

CHAPTER 5

Whitney Elements

We now leave the first part of this book, devoted to the study of the “div-side” of the modelling of Chapter 2, and will turn to the “curl-side”. As we need a more encompassing viewpoint to survey this enlarged landscape, we shall use more sophisticated mathematical tools. Hence this transition chapter. First, we enlarge the mathematical framework, studying the three fundamental operators grad , rot , div , from the functional point of view, thus making visible a rich structure, which happens to be the right functional framework for Maxwell’s equations. Then, we present a family of geometrical objects introduced around 1957 by Whitney (Hassler Whitney, 1907–1989, one of the masters of differential geometry), known as “Whitney (differential) forms” [W h]. They constitute a *discrete* realization of the previous structure, and therefore, the right framework in which to develop a finite element discretization of electromagnetic theory. (This is why I call them “Whitney elements” here, rather than “Whitney forms”.) Finally, now-popular “tree and cotree” techniques are addressed.

5.1 A FUNCTIONAL FRAMEWORK

In Section 3.2, when we had to complete the space of potentials, we saw a connection between the physically natural idea of “generalized solution” of an equation $Ax = b$, and the prolongation of operator A beyond its initial domain of definition. This will now be systematized, and applied to the classical differential operators grad , rot , and div . The idea is extremely simple: We take the *closures* of the graphs of all operators in sight, thus finding extensions of them with good properties. But the proofs along the way can be quite involved, so they are placed in such positions as to make it easy to ignore them at first reading. Familiarity with the Hilbert spaces $L^2(D)$ and $\mathbb{L}^2(D)$ is now assumed. (Cf. 3.2.3 and Appendix A, Section A.4.)

5.1.1 The “weak” grad, rot, and div

Let D be a regular bounded domain of E_3 and denote, as in Chapter 2, $C^\infty(\overline{D})$ and $C^\infty_0(\overline{D})$ the spaces of restrictions to D of smooth functions or fields with compact support in E_3 . All three components of a smooth field b have partial derivatives at all points of D and its boundary, hence a function $f = \operatorname{div} b$ that belongs to $C^\infty(\overline{D})$, and hence a linear operator, denoted div , the standard, or “strong” one.

We found it not so convenient a tool, back in Chapter 2. For instance, if $\{b_n\}$ is a sequence of smooth solenoidal vector fields of finite energy which converge in energy toward a field b , we expect b to be solenoidal as well. And yet, we would have “no right” to say that, because “ $\operatorname{div} b = 0$ ” doesn’t make sense if b is not smooth! A silly situation, from which we escaped thanks to the notion of weak formulation, but there is a more direct approach, as suggested by the very idea of completion, as follows. Set $f_n = \operatorname{div} b_n$, not necessarily zero for more generality. Suppose that $\lim_{n \rightarrow \infty} b_n = b$ and $\lim_{n \rightarrow \infty} f_n = f$ in $\mathbb{L}^2(D)$ and $L^2(D)$ respectively. Why not *decree* that $\operatorname{div} b$ does exist, as a scalar field, and is equal to f , thus enlarging the domain of div ? This is quite in the spirit of generalized solutions. By doing that for all similar sequences, we may expect the extension¹ of div thus obtained to be free of the inadequacies of the strong divergence.

So let us denote by $\overline{\operatorname{DIV}}$ the graph in $\mathbb{L}^2(D) \times L^2(D)$ of the strong divergence, i.e., the set of pairs $\{b, f\} \in C^\infty(\overline{D}) \times C^\infty(\overline{D})$ such that $\operatorname{div} b = f$. The recipe just described—enlarge the graph in order to include limits of related pairs $\{b_n, f_n\}$ —simply consists in taking its *closure*, denoted $\overline{\operatorname{DIV}}$, in $\mathbb{L}^2(D) \times L^2(D)$. Hence a new operator, that we shall provisionally denote “ div ” and call the *weak* divergence, for reasons which will be obvious in a moment.

But . . . *does* this subset $\overline{\operatorname{DIV}}$ define a function? Is it a *functional* graph? Conceivably, two sequences $\{b_n, f_n\}$ and $\{\tilde{b}_n, \tilde{f}_n\}$ could converge toward the same b but different f ’s, hence a multivalued extension of div . We say that a linear operator (or, for that matter, any function) is *closable* if such mishaps cannot occur, i.e., if the closure of its graph is functional.² And indeed,

Proposition 5.1. $\overline{\operatorname{DIV}}$ is a functional graph.

Proof. Otherwise, there would exist a nonzero f such that $\{0, f\}$ be in the

¹See Appendix A, Subsection A.1.2, for the basic notions about relations, functional or not, their graphs, their restrictions, their extensions, etc., and A.3.2 for metric-related notions.

²Of course, *closed* operators are those with a closed graph. Cf. A.4.4.

closure of DIV . Let then $\{b_n, f_n\} \in \text{DIV}$ go to $\{0, f\}$ in the sense of the $\mathbb{L}^2(D) \times L^2(D)$ norm. For all test functions $\varphi' \in C_0^\infty(D)$, one would have

$$(1) \quad \int_D b_n \cdot \text{grad } \varphi' = - \int_D \text{div } b_n \varphi',$$

and since the two sides tend to 0 and $\int_D f \varphi'$ respectively, by continuity of the scalar product, this implies $\int_D f \varphi' = 0 \quad \forall \varphi' \in C_0^\infty(D)$, hence $f = 0$ by density of $C_0^\infty(D)$ in $L^2(D)$ (cf. A.2.3), which proves the point. \diamond

The relation of this procedure with the weak formulation of the equation $\text{div } b = f$ is now patent, which stirs us to try and prove the following clincher result:

Proposition 5.2. *The closure of DIV coincides with the set ${}^w\text{DIV}$ of pairs $\{b, f\}$ in $\mathbb{L}^2(D) \times L^2(D)$ such that*

$$(2) \quad \int_D b \cdot \text{grad } \varphi' + \int_D f \varphi' = 0 \quad \forall \varphi' \in C_0^\infty(D).$$

The proof will qualify ${}^w\text{div}$ as the proper generalization of the “weak divergence” of Eq. (2.11). (The residual and a bit awkward restriction to “piecewise smooth” fields, more or less forced upon us in Chapter 2, has now been lifted for good.) However, it’s surprisingly difficult, so let me postpone it for a moment, in order to keep the main ideas in focus.

So—provisionally accepting Prop. 5.2 as valid—what we called earlier “weak solenoidality” corresponds to ${}^w\text{div } b = 0$, the fact for a field to have a null weak divergence in the present sense, and this justifies the terminology.

Let’s generalize. First, give names to the graphs of the strong operators:

GRAD , the graph of $\text{grad} : C^\infty(\bar{D}) \rightarrow C^\infty(\bar{D})$ in $L^2(D) \times \mathbb{L}^2(D)$,

ROT , the graph of $\text{rot} : C^\infty(\bar{D}) \rightarrow C^\infty(\bar{D})$ in $\mathbb{L}^2(D) \times \mathbb{L}^2(D)$,

DIV , the graph of $\text{div} : C^\infty(\bar{D}) \rightarrow C^\infty(\bar{D})$ in $\mathbb{L}^2(D) \times L^2(D)$,

then define the weak operators ${}^w\text{grad}$, ${}^w\text{rot}$, and ${}^w\text{div}$ via their graphs, which are the closures $\overline{\text{GRAD}}$, $\overline{\text{ROT}}$, and $\overline{\text{DIV}}$ of the former ones. (**Exercise 5.1:** Imitate the proof of Prop. 5.1 to show that $\overline{\text{GRAD}}$ and $\overline{\text{ROT}}$ are functional.) Note that functions may have a weak gradient without being differentiable in the classical sense (**Exercise 5.2:** Provide examples), and fields have a weak curl or a weak divergence in spite of their components not being differentiable at places.

We shall denote the domains of these weak operators by $L^2_{\text{grad}}(D)$, $\mathbb{L}^2_{\text{rot}}(D)$, and $\mathbb{L}^2_{\text{div}}(D)$. You may see them defined as follows, in the

literature:

$$L^2_{\text{grad}}(D) = \{\varphi \in L^2(D) : \text{grad } \varphi \in \mathbb{L}^2(D)\},$$

$$\mathbb{L}^2_{\text{rot}}(D) = \{\mathbf{u} \in \mathbb{L}^2(D) : \text{rot } \mathbf{u} \in \mathbb{L}^2(D)\},$$

$$\mathbb{L}^2_{\text{div}}(D) = \{\mathbf{u} \in \mathbb{L}^2(D) : \text{div } \mathbf{u} \in L^2(D)\}.$$

In such cases, grad , rot , and div are understood in the weak sense; they are actually what we denote here ${}^w\text{grad}$, ${}^w\text{rot}$, ${}^w\text{div}$. Thus stretching the scope of the notation is so convenient that we'll practice it systematically: *From now on, when grad , rot , div appear somewhere, it will be understood that their weak extensions ${}^w\text{grad}$, ${}^w\text{rot}$, ${}^w\text{div}$ are meant.*

5.1.2 New functional spaces: L^2_{grad} , $\mathbb{L}^2_{\text{rot}}$, $\mathbb{L}^2_{\text{div}}$

Up to this point, $L^2_{\text{grad}}(D)$, $\mathbb{L}^2_{\text{rot}}(D)$, and $\mathbb{L}^2_{\text{div}}(D)$ have been mere subspaces of $L^2(D)$, $\mathbb{L}^2(D)$, and $\mathbb{L}^2(D)$. Beware, they are *not* closed, contrary to the graphs! They are dense in L^2 or \mathbb{L}^2 , actually, since they contain all smooth functions or fields. So they are not complete with respect to the scalar product of L^2 or \mathbb{L}^2 . We can turn them into Hilbert spaces on their own right by endowing them with new scalar products, as follows:

$$((\varphi, \varphi')) = \int_D \varphi \cdot \varphi' + \int_D \text{grad } \varphi \cdot \text{grad } \varphi' \quad \text{for } L^2_{\text{grad}}(D),$$

$$((\mathbf{u}, \mathbf{u}')) = \int_D \mathbf{u} \cdot \mathbf{u}' + \int_D \text{rot } \mathbf{u} \cdot \text{rot } \mathbf{u}' \quad \text{for } \mathbb{L}^2_{\text{rot}}(D),$$

$$((\mathbf{u}, \mathbf{u}')) = \int_D \mathbf{u} \cdot \mathbf{u}' + \int_D \text{div } \mathbf{u} \text{ div } \mathbf{u}' \quad \text{for } \mathbb{L}^2_{\text{div}}(D),$$

where of course grad , rot , and div are the weak ones.

Let us then set, for instance (the two other lines can be treated in parallel fashion)

$$(3) \quad |||\varphi||| = (\int_D |\text{grad } \varphi|^2 + \int_D |\varphi|^2)^{1/2}$$

(we reserve the notation $\|\cdot\|$ for the L^2 norm). This is called the *graph norm*, because (cf. A.1.2) it combines the norms of both elements of the pair $\{\varphi, \text{grad } \varphi\}$, which spans $\overline{\text{GRAD}}$. With this norm, $L^2_{\text{grad}}(D)$ is complete, and hence a Hilbert space, since its Cauchy sequences $\{\varphi_n\}$ are in one-to-one correspondence with sequences $\{\varphi_n, \text{grad } \varphi_n\}$ belonging to the graph. Moreover, grad is continuous from the new normed space to $\mathbb{L}^2(D)$, since $\|\text{grad } \varphi\| \leq |||\varphi|||$ by construction.

