''_p.

Let the boundary be split such that $\Gamma = \Gamma^b \cup \Gamma^h$. The boundary conditions of $b = B$ on Γ^b and of $h = H$ on Γ^h can now be characterized using induced relations $R_i(\eta_2^b, \int^2)$ and $R_i(\eta_1^h, \int^1)$, where the corresponding operators are defined by

$$\eta_2^b \;:\; C_2(\Gamma^b) \to C_2(\Omega)\,, \tag{14}$$

$$\eta_1^h \;:\; C_1(\Gamma^h) \to C_1(\Omega)\,. \tag{15}$$

There may also be non-local conditions, for instance due to external circuits, which set the flux of b to Φ and the circulation of h to Ψ over (possibly relative) nonbounding 2-cycles and over nonbounding 1-cycles, respectively. The non-local conditions correspond with relations $R_i(\kappa_2^b, \int^2)$ and $R_i(\kappa_1^h, \int^1)$ defined by

$$\kappa_2^b \;:\; Z_2(\Omega,\Gamma^b) \;\to\; H_2(\Omega,\Gamma^b)\,, \tag{16}$$

$$\kappa_1^h \;:\; Z_1(\Omega,\Gamma^h) \;\to\; H_1(\Omega,\Gamma^h)\,. \tag{17}$$

Putting everything together, in a bounded domain with given $\mu \in M$, $i = j + \partial_t d \in F^2(\Omega)$, $q_m \in F^3(\Omega)$, given trace of b which equals to $B \in F^2(\Gamma^b)$, given trace of h which is $H \in F^1(\Gamma^b)$, $\int_z b = \Phi \in \mathbb{R}$ for some $z \in Z_2'$, and $\int_z h = \Psi \in \mathbb{R}$ for some $z \in Z_1'$, the magnetic field can be expressed as the solution of the problem:

Problem 3: *Find* $(b, h) \in F^2(\Omega) \times F^1(\Omega)$ *such that*

$$
\begin{aligned}
&(b, h) \in R_{1-1}(\mu)\,,\\
&(i, h) \in R_i(\partial_2^h, \textstyle\int^2)\,,\\
&(q_m, b) \in R_i(\partial_3^b, \textstyle\int^3)\,,\\
&(B, b) \in R_i(\eta_2^b, \textstyle\int^2)\,,\\
&(H, h) \in R_i(\eta_1^h, \textstyle\int^1)\,,\\
&(\Phi, b) \in R_i(\kappa_2^b, \textstyle\int^2) \;\; \text{and/or} \;\; (\Psi, h) \in R_i(\kappa_1^h, \textstyle\int^1)\,,
\end{aligned}
$$

hold.[4]

This problem has precisely the same structure as problem 2. When it comes to numerical computing there also remains the same problem of linear algebra to construct a linearly independent bases for the underlying spaces of the relations. Thence, once again, there is a call for an algorithm decomposing the groups of an exact sequence into appropriate subgroups and yielding a basis for them.

6. IMPLEMENTATION

A short exact sequence which is general enough for our purpose can be given by

$$U \xrightarrow{\alpha} V \xrightarrow{\beta} W/W_0\,, \tag{18}$$

where W/W_0 is a quotient group. (The quotient group W/W_0 coincides with group W if one selects $W_0 = \{0\}$.)

In finite dimensional spaces operators correspond with matrices and the elements of the linear vector spaces can be represented by vectors of coefficients. As a linear space is also a module and a group, theorem 1 of the decomposition of groups applies to linear spaces as

[4] For each pair of "magnetic connectors" it is enough to know *either* Φ or Ψ. This is in full analogy with voltages and currents in circuit theory: For each pair of entry ports one needs to know either the voltage or current [19]. If they both are known, then there is nothing to solve, as the impedance $Z = U/I$ is fixed. (Solving a boundary value problem corresponds with finding the impedance [8, 19].) In more precise terms, relations $R_i(\kappa_2^b, \int^2)$ and $R_i(\kappa_1^h, \int^1)$ are isomorphic [18, 20, 21].

well. This enables us to employ tools of linear algebra to develop an algorithm yielding the decompositions we need.