This can be seen as the real achievement of the whole procedure: *By putting the graph norms on the domains of the weak operators ${}^w\text{grad}$,*

${}^w\text{rot}$, ${}^w\text{div}$, we obtain Hilbert spaces on which these operators are continuous. From now on, $L^2_{\text{grad}}(D)$, $L^2_{\text{rot}}(D)$, $L^2_{\text{div}}(D)$ will thus be understood as these Hilbert spaces, duly furnished with the graph norm.

Remark 5.1. The Hilbert space $\{L^2_{\text{grad}}(D), \|\cdot\|_{\text{grad}}\}$ is the Sobolev space usually denoted $H^1(D)$. We shun this standard notation here for the sake of uniform treatment of grad , rot , and div , which is reason enough to so depart from tradition.³ \diamond

This graph closing is quite similar to the “hole plugging” of Chapter 3, where we invoked completion the first time. However, the link between the foregoing procedure and completion is much stronger than a mere analogy. There is a way in which what we have just done *is* completion of a space, followed by an application of the principle of extension by continuity of A.4.1.

Let’s show this by discussing the case of grad . Start from the space $C^\infty(\bar{D})$, and put on it the norm (3). Now, the strong grad is continuous from the new normed space $\{C^\infty(\bar{D}), \|\cdot\|_{\text{grad}}\}$ into $L^2(D)$. Let us take the completion of $C^\infty(\bar{D})$ with respect to the $\|\cdot\|_{\text{grad}}$ norm. Limits of Cauchy sequences of pairs belonging to GRAD span its closure, $\overline{\text{GRAD}}$, so there is no problem this time in identifying this completion with a functional space: The completion is in one-to-one correspondence with $\overline{\text{GRAD}}$, and therefore—since the latter is a *functional* graph, as we know (Exer. 5.1)—with its projection on $L^2(D)$. The completion is thus (identifiable with) a subspace of $L^2(D)$, which is the classical $H^1(D)$ —our $L^2_{\text{grad}}(D)$.

By construction, $C^\infty(\bar{D})$ is dense in $H^1(D)$, so we are in a position to apply this principle of extension by continuity of Appendix A (Theorem A.4): A uniformly continuous mapping f_U from a metric space X to a *complete* metric space Y , the domain of which is not all of X but only a dense subset U , can be extended by continuity to a map from all X to Y . Here, f_U is the strong gradient, U and X are $C^\infty(\bar{D})$ and $H^1(D)$, and Y is $L^2(D)$. The extension of the strong gradient thus obtained, on the one hand, and the weak gradient, on the other hand, are the same operator, because their graphs coincide, by construction.

Let us now update these integration by parts formulas which were so useful up to now. This will essentially rely on the fact that $L^2_{\text{grad}}(D)$, etc., are *complete* spaces, and justify the work invested in various completions up to this point.

First, over all space, the formulas

³Some Sobolev diehards insist that $L^2_{\text{rot}}(D)$ and $L^2_{\text{div}}(D)$ be denoted $H(\text{rot}; D)$ and $H(\text{div}; D)$ respectively, which would be just fine . . . if only they also used $H(\text{grad}; D)$ for $H^1(D)$.

$$\begin{aligned}\int_{E_3} \operatorname{div} u \cdot \varphi &= -\int_{E_3} u \cdot \operatorname{grad} \varphi \quad \forall \varphi \in L^2_{\operatorname{grad}}(E_3), u \in \mathbb{L}^2_{\operatorname{div}}(E_3), \\ \int_{E_3} \operatorname{rot} u \cdot v &= \int_{E_3} u \cdot \operatorname{rot} v \quad \forall u, v \in \mathbb{L}^2_{\operatorname{rot}}(E_3),\end{aligned}$$

are valid. We know they are when φ is in $C_0^\infty(E_3)$ and u and v both in $C_0^\infty(E_3)$. So if $\{u_n\}$ and $\{v_n\}$ are Cauchy sequences converging to u and v , then $\int \operatorname{rot} u_n \cdot v_m = \int u_n \cdot \operatorname{rot} v_m$ for all n and m , and one may pass to the limit, first with respect to n , then to m , by continuity (that is, if one insists on rigor, by applying the principle of extension by continuity to the linear continuous maps thus defined).

When D is not all E_3 , however, there are surface terms in these formulas, for smooth fields:

$$(4) \quad \int_D \operatorname{div} u \cdot \varphi = -\int_D u \cdot \operatorname{grad} \varphi + \int_S n \cdot u \cdot \varphi,$$

$$(5) \quad \int_D \operatorname{rot} u \cdot v = \int_D u \cdot \operatorname{rot} v + \int_S n \times u \cdot v,$$

and the extension by continuity becomes a very delicate affair because of the difficulty to give sense to the limits of the *restrictions* to the boundary of fields or functions that form a Cauchy sequence. Cf. A.4.2 for a glimpse of this problem of “traces”. We shall go in painful detail over only a *part* of it in Chapter 7. But one can do much mileage with the following idea, which borrows from the “distribution” point of view. Suppose u has a weak divergence in $L^2(D)$. Then, for a smooth φ , the expression $N_u(\varphi) = \int_D \operatorname{div} u \cdot \varphi + \int_D u \cdot \operatorname{grad} \varphi$ makes sense and vanishes for $\varphi \in C_0^\infty(D)$. It means⁴ that, for a smooth φ that doesn’t necessarily vanish on S , the values of $N_u(\varphi)$ depend on the *boundary* values of φ only. Therefore, we have there a linear map, $\varphi \rightarrow N_u(\varphi)$, which actually depends on the restriction φ_S of φ to S . In other words, this is a distribution defined on S (the required sequential continuity is obvious, in the case of a smooth surface). If u is smooth, $n \cdot u$ makes sense, and this distribution is seen to be the map $\varphi \rightarrow \int_S n \cdot u \cdot \varphi$, so we are entitled to identify it with the function $n \cdot u$. Now, moving backwards, we *define* $n \cdot u$, for u in $\mathbb{L}^2_{\operatorname{div}}(D)$, as precisely this distribution. A similar approach gives sense to $n \times u$ in (5).

It’s in this sense that fields of $\mathbb{L}^2_{\operatorname{rot}}(D)$ and $\mathbb{L}^2_{\operatorname{div}}(D)$ have well-defined tangential parts and normal parts, respectively, on the boundary, which may fail to be functions or fields in the usual sense of these words, but make sense as distributions, and reduce to the standard interpretation of $n \times u$ and $n \cdot u$ in case of regularity (of u and of S , of course). Note that, in contrast, $n \times u$ and $n \cdot u$ *don’t* make sense for $u \in \mathbb{L}^2(D)$ if u has no more

⁴Some cheating occurs here. See [LM] for a genuine proof.

regularity than that: Square-summable fields have no traces on boundaries!

Although I cut a few corners, I hope the foregoing was reason enough for you to *use* formulas (4) and (5), in both directions, without undue apprehension, provided of course $\varphi \in L^2_{\text{grad}}(D)$ and $u \in \mathbb{L}^2_{\text{div}}(D)$, as regards (4), and both u and v belong in $\mathbb{L}^2_{\text{rot}}(D)$, as regards (5). For extra security, however, note that we can always decide that, *by definition*, $n \cdot u = 0$ means “ $\int_D \text{div } u \cdot \varphi = -\int_D u \cdot \text{grad } \varphi$ for all φ in $L^2_{\text{grad}}(D)$ ”. This doesn’t go further than the weak formulation we adopted in Chapter 3: There it was for all φ in $C^\infty(\bar{D})$, but since the latter is dense in $L^2(D)$, the present interpretation is simply the application of the principle of extension by continuity. Same remark for $n \times u$, so from now on, we’ll agree that

$$\begin{aligned} n \cdot u = 0 \text{ on } S &\Leftrightarrow \int_D \text{div } u \cdot \varphi + \int_D u \cdot \text{grad } \varphi = 0 \quad \forall \varphi \in L^2_{\text{grad}}(D), \\ n \times u = 0 \text{ on } S &\Leftrightarrow \int_D \text{rot } u \cdot v - \int_D u \cdot \text{rot } v = 0 \quad \forall v \in \mathbb{L}^2_{\text{rot}}(D), \end{aligned}$$

with obvious adaptations in case we want such equalities on a part of S only.

Exercise 5.3. Show that the subspace $\{b \in \mathbb{L}^2_{\text{div}}(D) : \text{div } b = 0\}$ is closed, not only with respect to the graph norm (which is trivial) but in the \mathbb{L}^2 norm as well. Same thing for $\{h \in \mathbb{L}^2_{\text{rot}}(D) : \text{rot } h = 0\}$. Same question for $\{b \in \mathbb{L}^2_{\text{div}}(D) : n \cdot b = 0\}$ and for $\{h \in \mathbb{L}^2_{\text{rot}}(D) : n \times h = 0\}$.

5.1.3 Proof of Proposition 5.2

Before moving on, let’s give the deferred proof.

By (1), ${}^w\text{DIV}$ contains DIV , and is closed, as the orthogonal of the subspace $\{\{\text{grad } \varphi', \varphi'\} : \varphi' \in C_0^\infty(D)\}$. So if it were strictly larger than DIV , there would exist⁵ a pair $\{b, f\}$ in $\mathbb{L}^2(D) \times L^2(D)$ satisfying both (2) (p. 127) and

$$(6) \quad \int_D b \cdot b' + \int_D f \text{div } b' = 0 \quad \forall b' \in C^\infty(\bar{D}),$$

which expresses orthogonality to DIV . Taking $b' = \text{grad } \varphi'$ in (6), the same φ' as in (2), we see that $\int_D f (\varphi' - \Delta \varphi') = 0 \quad \forall \varphi' \in C_0^\infty(D)$. If f was smooth, this would imply $f = \Delta f$ in D , and therefore, $0 = \int_D (f - \Delta f) f = \int_D |f|^2 + \int_D |\nabla f|^2$, hence $f = 0$, then $b = 0$ by (6) and density. The idea of the proof is to smooth out f by convolution before applying this trick. So

⁵By the projection theorem of A.4.3, applied in the Hilbert space $X = {}^w\text{DIV}$ (with the scalar product induced by $\mathbb{L}^2(D) \times L^2(D)$) in the case where C is the closure of DIV .

let $f_n = \rho_n * f$, where ρ_n is a sequence of mollifiers, as in A.2.3, but let's *not* restrict the f_n s to D yet. Set $\delta_n = \sup(|x| : \rho_n(x) \neq 0)$ and $D_n = \{x \in D : d(x, E_3 - D) > \delta_n\}$. Notice that δ_n tends to zero, so the domain D_n grows as n increases, to eventually fill D . Now select a fixed φ' with support inside D_n and note that $\rho_n * \varphi'$ has its support in D , so $\varphi'_n = \rho_n * \varphi'$ belongs to $C_0^\infty(D)$. After this preparation, we have, by using the Fubini theorem and the possibility of permuting $*$ and Δ ,

$$\begin{aligned} \int_{E_3} f_n (\varphi' - \Delta \varphi') &= \int_{E_3} (f * \rho_n) (\varphi' - \Delta \varphi') = \int_{E_3} f (\rho_n * (\varphi' - \Delta \varphi')) \\ &= \int_{E_3} f (\varphi'_n - \Delta \varphi'_n) = \int_D f (\varphi'_n - \Delta \varphi'_n) = 0, \end{aligned}$$

which shows that $f_n = \Delta f_n$ in D_n and hence, $f_n = 0$ in D_n by the previous argument. The limit f of the f_n s must therefore be 0. \diamond

5.1.4 Extending the Poincaré lemma

The three differential operators grad , rot , and div should not only be treated in parallel, but also as an integrated whole, which as one knows has a strong structure: curls of gradients vanish, curls are divergence-free, and to some extent, these properties have reciprocals. It's important to check whether such structure persists when we pass to the weak extensions.

To be more precise, we'll say that a domain of E_3 is *contractible* if it is simply connected with a connected boundary.⁶ A classical result of Poincaré (cf. A.3.3) asserts that, in such a domain, a smooth curl-free [resp. div-free] field is a gradient [resp. a curl]. Is that still true if we replace the strong operators by the weak ones?

To better discuss such issues, let us introduce some vocabulary. A family of vector spaces X^0, \dots, X^n (all on the same scalar field) and of linear maps A^p from X^{p-1} to X^p , $p = 1, \dots, d$, forms an *exact sequence at the level of X^p* if $\text{cod}(A^p) = \text{ker}(A^{p+1})$ in case $1 \leq p \leq d-1$, if A^1 is injective in case $p = 0$, and if A^d is surjective in case $p = d$. An *exact sequence* is one which is exact at all levels. It's customary to discuss sequences with help of diagrams of this form:

⁶Because it can then be contracted onto one of its points by continuous deformation. "Connected" means in one piece, "simply connected" that any closed path can be contracted to a point by continuous deformation. (This is not the case, for instance, for the inside of a torus, which is connected but not simply connected. On the other hand, the space between two nested spheres forms a simply connected domain, but one whose boundary is not connected.)

$$\{0\} \rightarrow X^0 \xrightarrow{A^1} X^1 \xrightarrow{A^2} \dots \xrightarrow{A^{d-1}} X^{d-1} \xrightarrow{A^d} X^d \rightarrow \{0\},$$

where $\{0\}$ is the space of dimension 0. In such diagrams, arrows are labeled with operators and the image, by any of these operators, of the space left to its arrow, is in the kernel of the next operator on the right.

The *Poincaré lemma* just evoked can then be stated as follows: For a contractible domain, the sequence

$$\{0\} \rightarrow C^\infty(\bar{D}) \xrightarrow{\text{grad}} C^\infty(\bar{D}) \xrightarrow{\text{rot}} C^\infty(\bar{D}) \xrightarrow{\text{div}} C^\infty(\bar{D}) \rightarrow \{0\}$$

is exact at levels 1 and 2 (at all levels⁷ from 1 to $d-1$, in dimension d). For a regular bounded⁸ contractible domain, we expect the following sequence, where grad , rot , and div are now the weak operators, to have the same structural property:

$$(7) \quad \{0\} \rightarrow L^2_{\text{grad}}(D) \xrightarrow{\text{grad}} \mathbb{L}^2_{\text{rot}}(D) \xrightarrow{\text{rot}} \mathbb{L}^2_{\text{div}}(D) \xrightarrow{\text{div}} L^2(D) \rightarrow \{0\}.$$

This is true, but the proof calls on some difficult technical results. Let us sketch it for level 1. By definition of the strong curl,

$$\ker(\text{rot} ; C^\infty(\bar{D})) = \{h : \int_D h \cdot \text{rot } a' = 0 \quad \forall a' \in C_0^\infty(D)\}.$$

If D is contractible, the left-hand side is $\text{grad}(C^\infty(\bar{D}))$, by the Poincaré lemma, so

$$\text{grad}(C^\infty(\bar{D})) = C^\infty(\bar{D}) \cap (\text{rot}(C_0^\infty(D)))^\perp.$$

Taking the closures of both sides, we find that

$$\overline{\text{grad}(C^\infty(\bar{D}))} = \ker(\text{rot} ; \mathbb{L}^2_{\text{rot}}(D)).$$

It means that if $\text{rot } h = 0$ in the weak sense, there is a sequence of functions φ_n smooth over D , such that $h = \lim_{n \rightarrow \infty} \text{grad } \varphi_n$. Now suppose D bounded. One may impose $\int_D \varphi_n = 0$, and by a variant of the Poincaré

⁷At level 0, $\text{grad } \varphi = 0$ does not imply $\varphi = 0$ but only φ equal to some constant, unless $D = E_d$. At level d , and if $D = E_d$ this time, $\text{div } u = f$ implies $\int f = 0$, so not all f 's qualify.

⁸One should be cautious with unbounded domains. For instance, as we shall have to worry about in Chapter 7, the image $\text{grad}(L^2_{\text{grad}}(E_3))$ is not closed, and thus does not fill out the kernel of rot . The closure of this image is $\ker(\text{rot})$, however, which is enough for the purposes of cohomology (see *infra*).

inequality (see Exercises 5.11 and 5.12, at the end of the chapter), one has then $\|\varphi_n\| \leq c(D) \|\text{grad } \varphi_n\|$, where $c(D)$ only depends on D . The φ_n 's thus form a Cauchy sequence. Let φ be its limit. Then $h = \text{grad } \varphi$, since grad is closed. Hence the result: $\ker(\text{rot} ; \mathbb{L}_{\text{rot}}^2) = \text{grad}(\mathbb{L}_{\text{grad}}^2)$. For a similar proof at level 2, aiming at $\ker(\text{div} ; \mathbb{L}_{\text{div}}^2) = \text{rot}(\mathbb{L}_{\text{rot}}^2)$, begin with Exercise 5.13, and use the "Coulomb gauge" ($\text{div } a = 0$).

As one sees, all this is difficult to establish with rigor, but the foundations are solid, and the results are easily summarized: At least in the case of bounded regular domains, *all structural properties of the sequence of operators $\text{grad} \rightarrow \text{rot} \rightarrow \text{div}$ carry over to their weak extensions.*

5.1.5 "Maxwell's house"

We'll take this remark quite seriously and *base further study of models derived from Maxwell equations on the systematic exploitation of these structural properties* (an ambitious working program, to which the present book can only begin to contribute). Figure 5.1 should help convey the idea.

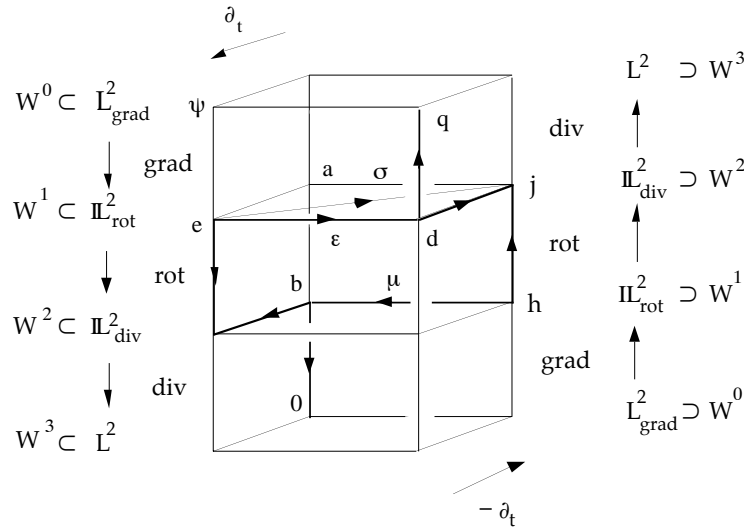


FIGURE 5.1. The functional framework for Maxwell's equations. Note how Ohm's law spoils the otherwise perfect symmetry of the structure.

The structure depicted by Fig. 5.1 is made of four copies of the sequence (7), placed vertically. The two on the left go downwards, the two on the right go upwards, which reflects the symmetry of the Maxwell equations. We need two such "pillars" on each side, linked by the time-derivative,

to account for time-dependence. The four pillars are connected by horizontal beams, which link entities related by constitutive laws. This is like a building, in which as we'll see Maxwell's equations are well at home: "Maxwell's house", let's say.

Joints between pillars and beams make as many niches for electromagnetic-related entities. For instance, magnetic field, being associated with lines (dimension 1) is at level 1 on the right, whereas b , associated with surfaces (dimension 2), is at level 2 on the left, at the right position to be in front of h . Note how the equations can be read off the diagram. Ampère's relation, for instance, is obtained by gathering at level 2, right, back, the outcomes of the arrow actions on nearby fields: $-\partial_t d$ comes from the front and $\text{rot } h$ from downstairs, and they add up to j . All aspects of the diagram should be as easy to understand, except the leftmost and rightmost columns. These concern the finite dimensional spaces W^p of *Whitney elements* announced in the introduction, which we now address.

5.2 THE WHITNEY COMPLEX

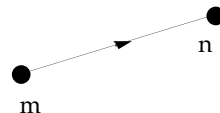
Let us start back from the notion of finite element mesh of Chapter 3: Given a regular bounded domain $D \subset \mathbb{E}_3$, with a piecewise smooth boundary S , a *simplicial mesh* is a tessellation of D by tetrahedra, subject to the condition that any two of them may intersect along a common face, edge or node, but in no other way. We denote by \mathcal{N} , \mathcal{E} , \mathcal{F} , \mathcal{T} (nodes, edges, faces, and tetrahedra, respectively) the sets of simplices of dimension 0 to 3 thus obtained,⁹ and by m the mesh itself. (The possibility of having curved tetrahedra is recalled, but will not be used explicitly in this section, which means that D is assumed to be a polyhedron.)

Besides the list of nodes and of their positions, the mesh data structure also contains *incidence matrices*, saying which node belongs to which edge, which edge bounds which face, and so on. Moreover, there is a notion of orientation of the simplices, which was downplayed up to now. In short, an edge, face, etc., is not only a two-node, three-node, etc., subset of \mathcal{N} , but such a set *plus* an *orientation* of the simplex it subtends. Let's define these concepts (cf. A.2.5 for more details).

⁹Note that if a simplex s belongs to the mesh, all simplices that form the boundary ∂s also belong. Moreover, each simplex appears only once. (This restriction may be lifted to advantage in some circumstances, for instance when "doubling" nodes or edges, as we'll do without formality in Chapter 6.) The structure thus defined is called a *simplicial complex*.