We assume now that domain Ω and the boundary Γ are split into a *cellular mesh*. In common words, the question is of any mesh of the *finite element* type. Hence, all our spaces will also be of finite dimension. In general, finite dimensional spaces are, as is well known, isomorphic to spaces of vectors of coefficients. Here, the sets of nodes, edges, faces, and volumes –i.e., the sets of p-cells, $p = 0, \dots, 3$– equipped with some coefficients correspond with the chains of C_p, $p = 0, \dots, 3$, respectively. For instance, the ith edge of the finite element mesh corresponds with a vector $[0, \dots, 1, \dots, 0]^T$, where only the ith entry is nonzero and equal to one. A 1-chain (a p-chain) corresponds then with any vector or array of coefficients assigned in a 1-to-1 sense with the edges (with the p-cells, resp.). To guarantee exact arithmetics, we shall assume that the coefficients belong to the field $\mathbb{Q}$ of rational numbers.

According to theorem 1, sequence (18) implies decomposition

$$V = \ker(\beta) \oplus V' \,, \tag{19}$$

such that $R_i(\beta) \subset V' \times \mathrm{cod}(\beta)$. So, the algorithm should yield a linearly independent basis for $\ker(\beta)$ and for the isomorphic relation $R_i(\beta)$. Next, such an algorithm is presented.

6.1. Algorithm

Let U be a n-dimensional vector space. Assuming a basis for U, the corresponding *coefficient space* isomorphic to U is denoted by $\bar{U}$.

PURPOSE: Assuming finite dimensional spaces V, W, subspace W_0 of W, operator β such that

$$\beta : V \longrightarrow W/W_0 \,,$$

and matrix $\boldsymbol{\beta}$ representing operator β in the coefficient spaces, the algorithm decomposes space $\bar{V}$ such that

$$\bar{V} \;=\; \ker(\boldsymbol{\beta}) \oplus \bar{V}' \,,$$

and creates the basis of $\ker(\boldsymbol{\beta})$, $\bar{V}'$, and of $\mathrm{cod}(\boldsymbol{\beta})$ such that $\boldsymbol{\beta}$ maps the ith basis vector of V' to the ith basis vector of $\mathrm{cod}(\boldsymbol{\beta})$.

INPUT: First, the $nv = \dim(\bar{V})$ and $nw = \dim(\bar{W}_0)$ vectors forming the linearly independent bases of $\bar{V}$ and $\bar{W}_0$ have to be inserted in input:

$$\begin{aligned}\bar{V} \; &= \mathrm{span}\{\mathbf{v}_i\}_{i=1}^{nv}\,,\\ \bar{W}_0 &= \mathrm{span}\{\mathbf{w}_i\}_{i=1}^{nw}\,,\end{aligned}$$

Second, matrix $\boldsymbol{\beta}$ has to be given in input.

STEP 1: Form matrices $\mathbf{V}$ and $\mathbf{W}_\beta$ such that

$$\begin{aligned}\mathbf{V} \;\; &:= [\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_{nv}]\,,\\ \mathbf{W}_\beta &:= [\mathbf{w}_1, \mathbf{w}_2, \ldots, \mathbf{w}_{nw}]\,.\end{aligned}$$

Next initialize two matrices $\mathbf{K}_\beta$ and $\mathbf{V}_\beta$, and counters nk and nv':

$$\begin{aligned}\mathbf{K}_\beta &:= [\,]\,,\\ \mathbf{V}_\beta &:= [\,]\,,\\ nk \; &:= 0\,,\\ nv' &:= 0\,.\end{aligned}$$

(Symbol [ ] denotes to a matrix with no columns.)

STEP 2: FOR $i = 1$ TO nv
    $\mathbf{a} := \boldsymbol{\beta}\mathbf{v}_i$

  % Test whether $\mathbf{a} \in \mathrm{cod}(\mathbf{W}_\beta)$
    Solve vector $\mathbf{x}$ such that $\mathbf{W}_\beta^T\mathbf{W}_\beta\mathbf{x} = \mathbf{W}_\beta^T\mathbf{a}$
    Boolean TEST := ($\mathbf{W}_\beta\mathbf{x}$ EQUAL $\mathbf{a}$)

    IF (TEST) THEN
      $nk := nk + 1$
    % Take elements $nw + 1, \ldots, nv'$ of vector $\mathbf{x}$
      Vector $\mathbf{x}' := \mathbf{x}(nw + 1, \ldots, nv')$
      Vector $\mathbf{d} := \mathbf{v}_i - \mathbf{V}_\beta\mathbf{x}'$
    % Add $\mathbf{d}$ into the basis of $\ker(\boldsymbol{\beta})$.
      $\mathbf{K}_\beta := [\mathbf{K}_\beta, \mathbf{d}]$
    ELSE
      $nv' := nv' + 1$
    % Add $\mathbf{v}_i$ and $\mathbf{a}$ to the basis of
    % $\bar{V}'$ and $\mathrm{cod}(\boldsymbol{\beta})$, respectively.
      $\mathbf{V}_\beta := [\mathbf{V}_\beta, \mathbf{v}_i]$
      $\mathbf{W}_\beta := [\mathbf{W}_\beta, \mathbf{a}]$
    END IF