5.2.1 Oriented simplices

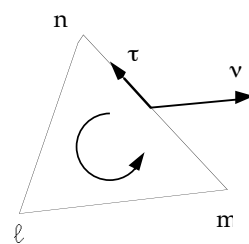
An edge $\{m, n\}$ of the mesh is oriented when, standing at a point of e , one knows which way is “forward” and which way is “backward”. This amounts to distinguishing two classes of vectors along the line that supports e , and to select one of these classes as the “forward” (or positively oriented) one. To denote the orientation without too much fuss, we’ll make the convention that edge $e = \{m, n\}$ is oriented from m to n . All edges of the mesh are oriented, and the opposite edge $\{n, m\}$ is not supposed to belong to \mathcal{E} if e does.



Now we define the so-called *incidence numbers* $\mathbf{G}_{e_n} = 1$, $\mathbf{G}_{e_m} = -1$, and $\mathbf{G}_{e_k} = 0$ for nodes k other than n and m . They form a rectangular matrix \mathbf{G} , with \mathcal{N} and \mathcal{E} as column set and row set, which describes how edges connect to nodes. (See A.2.2 for the use of boldface.)

Faces also are oriented, and we shall adopt a similar convention to give the list of nodes that define one and its orientation, all in one stroke: A face $f = \{\ell, m, n\}$ has three vertices, which are nodes ℓ , m , and n ; we regard even permutations of nodes, $\{m, n, \ell\}$ and $\{n, \ell, m\}$, as being the same face, and odd permutations as defining the oppositely oriented face, which is not supposed to belong to \mathcal{F} if f does. This does orient the face, for when sitting at a point of f , one knows what it means to “turn left” (i.e., clockwise) or to “turn right”. In more precise terms, vectors ℓm and ℓn , for instance, form a reference frame in the plane supporting f . Given two independent vectors v_1 and v_2 at a point of the face, lying in its plane, one may form the determinant of their coordinates with respect to this basis. Its sign, $+$ or $-$, tells whether v_2 is to the left or to the right with respect to v_1 . Observe that v_1 and v_2 also form a frame, so this sign comparison defines an equivalence relation with two classes, *positively oriented* and *negatively oriented* frames. The positive ones include $\{\ell m, \ell n\}$, and also of course $\{mn, m\ell\}$ and $\{n\ell, nm\}$.

An orientation of f induces an orientation of its boundary: A tangent vector τ along the boundary is positively oriented if $\{v, \tau\}$ is a direct frame, where v is any outgoing vector¹⁰ in the plane of f , originating from the same point as τ (inset). Thus, with respect to the orientation of the face, an edge may “run along”, like



¹⁰No ambiguity on that: In the plane of f , the boundary is a closed curve that separates two regions of the plane, so “outwards” is well defined. Same remark for the surface of a tetrahedron (Fig. 5.2).

$e = \{m, n\}$, when its orientation matches the orientation of the boundary, or “run counter” when it doesn’t.

We can now define the incidence number R_{fe} : it’s $+1$ if e runs along the boundary, -1 otherwise, and of course 0 if e is not one of the edges of f . Hence a matrix R , indexed over \mathcal{E} and \mathcal{F} .

A matrix D , indexed over \mathcal{F} and \mathcal{T} , is similarly defined: $D_{\tau f} = \pm 1$ if face f bounds tetrahedron τ , the sign depending on whether the orientations of f and of the boundary of τ match or not. This makes sense only after the tetrahedron τ itself has been oriented, and our convention will be that if $\tau = \{k, \ell, m, n\}$, the vectors $k\ell$, km , and kn , in this order, define a positive frame. (Beware: $\{\ell, m, n, k\}$ has the opposite orientation, so it does not belong to \mathcal{T} if τ does.) The orientation of τ may or may not match the usual orientation of space (as given by the corkscrew rule): these are independent things (Fig. 5.2).

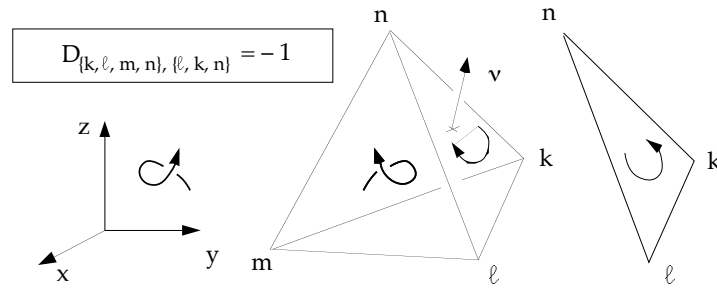
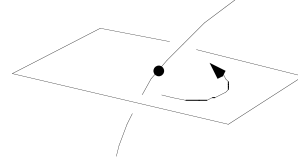


FIGURE 5.2. Left: Standard orientation of space. Right: The tetrahedron $\tau = \{k, \ell, m, n\}$, “placed” this way in E_3 , has “counter-corkscrew” orientation. See how, thanks to the existence of a canonical “crossing direction” (here inside-out, materialized by the outgoing vector v), this orientation induces one on the boundary of the tetrahedron, which here happens to be opposite to the orientation of $f = \{k, n, \ell\}$. Concepts and graphic conventions come from [VW] and [Sc], via [Bu].

Remark 5.2. The orientation of faces is often casually defined by providing each face with its own normal vector, which is what we did earlier when we had to consider crossing directions. This is all right if the ambient space E_3 has been oriented, which is what we assume as a rule (the standard orientation is that of Fig. 5.2, left). In that case, the normal vector and the ambient orientation join forces to orient the face. But there are two distinct concepts of orientation here. What we have described above is *inner* orientation, which is intrinsic and does not depend on the simplex being embedded in a larger space. In contrast, giving a crossing direction¹¹ for a surface is *outer*, or *external* orientation. More generally, when a manifold (line, surface, . . .) is immersed in a space of higher

dimension, an outer orientation of the tangent space at a point is by definition an inner orientation of its complement. (Outer orienting a line is thus the same as giving a way to turn around it, cf. the inset.) So if the encompassing space is oriented, outer orientation of the tangent space at a point of the manifold determines its inner orientation, and the other way around. (Cf. A.2.2 for more detail.) It's better not to depend on the orientation of E_x , however, so let it be clear that faces have inner orientations, like edges and tetrahedra. \diamond



Remark 5.3. For consistency, one is now tempted to attribute an orientation to nodes as well, which is easy to do: just assign a sign, $+1$ or -1 , to each node, and for each node n with “orientation” -1 , change the sign of all entries of column n in the above \mathbf{G} . Implicitly, we have been orienting all nodes the same way ($+1$) up to now, and we'll continue to do so, but all proofs below are easily adapted to the general case. \diamond

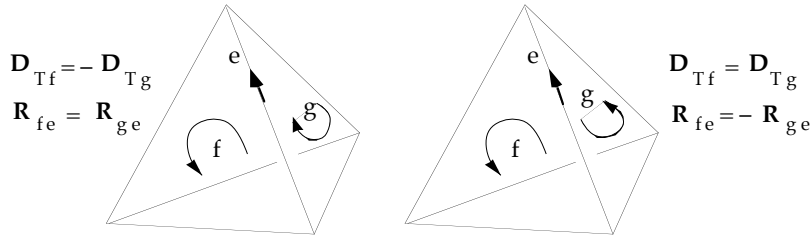


FIGURE 5.3. Opposition of incidence numbers, leading to $\mathbf{DR} = 0$, whatever the orientations.

Next point:

Proposition 5.3. *One has $\mathbf{DR} = 0$, $\mathbf{RG} = 0$. (Does that ring a bell?)*

Proof. For $e \in \mathcal{E}$ and $\tau \in \mathcal{T}$, the $\{\tau, e\}$ -entry of \mathbf{DR} is $\sum_{f \in \mathcal{F}} \mathbf{D}_{\tau f} \mathbf{R}_{fe}$. The only nonzero terms are for faces that both contain e and bound τ , which means that e is an edge of τ , and there are exactly two faces f and g of τ hinging on e (Fig. 5.3). If $\mathbf{D}_{\tau g} = \mathbf{D}_{\tau f}$, their boundaries are oriented in such a way that e must run along one and counter the other, so $\mathbf{R}_{ge} = -\mathbf{R}_{fe}$, and the sum is zero. If $\mathbf{D}_{\tau g} = -\mathbf{D}_{\tau f}$, the opposite happens, $\mathbf{R}_{ge} = \mathbf{R}_{fe}$, with the same final result. The proof of $\mathbf{RG} = 0$ is similar. \diamond

¹¹Which doesn't require a *normal* vector, for any outgoing vector will do; cf. Fig. 5.2, middle.

Let us finally mention some facts about the dual mesh m^* of 4.1.2, obtained by barycentric subdivision and reassembly (although we shall not make use of it as such). Each dual cell s^* inherits from s an *outer* orientation (and hence, an inner one if space E_3 is oriented). Incidence relations between dual cells are described by the same matrices \mathbf{G} , \mathbf{R} , \mathbf{D} , only transposed: $\mathbf{R}_{f_e} \neq 0$, for instance, means that the bent edge f^* is part of the boundary of the skew face e^* (cf. Fig. 4.4), and so on.

5.2.2 Whitney elements

Now, we assign a function or a vector field to all simplices of the mesh. For definiteness, assume the usual orientation of space, although concepts and results do not actually depend on it.

For notational consistency, we make a change with respect to Chapter 3, which consists of denoting by w_n the continuous, piecewise affine function, equal to 1 at n and to 0 at other nodes, that was there called λ^n . The w stands for “Whitney”, and as we shall see, the hat function λ^n , now w_n , is the Whitney element of lowest “degree”, this word referring not to the degree of w_n as a polynomial, but to the dimension of the simplices it is associated with (the nodes). We shall have Whitney elements associated with edges, faces, and tetrahedra as well, and the notation for them, as uniform as we can manage, will be w_e , w_f , and w_T . Recall the identity

$$(8) \quad \sum_{n \in \mathcal{N}} w_n = 1$$

over D . We shall denote by W^0 the span of the w_n s (that was, in Chapter 3, space Φ_m). Finite-dimensional spaces W^p will presently be defined also, for $p = 1, 2, 3$. They all depend on m , and should therefore rather be denoted by $W^0(m)$, or W_m^0 , but the index m can safely be understood and is omitted in what follows.

Next, degree, 1. To edge $e = \{m, n\}$, let us associate the vector field

$$(9) \quad w_e = w_m \nabla w_n - w_n \nabla w_m$$

(cf. Fig. 5.4, left), and denote by W^1 the finite-dimensional space generated by the w_e s. Similarly, W^2 will be the span of the w_f s, one per face $f = \{\ell, m, n\}$, with

$$(10) \quad w_f = 2(w_\ell \nabla w_m \times \nabla w_n + w_m \nabla w_n \times \nabla w_\ell + w_n \nabla w_\ell \times \nabla w_m)$$

(cf. Fig. 5.4, right). Last, W^3 is generated by functions w_T , one for each

tetrahedron τ , equal to $1/\text{vol}(\tau)$ on τ and 0 elsewhere. (Its analytical expression in the style of (9) and (10), which one may guess as an exercise, is of little importance.)

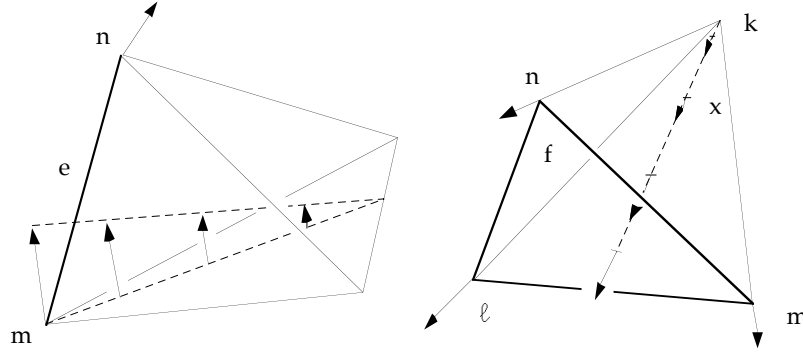


FIGURE 5.4. Left: The “edge element”, or Whitney element of degree 1 associated with edge $e = \{m, n\}$, here shown on a single tetrahedron with e as one of its edges. Right: The “face element”, or Whitney element of degree 2 associated with face $f = \{l, m, n\}$, here shown on a single tetrahedron with f as one of its faces. The arrows suggest how the vector fields w_e and w_f as defined in (9) and (10), behave. At point m on the left, for instance, $w_e = \nabla w_n$, after (9), and this vector is orthogonal to the face opposite m . At point m on the right, $w_f = \nabla w_n \times \nabla w_l$, after (10); this vector is orthogonal to both ∇w_n and ∇w_l , and hence parallel to the planes that support faces $\{l, m, k\}$ and $\{k, m, n\}$, that is, to their intersection, which is edge $\{k, m\}$.

Thus, to each simplex s is attached a field, scalar- or vector-valued. These fields are the Whitney elements. (The proper name is “Whitney forms” in the context in which they were introduced [Wh].) We’ll review their main properties, all easy to prove. First,

- The value of w_n at node n is 1 (and 0 at other nodes),
- The circulation of w_e along edge e is 1,
- The flux of w_f across face f is 1,
- The integral of w_τ over tetrahedron τ is 1,

(and also, in each case, 0 for other simplices).

For degree 0, we already knew that, and for degree 3, it is so by way of definition. Let us prove the point for degree 1, i.e., about the circulation of w_e . Since the tangent vector τ is equal to $mn/|mn|$, one has, with help of Lemma 4.1,

$$\int_e \tau \cdot (w_m \nabla w_n) = mn \cdot \nabla w_n (\int_e w_m) / |mn| = (\int_e w_m) / |mn|,$$

and hence

$$\int_e \tau \cdot w_e = \int_e \tau \cdot (w_m \nabla w_n - w_n \nabla w_m) = \int_e (w_m + w_n) / |mn| = 1,$$

since $w_m + w_n = 1$ on edge $\{m, n\}$.

The reader will easily treat the case of faces. (Doing Exercise 5.4 before may help.) Note the convoluted way in which *orientation* of the ambient space intervenes (in the definition of both the cross product and the crossing direction), without influencing the final result, in spite of what one may have feared.

Exercise 5.4. Review Exer. 3.9, showing that the volume of a tetrahedron $T = \{k, \ell, m, n\}$ is $\text{vol}(T) = 4 \int_T w_n$. Show that the area of face $\{k, \ell, m\}$ is $3 \text{vol}(T) |\nabla w_n|$, the length of vector $\{k, \ell\}$ is $6 \text{vol}(T) |\nabla w_m \times \nabla w_n|$, and that $6 \text{vol}(T) \det(\nabla w_k, \nabla w_\ell, \nabla w_m) = 1$.

Exercise 5.5. Compute $\int_T w_e \cdot w_{e'}$, according to the respective positions of edges e and e' , in terms of the scalar products $\nabla w_n \cdot \nabla w_m$.

Exercise 5.6. Show that field (9) is of the form $x \rightarrow a \times x + b$ in a given tetrahedron, where a and b are three-component vectors, vector a being parallel to the edge opposite $\{m, n\}$. Show that the field (10) is of the form $x \rightarrow \alpha x + b$ (where now $\alpha \in \mathbb{R}$).

A second group of properties concerns the continuity, or lack thereof, of the w 's across faces of the mesh. Function w_n is continuous. For the field w_e , it's more involved. Let us consider two tetrahedra with face $\{\ell, m, n\}$ in common, and let x be a point of this face. Then the vector field ∇w_n is not continuous at x , since w_n is not differentiable. But on the other hand, the tangential part (cf. Fig. 2.5) of ∇w_n on face $\{\ell, m, n\}$ changes in a continuous way when one crosses the face from one tetrahedron to its neighbor; indeed, it only depends on the values of w_n on this face, whatever the tetrahedron one considers. As this goes the same for ∇w_m , and for all faces of the mesh, one may conclude that the tangential part of w_e is continuous across faces. Similar reasoning shows that the *normal* part of w_f is continuous across faces. As for w_T , it is just discontinuous.

Thanks to these continuity properties, W^0 is contained in L^2_{grad} , W^1 in L^2_{rot} , and W^2 in L^2_{div} . The W^p are of finite dimension. They *can therefore play the role of Galerkin approximation spaces* for the latter functional spaces. We knew that as far as W^0 is concerned. For $p = 1$ or 2, however, this calls for an unconventional interpretation of the degrees of freedom. Take h in W^1 , for instance. Then, by definition,

$$(11) \quad h = \sum_{e \in \mathcal{E}} \mathbf{h}_e w_e,$$

where each \mathbf{h}_e (set in boldface) is a scalar coefficient. As the circulation of w_e is 1 along edge e and 0 along others, the circulation of h along edge e is the degree of freedom \mathbf{h}_e . So the DoFs are associated with *edges* of the mesh, not with *nodes*, which is the main novelty with respect to classical finite elements. In the same way, if $b \in W^2$, one has $b = \sum_{f \in \mathcal{F}} \mathbf{b}_f w_f$ and the \mathbf{b}_f s are the fluxes of b through faces. So in this case, degrees of freedom sit at faces. Last, there is one DoF for each tetrahedron in the case of functions belonging to W^3 .

Remark 5.4. So the w_e s (as well as other Whitney elements) are linearly independent, for $h = 0$ in (11) implies $\mathbf{h}_e = 0$ for all e (cf. Exer. 3.8). \diamond

The convergence properties of Whitney elements are quite similar to those we already know as regards W^0 . Let φ be a smooth function, and set $\varphi_m = \sum_{n \in \mathcal{N}} \varphi_n w_n$, where φ_n is the value of φ at node n . (This is the m -interpolate of Subsection 4.3.1, with adapted notation.) When the mesh is refined, so that the grain tends to zero, while avoiding “asymptotic flattening” of the simplices, φ_m converges towards φ in $L^2_{\text{grad}}(D)$, as we proved in Chapter 4. In the same way, if h is a smooth vector field, if \mathbf{h}_e is the circulation of h along edge e , and if one sets $\mathbf{h}_m = \mathbf{r}_m h = \sum_{e \in \mathcal{E}} \mathbf{h}_e w_e$, then \mathbf{h}_m converges to h in $\mathbb{L}^2_{\text{rot}}(D)$. Same thing for $\mathbf{b}_m = \sum_{f \in \mathcal{F}} \mathbf{b}_f w_f$, where \mathbf{b}_f is the flux of b through f , with convergence with respect to the norm of $\mathbb{L}^2_{\text{div}}(D)$. See [Do] for proofs.

5.2.3 Combinatorial properties of the complex

The properties we have noticed (nature of the degrees of freedom, continuity, convergence) concerned spaces W^p as taken one by one, for different values of p . But there is more: properties of the structure made by all the W^p s when taken together, or “Whitney complex”, which are even more remarkable. These structural properties are what makes possible a discretization of the structure of Fig. 5.1 as a whole. First:

Proposition 5.4. *The following inclusions hold:*

$$(12) \quad \text{grad}(W^0) \subset W^1, \quad \text{rot}(W^1) \subset W^2, \quad \text{div}(W^2) \subset W^3.$$

Proof. Let us consider node m . If $\mathbf{G}_{e_n} \neq 0$, either $e = \{m, n\}$ or $e = \{n, m\}$, but in both cases, $\mathbf{G}_{e_m} w_e = w_n \nabla w_m - w_m \nabla w_n$ by definition of the incidence numbers \mathbf{G}_{e_n} . Therefore,

$$\begin{aligned}\sum_{e \in \mathcal{E}} \mathbf{G}_e \mathbf{w}_e &= \sum_{n \in \mathcal{N}} (\mathbf{w}_n \nabla \mathbf{w}_m - \mathbf{w}_m \nabla \mathbf{w}_n) \\ &= (\sum_{n \in \mathcal{N}} \mathbf{w}_n) \nabla \mathbf{w}_m - \mathbf{w}_m \nabla (\sum_{n \in \mathcal{N}} \mathbf{w}_n) \equiv \nabla \mathbf{w}_m\end{aligned}$$

since $\sum_{n \in \mathcal{N}} \mathbf{w}_n \equiv 1$, hence $\text{grad } \mathbf{w}_m \in W^1$, and hence the first inclusion by linearity. Similarly, for $e = \{m, n\}$, one has $\text{rot } \mathbf{w}_e = 2 \nabla \mathbf{w}_m \times \nabla \mathbf{w}_n = \sum_{f \in \mathcal{F}} \mathbf{R}_{fe} \mathbf{w}_f$, hence $\text{rot } \mathbf{w}_e \in W^2$, and $\text{div } \mathbf{w}_f = \sum_{T \in \mathcal{T}} \mathbf{D}_{Tf} \mathbf{w}_T$, that is to say, $\text{div } \mathbf{w}_f \in W^3$ (**Exercise 5.7**: prove all this). Hence (12). \diamond

This result has the following important implication. If one sets $\mathbf{h} = \text{grad } \varphi$, where $\varphi = \sum_{n \in \mathcal{N}} \varphi_n \mathbf{w}_n$ is an element of W^0 , this field \mathbf{h} can also be expressed as in (11), the edge DoF being $\mathbf{h}_{[m,n]} = \varphi_n - \varphi_m$. Let \mathbf{h} be the vector of the \mathbf{h}_e s (of length E , the number of edges), and $\boldsymbol{\varphi}$ the vector of the φ_n s (of length N , the number of nodes). Then $\mathbf{h} = \mathbf{G}\boldsymbol{\varphi}$, where \mathbf{G} is the above $E \times N$ incidence matrix, which thus appears as a discrete analogue of the gradient operator, via the correspondence between the potential φ [resp. the field \mathbf{h}] and the associated **vector**¹² of DoFs $\boldsymbol{\varphi}$ [resp. \mathbf{h}].