  END FOR

OUTPUT: The columns of matrices $\mathbf{K}_\beta$, $\mathbf{V}_\beta$, and $\mathbf{W}_\beta$ yield the basis vectors of $\ker(\boldsymbol{\beta})$ and $R_i(\boldsymbol{\beta})$ such that

$$\begin{aligned}\ker(\boldsymbol{\beta}) &= \operatorname{span}\left\{(\mathbf{K}_\beta)_i\right\}_{i=1}^{nk}, \\ R_i(\boldsymbol{\beta}) &= \operatorname{span}\left\{\left((\mathbf{V}_\beta)_j, (\mathbf{W}_\beta)_{nw+j}\right)\right\}_{j=1}^{nv'},\end{aligned}$$

where $(\ )_i$ denotes the ith column of a matrix.

USAGE: Assume one has an exact sequence

$$U \xrightarrow{\alpha} V \xrightarrow{\beta} W/W_0\,, \tag{20}$$

where U, V, and W are finite dimensional spaces and W_0 is a subspace of W. Now, by running the algorithm one gets the decomposition

$$\bar{V} = \ker(\boldsymbol{\beta}) \oplus \bar{V}'\,,$$

and immediately from this one also has

$$\bar{V} = \operatorname{cod}(\boldsymbol{\alpha}) \oplus \bar{V}'\,, \tag{21}$$

as $\operatorname{cod}(\boldsymbol{\alpha})$ and $\ker(\boldsymbol{\beta})$ coincide due to the exactness of sequence (20). But now, (21) is nothing else than a realization of theorem 1 in coefficient spaces, and thus –as the construction of the decomposition was a central question– the algorithm is truly all what is needed to solve the topological problem. In order to generate decompositions such as (7) and (13) the algorithm has to be run recursively.

6.2. Example

Let us denote by $\mathbf{C}_0$, $\mathbf{C}_1$, $\mathbf{C}_2$, and $\mathbf{C}_3$ (identity) matrices whose columns are the vectors of coefficients corresponding with the nodes, edges, faces, and volumes of the cellular mesh of Ω, respectively. These matrices represent on the discrete level the bases of the spaces of chains C_p, $p = 0, \ldots, 3$. The number of columns in matrix $\mathbf{C}_p$ is denoted by n_p.

A so called *incidence matrix* [8] $\mathbf{D}_p$ is a rectangular matrix, with $\mathbf{C}_{p-1}$ and $\mathbf{C}_p$ as column and row set, which describes how p-cells connect to $(p-1)$-cells. The entries of matrix $\mathbf{D}_p$ are either 0, 1, or -1: The entry $\{c, c'\}$ of $\mathbf{D}_p$ is ± 1 only if $(p-1)$-cell c' bounds p-cell c and otherwise equal to zero. The sign of the entry depend on whether the orientations of c and c' match or not. On the discrete level the boundary operator ∂_p corresponds with the transpose $\mathbf{D}_p^T$ of the incidence matrix.

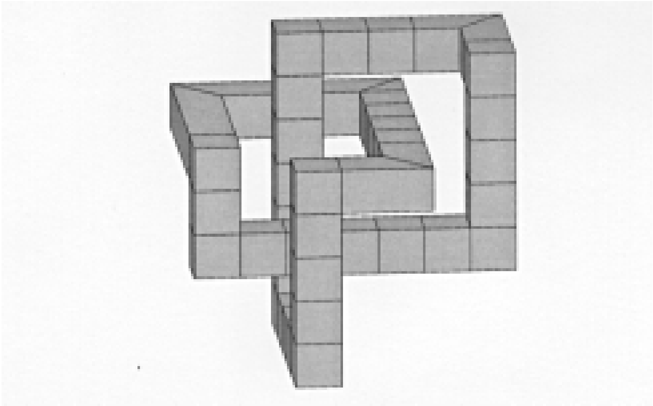

Figure 1. A cellular mesh forming a trefoil knot.

As an example, let's see how the topological properties of the (be aware) complement of a so called *trefoil knot* [22] in a box can be computed with the algorithm, Fig. 1.