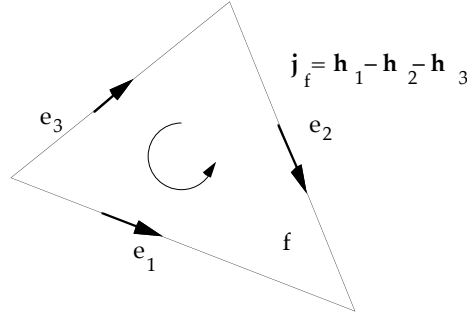


FIGURE 5.5. Computing \mathbf{j}_f (flux through face f of field $\mathbf{j} = \text{rot } \mathbf{h}$), from the DoFs of \mathbf{h} . Here, \mathbf{h}_i is the circulation of \mathbf{h} along edge e_i , the orientation of the e_i s with respect to f is indicated by the arrows, and the terms of the incidence matrix \mathbf{R} are $\mathbf{R}_{fe1} = 1$, $\mathbf{R}_{fe2} = \mathbf{R}_{fe3} = -1$.

Similarly (Fig. 5.5), if $\mathbf{h} = \sum_{e \in \mathcal{E}} \mathbf{h}_e \mathbf{w}_e$, then $\mathbf{j} \equiv \text{rot } \mathbf{h} = \sum_{f \in \mathcal{F}} \mathbf{j}_f \mathbf{w}_f$, where the \mathbf{j}_f s form the components of **vector** $\mathbf{j} = \mathbf{R}\mathbf{h}$, of dimension F (the number of faces). Last, one has $\text{div } \mathbf{b} = \sum_{T \in \mathcal{T}} \boldsymbol{\psi}_T \mathbf{w}_T$, where $\boldsymbol{\psi} = \mathbf{D}\mathbf{b}$, when $\mathbf{b} = \sum_{f \in \mathcal{F}} \mathbf{b}_f \mathbf{w}_f$. Matrices \mathbf{R} and \mathbf{D} , of respective dimensions $F \times E$ and $T \times F$ (where T is the number of tetrahedra), thus correspond to the curl and the divergence. We now understand the equalities $\mathbf{D}\mathbf{R} = 0$ and $\mathbf{R}\mathbf{G} = 0$: They are the discrete counterparts of the differential relations $\text{div}(\text{rot } \cdot) = 0$ and $\text{rot}(\text{grad } \cdot) = 0$.

¹²See A.2.2 about this use of boldface for DoF-vectors. This is only an attention-catching device, which will not be used throughout.

We'll denote by W^p , $p=0$ to 3 , the spaces $\mathbb{R}^{\mathcal{N}}, \mathbb{R}^{\mathcal{E}}, \mathbb{R}^{\mathcal{F}}, \mathbb{R}^{\mathcal{T}}$, isomorphic to the Cartesian products $\mathbb{R}^{\mathcal{N}}, \mathbb{R}^{\mathcal{E}}$, etc. These spaces are isomorphic, for a given m , to the W_m^p , but conceptually distinct from them. We can summarize all our findings by the following sketch, called a *commutative diagram*,¹³ which describes the structure of Whitney element spaces:

$$(13) \quad \begin{array}{ccccccc} & \text{grad} & & \text{rot} & & \text{div} & \\ W^0 & \rightarrow & W^1 & \rightarrow & W^2 & \rightarrow & W^3 \\ | & & | & & | & & | \\ W^0 & \rightarrow & W^1 & \rightarrow & W^2 & \rightarrow & W^3 \\ & \mathbf{G} & & \mathbf{R} & & \mathbf{D} & \end{array} .$$

Graphic conventions should be obvious, once it is understood that vertical arrows denote isomorphisms.

Whether the top and bottom sequences in (13) are exact is then a natural question. The answer depends on the topology of D .

Proposition 5.5. *If the set-union of all tetrahedra in the mesh is contractible, one has the following identities:*

$$W^1 \cap \ker(\text{rot}) = \text{grad } W^0, \quad W^2 \cap \ker(\text{div}) = \text{rot } W^1,$$

in addition to (12).

Proof. Let h be an element of W^1 such that $\text{rot } h = 0$. Then (D being simply connected) there exists a function φ such that $h = \text{grad } \varphi$. The φ_n s being the values of φ at nodes, let us form $k = \text{grad}(\sum_{n \in \mathcal{N}} \varphi_n w_n)$. Then $k \in W^1$ by the first inclusion of Prop. 5.4, and its DoFs are those of h by construction, so $h = k \in \text{grad } W^0$. As for the second equality, take an element b of W^2 such that $\text{div } b = 0$. There exists¹⁴ a vector field a such that $b = \text{rot } a$. The a_e s being the circulations of a along the edges, let us form $c = \text{rot}(\sum_{e \in \mathcal{E}} a_e w_e)$. Then $c \in W^2$ by the second inclusion, and its DoFs are those of b by construction, hence $b = c \in \text{rot } W^1$. \diamond

¹³In practice, it means that, by following a path on the diagram, and by composing the operators encountered along the way, the operator thus obtained depends only on the points of departure and arrival. Allowed paths are along the arrows (in the direction indicated) and along unarrowed segments (in both directions).

¹⁴Beware, “ D simply connected” is not enough for that, and the hypothesis “ S connected” cannot be forgotten. For instance, if $D = \{x \in E_3 : 1 < |x| < 2\}$, the field $\text{grad}(x \rightarrow 1/|x|)$ is divergence-free, since the function $x \rightarrow 1/|x|$ is harmonic, but is not a curl, since its flux across the closed surface $\{x : |x| = 1\}$ does not vanish.

So the image fills the kernel at both middle positions of diagram (13) if D is topologically trivial, i.e., contractible. But things are more interesting the other way around, for if the sequences in (13) *fail* to be exact at one of these positions or both, this tells something about the topology of D . For instance, the existence of curl-free fields that are not gradients implies the presence of one or more “loops” in the domain (as for a torus, which has one such loop). Solenoidal fields which are not curls can’t exist unless there is a “hole”, as when D is the volume between two nested spheres. The sequences are thus an algebraic tool by which the topology of D can be explored (and this of course was Whitney’s concern). Although topological difficulties are avoided in this book as a rule, the reader may be interested by the information on all this contained in the next subsection.

The main interest of the Whitney complex from our point of view lies elsewhere, however. Propositions 5.4 and 5.5 justify the replacement of each pillar of Maxwell’s house, Fig. 5.1, by one of the isomorphic sequences of (13). Hence, for a given mesh, a “discrete” building, or “Maxwell–Whitney house”, in which we’ll try to embed any problem at hand, thus obtaining a modelling in finite terms. It is already clear that the two “vertical” equations, $-\partial_t \mathbf{d} + \text{rot } \mathbf{h} = \mathbf{j}$ and $\partial_t \mathbf{b} + \text{rot } \mathbf{e} = 0$, will be discretized as $-\partial_t \mathbf{d} + \mathbf{R} \mathbf{h} = \mathbf{j}$ and $\partial_t \mathbf{b} + \mathbf{R} \mathbf{e} = 0$. The difficulty, therefore, lies in the discretization of the constitutive laws. This will be our main concern in Chapters 6 to 9.

5.2.4 Topological properties of the complex

(This subsection is independent, and can be skipped.) In the case of a contractible domain, we just proved the sequence

$$\{0\} \rightarrow W^0 \xrightarrow{\text{grad}} W^1 \xrightarrow{\text{rot}} W^2 \xrightarrow{\text{div}} W^3 \rightarrow \{0\}$$

exact at all levels except 0. As we knew beforehand, the following sequence has the same property, in the case of a regular bounded domain:

$$(14) \quad \{0\} \rightarrow L_{\text{grad}}^2 \xrightarrow{\text{grad}} \mathbb{L}_{\text{rot}}^2 \xrightarrow{\text{rot}} \mathbb{L}_{\text{div}}^2 \xrightarrow{\text{div}} L^2 \rightarrow \{0\}.$$

This is no coincidence, as we shall verify for two particular cases where D is not contractible.

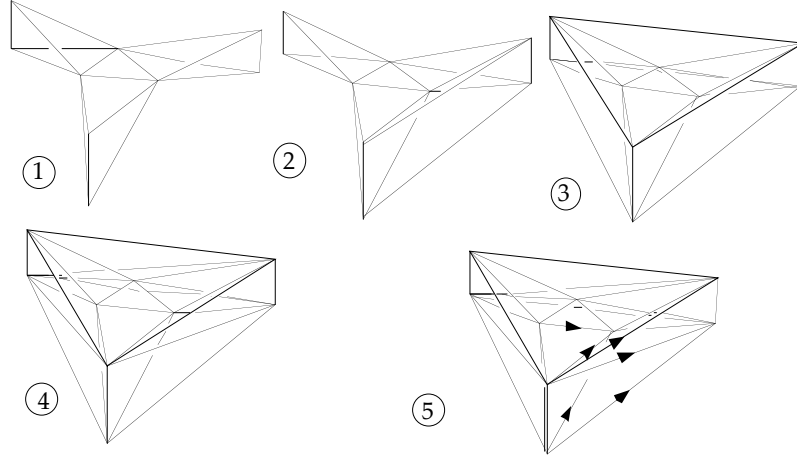


FIGURE 5.6. Steps in the construction of a “simplicial torus”: Join three tetrahedra around a triangle (1), add a pyramid (2), then two others (3), in order to form a solid ring, then cut each pyramid in two tetrahedra (4). The toric polyhedron thus obtained comprises 9 tetrahedra, 27 faces, 27 edges, and 9 vertices ($\chi = 0$). In (5), how to assign DoFs to edges in order to get a curl-free field in W^1 which is not a gradient.

Let's first consider the case of the mesh¹⁵ of a torus, Fig. 5.6. Let us assign the DoF $\mathbf{h}_e = 0$ to all edges, except the six shown in Fig. 5.6, for which $\mathbf{h}_e = 1$ (the arrows mark orientation). One obtains this way an element \mathbf{h} of W^1 which is curl-free (this can be checked by summing the \mathbf{h}_e s along the perimeters of all faces, hence $\mathbf{R}\mathbf{h} = 0$), but is certainly not a gradient, since its circulation does not vanish along some closed circuits, such as the one formed by the boundary of the empty central triangle, for instance.

So $\text{grad } W^0$ is strictly contained in $\ker(\text{rot} ; W^1)$. The quotient¹⁶ $\ker(\text{rot} ; W^1) / \text{grad}(W^0)$ then does not reduce to 0, and it's easy to see its dimension is 1 in the present case. In the general case, this dimension is called the *Betti number of dimension 1* of the mesh. This number measures the lack of exactitude at level 1 of the Whitney sequence. Let's denote it $b_1(m)$, or just b_1 .

Now, if one considers the sequence (14) relative to this toric volume, one sees the same lack of exactitude. Indeed, curl-free fields in this torus which are not gradients can all be obtained by adding some gradient to a

¹⁵A very coarse mesh, but this doesn't matter: Properties proved this way are mesh-independent.

¹⁶This notion is discussed in A.1.6 and A.2.2.

multiple of the just constructed special field. The dimension of the quotient $\ker(\text{rot} ; \mathbb{L}_{\text{rot}}^2) / \text{grad}(\mathbb{L}_{\text{grad}}^2)$ is therefore equal to 1.

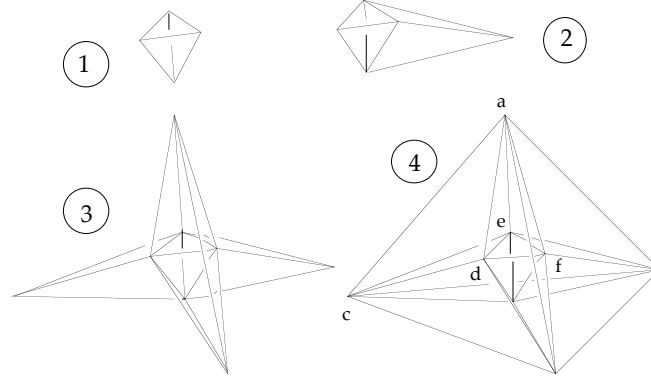


FIGURE 5.7. Steps in the construction of a “hollow tetrahedron”: To the faces of a regular tetrahedron (1), stick four tetrahedral spikes (2–3), then six tetrahedra that share an edge with the central one (4), and finally the four tetrahedra necessary to fill up the flanks. Remove the central tetrahedron. The hollow solid that remains comprises 14 tetrahedra, 32 faces, 24 edges, and 8 vertices ($\chi = 2$).

A similar phenomenon can be observed in the case of the hollow tetrahedron of Fig. 5.7. By assigning the DoF 0 to all faces except $\{a, c, e\}$, $\{a, d, e\}$, and $\{d, e, f\}$, which are given the DoF 1, one obtains a solenoidal field \mathbf{b} in W^2 (add fluxes through faces for all tetrahedra, hence $\mathbf{D}\mathbf{b} = 0$), but not the curl of any field, since its flux through some closed surfaces, such as for instance the boundary of the inner tetrahedron, does not vanish. This time, $\text{rot } W^1$ is strictly contained in $\ker(\text{div} ; W^2)$, and the dimension of the quotient $\ker(\text{div} ; W^2) / \text{rot}(W^1)$ is 1. In the general case, this dimension is called the *Betti number of dimension 2* of the mesh (denoted b_2) and measures the lack of exactitude of the sequence at level 2.

These departures from exactitude thus appear as *global topological properties* of the meshed domain. From what precedes, one can guess that the Betti numbers b_1 and b_2 are respectively the numbers of “loops” and “holes” in D , and do not depend on the mesh. The foregoing observations thus suggest that the Whitney sequence is a tool of algebraic and combinatorial nature that is able to convey topological information.

Indeed, this sequence is one of the constructions of *algebraic topology*, the part of mathematics that is concerned with associating algebraic objects (invariant by homeomorphism) to topological spaces, in order to study topology by the methods of algebra. Thus, for instance, what we said

about loops and holes actually goes the other way: These intuitive notions receive a proper definition by considering basis elements of some quotient spaces, the dimensions of which are the Betti numbers, as in the two foregoing examples. Algebraic topology offers several constructions of this kind. One is *homology*, which we used extensively up to now without being formal about it (but see next subsection). Another is *cohomology*, which roughly speaking consists in setting up sequences similar to (13) or (14). For instance, the grad-rot-div sequence is the three-dimensional case of *de Rham's cohomology* (for which, as we saw, it's unimportant whether strong or weak operators are meant, at least for regular bounded domains). The Whitney sequence thus appears as a kind of *discretized cohomology*, lending itself to (combinatorial) computations, a definite advantage over de Rham's one, and this is why it was developed [Wh].

Though following this direction would be of the utmost interest, this is not the place, and anyway, the only result of topology we really need is the following one. Having defined the Betti numbers by $b_p = \dim(\ker(d; W^p)/dW^{p-1})$, $p = 1$ to 3 , where d stands for grad, rot, div, according to the value of p , and b_0 as the dimension of the kernel $\ker(\text{grad})$ in W^0 (equal to the number of connected components of D), one proves these numbers are *topological invariants*, meaning they depend on D up to homeomorphism, but not on the mesh. The integer $\chi = b_0 - b_1 + b_2 - b_3$ is called the *Euler-Poincaré constant* of the domain. By the very definition of the b_p s, one has the already met *Euler-Poincaré formula*:

$$(15) \quad N - E + F - T = \chi(D),$$

where N, E, F, T are the numbers of simplices of all kinds, as previously defined. The constant χ is typically equal to $0, 1$ or 2 (cf. Figs. 5.6 and 5.7). When the meshed region is bounded and contractible, $\chi = 1$. A similar formula holds of course in all dimensions (we had use for the two-dimensional one already), and not only for domains of E_d , but for all topological spaces that admit of simplicial meshes.

Exercise 5.8. In dimension 2, prove by direct counting that $N - E + F$ is the same for meshes m and $m/2$ (Subsection 4.1.2).

5.2.5 Metric properties of the complex

All that precedes was of *combinatorial* character. Matrices $\mathbf{G}, \mathbf{R}, \mathbf{D}$ encompass all the knowledge on the topology of the mesh, but say nothing of *metric* properties: lengths, angles, areas, etc. To take these into account, we introduce the following “mass matrices”.

Let α be a function over D , strictly positive. (For our needs here, it will be one of the coefficients ε , μ , etc., or its inverse.) We denote by $\mathbf{M}_p(\alpha)$, $p = 0, 1, 2, 3$, the square matrices of size $N \times N$, $E \times E$, $F \times F$, $T \times T$, whose entries are

$$(16) \quad (\mathbf{M}_p(\alpha))_{s s'} = \int_D \alpha w_s \cdot w_{s'} \quad \text{if } p = 1 \text{ or } 2, \\ = \int_D \alpha w_s w_{s'} \quad \text{if } p = 0 \text{ or } 3,$$

where s and s' are two simplices of dimension p . The \mathbf{M}_p s are called *mass matrices* because one of them (\mathbf{M}_1) is found in the same position as the mass matrix of a vibrating mechanical system when one sets up the numerical scheme for computing the modes of a resonating cavity, as we'll see in Chapter 9.

Note that in the first line, the coefficient α can be replaced by a symmetrical tensor of Cartesian components α_{ij} :

$$(\mathbf{M}_p(\alpha))_{s s'} = \int_D \sum_{i,j=1,2,3} \alpha_{ij} w_s^i w_{s'}^j.$$

This makes possible the consideration of *anisotropic* materials.

5.3 TREES AND COTREES

In the practice of computation, the need arises to sort out the curl-free fields among fields in W^1 and (though less often) the solenoidal fields among fields in W^2 .

Why is that a problem? Aren't curl-free fields sufficiently characterized, in terms of the DoF vector \mathbf{h} , by $\mathbf{R}\mathbf{h} = 0$? They are, but this is an *implicit* characterization, by algebraic constraints on \mathbf{h} . That such vectors be of the form $\mathbf{h} = \mathbf{G}\boldsymbol{\varphi}$, at least in the contractible case, often helps, because there are no constraints on $\boldsymbol{\varphi}$. (It *did* help in Chapters 2 and 3, where we treated the equation $\text{rot } \mathbf{h} = 0$ by the introduction of a magnetic potential.) But one may ask for more and better: an *explicit* representation of the subspace $\{\mathbf{h} \in W^1 : \mathbf{R}\mathbf{h} = 0\}$ by way of a *basis* for it, that is, some family $\{\mathbf{h}^1, \mathbf{h}^2, \dots, \mathbf{h}^{N-1}\}$ of independent DoF vectors¹⁷ that would generate $\ker(\mathbf{R})$. A similar problem arises in relation with gauging: One may wish to select a basis of independent vectors $\{\mathbf{a}^1, \dots, \mathbf{a}^A\}$ in W^1 the span of which is the codomain $\mathbf{R}W^1$ (equal to $\{\mathbf{b} \in W^2 : \mathbf{D}\mathbf{b} = 0\}$ in the contractible

¹⁷It should be clear that their number will be $N - 1$ (where N is the number of nodes), in the contractible case.

case), for this singles out a unique $\mathbf{a} \in W^1$ such that $\mathbf{b} = \text{rot } \mathbf{a}$, given a solenoidal \mathbf{b} in W^2 . This is what “trees” and “cotrees” are about.

Exercise 5.9. Show that, if D is contractible, the dimension A of $\ker(\mathbf{D})$ is $E - N + 1$.

In Chapters 6 and 8, and in Appendix C, we shall have several examples of use of such techniques, which are popular nowadays [AR, Fu, GT, Ke, PR, RR, T&, . . .]. Alas, due to their origins in circuit-graphs theory [Ha], their intimate connection with *homology* is generally overlooked, which is a pity. So this may be the right time to disclose a few elements of homology, at least those necessary to understand trees and cotrees.

5.3.1 Homology

The basic concept is that of “chain”. Call S_p the sets of p -simplices of the mesh. A p -chain \mathbf{c} is then simply the assignment to each $s \in S_p$ of a number \mathbf{c}_s , i.e., a family of numbers indexed on S_p . This is conveniently denoted by $\mathbf{c} = \sum_{s \in S_p} \mathbf{c}_s s$. (Note, as usual, the one-to-one correspondence between the chain \mathbf{c} and the **vector** $\mathbf{c} = \{\mathbf{c}_s : s \in S_p\}$.)

This may sound more abstract than it really is: Think for instance—in connection with our model problem—about a path of edges of the mesh, going from S_0^h to S_1^h . It’s an oriented line, so each edge runs either “along” or “counter” this orientation (cf. p. 137), hence a number $\mathbf{c}_e = \pm 1$ for each edge of the path. Assigning the number 0 to all other edges of the mesh, we do have a 1-chain. This makes precise the fuzzy notion of “circuit” by which, obviously, we mean more than the supporting line: A circuit is a line *plus* a way to run along it; so when the line is made of oriented edges, we need to tell the proper direction along each edge, which is precisely what the chain coefficients do.

In dimension 2, the concept is just as useful to make precise the notion of “polyhedral surface composed of faces of the mesh” that we repeatedly invoked. (Think about it.) What we had to call up to now, in a rather clumsy way, m^* -lines and m^* -surfaces, are just chains over the *dual* simplices, with $p = 1$ or 2.

Note that chains encompass more than that. Rendering the concept of a circuit “run k times”, for instance, is obvious: a 1-chain with coefficients $\pm k$. A collection of m -paths (“open circuits” composed of edges of the mesh), not necessarily connected, also is a chain, and so on. Non-integer coefficients make less intuitive sense, of course (although one can think of various useful interpretations in electromagnetism). Indeed, there are several versions of homology, depending on which kind of numbers the coefficients \mathbf{c}_s are allowed to be. Most often, they are taken as relative

integers. But there is some gain in simplicity in assuming real-valued coefficients, as we shall do here.