First, the bases for the subspaces of cycles, and bounding cycles are found as follows:

INPUT OF RUNS $p = 1, 2, 3$*:*

$$\begin{aligned} \bar{V} &:= \mathrm{span}\{(\mathbf{C}_p)_i\}_{i=1}^{n_p}, \\ \bar{W}_0 &:= [\,], \\ \boldsymbol{\beta} &:= \mathbf{D}_p^T. \end{aligned}$$

OUTPUT: The algorithm yields the bases of spaces $\bar{Z}_p$, $\bar{B}_{p-1}$, and $\bar{C}'_p$ such that

$$\begin{aligned} \bar{Z}_p &= \ker(\mathbf{D}_p^T), \\ \bar{B}_{p-1} &= \mathrm{cod}(\mathbf{D}_p^T), \\ \bar{C}_p &= \ker(\mathbf{D}_p^T) \oplus \bar{C}'_p, \end{aligned}$$

and where $\mathbf{D}_p^T$ is a map from $\bar{C}'_p$ onto $\bar{B}_{p-1}$ in a one-to-one sense. □

The output of the first stage gives discrete counterparts of the decompositions (3) when $p = 0, 1, 2, 3$. In three dimensions the 3-chains cannot be boundaries of 4-chains, and thus, space B_3 is trivial. In addition, by definition a 0-chain does not have a boundary, and therefore, Z_0 coincides with C_0.

Next, the representatives of the quotient spaces H_p are found by constructing a discrete counterpart of decompositions (6). In this case the identity matrix represents operator κ_p on the discrete level. The output of the first run is now the input for the second stage:

INPUT OF RUNS $p = 0, \ldots, 3$*:*

$$\begin{aligned} \bar{V} &:= \bar{Z}_p \\ \bar{W}_0 &:= \bar{B}_p \,, \\ \boldsymbol{\beta} &:= \mathbf{I} \,. \end{aligned}$$

OUTPUT: The algorithm yields a basis for space $\bar{Z}'_p$ consisting of the coefficient vectors representing the cosets of H_p, i.e.

$$\bar{Z}'_p \;=\; \operatorname{span}\{(\mathbf{V}_\beta)_i\}_{i=1}^{nv'} \,.$$

Space $\ker(\boldsymbol{\kappa}_p)$ coincides with $\bar{B}_p$, and thus, it does not yield anything new in this case. □

By calculating the dimension of spaces $\bar{Z}'_p$, $p = 0, \ldots, 3$, the *Betti numbers* [15]

$$\begin{aligned} \dim(H_0) = \dim(\bar{Z}'_0) &\;=\; 1 \,, \\ \dim(H_1) = \dim(\bar{Z}'_1) &\;=\; 1 \,, \\ \dim(H_2) = \dim(\bar{Z}'_2) &\;=\; 1 \,, \\ \dim(H_3) = \dim(\bar{Z}'_3) &\;=\; 0 \,, \end{aligned}$$

characterizing the topological properties of this problem can be found.

6.3. Practical Issues

In practice a critical part of the algorithm is the test whether $\boldsymbol{\beta}\mathbf{v}_i \in \operatorname{cod}(\mathbf{W}_\beta)$ holds. This is the same as asking whether there exists a vector $\mathbf{x}$ such that

$$\mathbf{W}_\beta \mathbf{x} \;=\; \boldsymbol{\beta}\mathbf{v}_i \tag{22}$$

holds.

A technique to answer this question is to employ the *Smith normal form* [23]. If the *invariant factors* obtained by finding the Smith normal forms of matrices $\mathbf{W}_\beta$ and $[\mathbf{W}_\beta, \boldsymbol{\beta}\mathbf{v}_i.]$ are the same, then the existence of a $\mathbf{x}$, such that (22) holds, is guaranteed. Furthermore, once the Smith normal form is found getting $\mathbf{x}$ thereafter is trivial.

Another possibility is to exploit the least square solver. One can always solve $\mathbf{x}$ from

$$\mathbf{W}_\beta^T \mathbf{W}_\beta \, \mathbf{x} \;=\; \mathbf{W}_\beta^T \boldsymbol{\beta}\mathbf{v}_i \,, \tag{23}$$

and then verify whether vector $\mathbf{x}$ fulfills also (22).

If the coefficients are rational numbers, then arithmetics is exact. In practice, however, computing with rational numbers (i.e., with pairs of integers) is inefficient when the matrices become large in size, and thus, one may have to use real numbers (in single or double precision) instead, But then, also an ϵ-test to check the equality between real numbers is needed.

As the topological properties have nothing to do with the cardinality of the sets of nodes, edges, faces and volumes, in practice, computing time can be minimized by employing as coarse cellular meshes as possible.

It is also useful to notice that the algorithm generalizes the *spanning-tree techniques* to construct trees and cotrees of graphs [24].

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