One can add chains ($c + c'$ is the chain $\sum_{s \in S} (c_s + c'_s) s$) and multiply a chain by a scalar. The set of all p -chains, that we shall denote by¹⁸ $W_p(D)$, is thus a vector space.¹⁹

Next concept: The *boundary* operator ∂ . This is a linear map, which assigns a $(p - 1)$ -chain ∂c to any p -chain c . By linearity, $\partial c \equiv \partial(\sum_{s \in S} c_s s) = \sum_{s \in S} c_s \partial s$. To fully specify ∂ , therefore, we need only state what the boundary ∂s is for any single simplex s . By definition,

$$\partial e = \sum_{n \in N} G_{en} n, \quad \partial f = \sum_{e \in E} R_{fe} e, \quad \partial T = \sum_{f \in F} D_{Tf} f.$$

This makes perfect sense: The boundary of $e = \{m, n\}$, for instance, is thus the chain $n - m$ (assuming all nodes have orientation $+1$), or if one prefers, the 0 -chain c with $c_n = 1$, $c_m = -1$, and $c_k = 0$ for other nodes. The ∂ of a 0 -chain we can define for thoroughness as a special (and unique) “ (-1) -chain” denoted 0 . (It doesn’t matter much.) Be aware that a boundary is more than the topological boundary, just as a chain is more than the set-union of simplices supporting it.

We’ll say a chain c is *closed* if $\partial c = 0$. (One often says, a bit improperly, that its boundary is “empty”.) Closed chains are rather called *cycles*, in standard texts, but the word “closed” is convenient to make contact with our observations of Chapter 4 (cf. Fig. 4.6). Notice that ∂ is represented by a matrix: G^t, R^t, D^t , depending on the dimension p . Observe also how the contents of Proposition 5.3 (cf. Fig. 5.3) can now elegantly be summarized: $\partial\partial = 0$, “the boundary of a boundary is empty”.

A p -chain c is a *boundary* if there is a $(p + 1)$ -chain γ such that $c = \partial\gamma$. Boundaries are cycles, of course. But not all cycles are boundaries . . . and from there we might go into topology again. See a specialized book (e.g., [HW]) for the way Betti numbers can be redefined, as dimensions of the quotients²⁰ $\ker(\partial; W_p)/\partial W_{p+1}$. That this technique and the foregoing

¹⁸It should rather be $W_p(S_p(D))$, where $S_p(D)$ denotes the set of p -simplices of the mesh m of D , but this is too heavy notation, and I hope the few abuses of this kind that follow will be harmless.

¹⁹If the case of \mathbb{Z} -valued chain-coefficients, $W_p(D)$, more classically denoted by $C_p(D)$ in algebraic topology, is only what algebraists call a *module* (the structure which is to a ring, here \mathbb{Z} , what a vector space is to a field).

²⁰Two p -chains c and c' are *homologous* modulo Δ if $\partial(c - c')$ is a chain on Δ , i.e., $\partial(c - c') \in W_p(\Delta)$. The classes of this equivalence relation are called [relative] *homology classes* mod Δ . These are the formal definitions of the notions evoked in Exercises 2.5 and 2.6, at least for paths and surfaces made of simplices of the mesh. (Lifting this restriction is not difficult; this is the concern of *singular homology* [GH].)

one, based on Whitney fields and the d operator, thus yield the same topological information, is one of the great *duality* features of algebraic topology. Rather than being formal about that, let's just point to the following fact: fields and 1-chains of W^1 and W_1 are in duality via the formula

$$(17) \quad \langle h, c \rangle = \sum_{e \in \mathcal{E}} h_e c_e = (h, c),$$

which stems from the basic property of edge elements, $\int_e \tau \cdot w_e = \delta_{e\tau}$. (Observe how (17) generalizes the concept of circulation of h along a path c .) What is meant by “in duality” is that $\langle h, c \rangle = 0 \quad \forall c$ implies $h = 0$ and the other way around. One should understand from this how the concepts of “curl-free field which is not a gradient” and “1-cycle which is not a 1-boundary” are dual, and be able to generalize to $p > 1$. It's also illuminating to think of the Stokes theorem as the statement $\langle dh, c \rangle = \langle h, \partial c \rangle$ for all $h \in W^p$ and $c \in W_{p+1}$, and to remark that the matrix representations of d and ∂ are transposed of each other. The duality (17) is also the key to an explanation of *why* the Whitney elements have the form they have ((9) and (10)); see [B1] on this.

To be really useful, all these notions need to be “relativized”, the same concepts being redefined “modulo something”, as follows. Suppose our simplices are those of the mesh of a domain D , and let Δ be a closed part of D which is itself a union of simplices of the mesh. (Often, Δ will be the surface of the domain, or a part of it, but it's not the only possibility; Δ might correspond, in some magnetostatics problems, to regions inside D occupied by bodies of high permeability, taken as infinite in the modelling.) Let us denote by $W_p(\Delta)$ the set of chains over Δ : all p -chains over D whose coefficients are all 0, except for p -simplices belonging to Δ . Now we say that a chain $c \in W_p(D)$ is *closed mod Δ* if $\partial c \in W_p(\Delta)$. A p -chain c *bounds mod Δ* if there exists a $(p+1)$ -chain γ such that $c - \partial\gamma \in W_p(\Delta)$. (Rather than puzzling over these definitions, look again at Fig. 4.6, take Δ as S^b or S^h as the case may be, and imagine the various paths and surfaces as made of edges and faces of the mesh.) Chains closed mod Δ , or boundaries mod Δ , are also called *relative cycles* or *boundaries* (meaning, relative to Δ).

5.3.2 Trees, co-edges

Now we have enough to introduce trees. To well understand the two definitions that follow, ignore the bracketed parts first, then think again about the “relative” version:

Definition 5.1. A set S^T of p -simplices of the mesh m such that $W_p(S^T)$ does not contain any cycle $[\text{mod } \Delta]$, except the null one, is called a tree of dimension p , or p -tree $[\text{mod } \Delta]$.

Definition 5.2. A p -tree is a spanning tree $[\text{mod } \Delta]$ if there is no strictly larger p -tree $[\text{mod } \Delta]$ containing it. The set of all left-over simplices [not belonging to Δ] is called the associated tree complement $[\text{mod } \Delta]$, or cotree $[\text{mod } \Delta]$. Its elements are the co-simplices with respect to this tree.

To grasp this, take $p = 1$ and an empty Δ . Then $\partial c = 0$ means that vector $G^t c$, of length N , which is a linear combination of rows of the matrix G , vanishes. Algebraically, therefore, extracting a spanning tree is equivalent to finding a maximal set of independent rows of G (or R , or D), which amounts to looking for a submatrix of maximal rank²¹—a standard problem in linear algebra, all the more easy than matrix entries are integers. When $\Delta \neq \emptyset$, relative trees are obtained by the same procedure, but after removal of all rows and columns corresponding to simplices that belong to Δ .

Other rows, those corresponding to co-edges, are thus expressible as linear combinations of the previous ones, and form a basis for $\ker(G^t)$. Co-edges thus furnish a basis for 1-cycles, in the sense that, given a co-edge e , there is a unique way to assign an integer c_ε to each edge ε of the tree in order to get a closed 1-chain: $\partial(e + \sum_{\varepsilon \in \mathcal{E}^T} c_\varepsilon \varepsilon) = 0$, where \mathcal{E}^T denotes the set of tree edges. In less formal language, one says that each co-edge “closes a circuit” in conjunction with edges of the tree.

In the general case $\Delta \neq \emptyset$, we have only $\partial(e + \sum_{\varepsilon \in \mathcal{E}^T} c_\varepsilon \varepsilon) \in W_0(\Delta)$, still with uniqueness of the c_ε s. In words, the co-edge e closes a circuit, in conjunction with edges of the tree, if passage through Δ is allowed. (The part of the circuit within Δ is not uniquely determined.)

Figure 5.8, which shows a spanning tree in a two-dimensional mesh, relative to a part of it, should help understand all this. Three kinds of co-edges are shown, each with its associated circuit. For co-edges like a , the circuit doesn’t pass through Δ , contrary to what happens for co-edges of the same type as b . Co-edges like c are special in that the cycles they generate do not bound, which reveals the existence of a loop in the meshed region. (All of this is valid in three dimensions, too.)

These notions, here explained for $p = 1$, have obvious counterparts for all simplex dimensions. For $p = 2$, a tree would be a maximal set of faces that doesn’t generate closed surfaces (2-cycles). Again, any extra face

²¹And hence, spanning the same range as the original matrix. We’ll return to the graph-theoretical origin of the expression “spanning tree” in a moment.

would generate one, and this surface may not bound, owing to the presence of a hole in D .

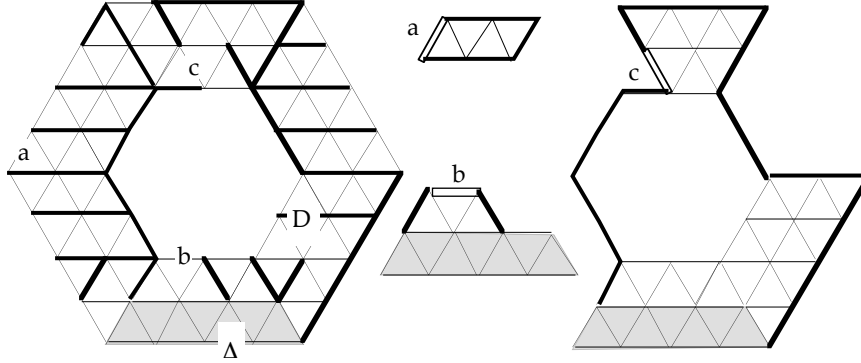


FIGURE 5.8. Notions of relative tree and co-edge. The tree on the left, with thick edges, is relative to the shaded region, Δ . On the right, closed chains $\text{mod } \Delta$ generated by three typical co-edges a , b , c .

How to *use* trees and cotrees will be explained by way of examples in Chapter 8 and Appendix C, but a few general indications can be given at this stage.

Suppose D contractible, and let \mathcal{E}^T be a spanning tree of edges. For each co-edge e , let us build a DoF-vector \mathbf{a}^e by setting $\mathbf{a}^e_\varepsilon = 0$ for all edges $\varepsilon \neq e$ and $\mathbf{a}^e_e = 1$. These (independent) **vectors** form a basis for $\ker(\mathbf{G}^d)$. We know already what $\mathbf{G}^d \mathbf{a}^e = 0$ means for the corresponding vector fields $\mathbf{a}^e \in W^1$: m -weak sinusoidality. So this is a kind of “discrete Coulomb gauge” imposed on the vector fields $\{\mathbf{a}^e : e \in \mathcal{E} - \mathcal{E}^T\}$, the curls of which will span $\ker(\text{div} ; W^2)$. On the other hand, thanks to the general algebraic relation $W^1 = \text{cod}(\mathbf{G}) \oplus \ker(\mathbf{G}^d)$ (cf. Appendix B), the DoF-vectors \mathbf{h}^e such that $\mathbf{h}^e_\varepsilon = 0$ for all edges $\varepsilon \neq e$ and $\mathbf{h}^e_e = 1$ form a basis for $\mathbf{G}W^0$, and hence the corresponding vector fields form a basis for $\text{grad } W^0$. Spanning trees of edges thus resolve the two problems mentioned at the beginning of this section.

In the general case, however, this will not work satisfactorily: We may not get enough \mathbf{h}^e s to span $\ker(\text{rot})$, if there exist curl-free fields which are not gradients, and too many \mathbf{a}^e s, for there can exist nonzero fields in W^1 which are simultaneously curl-free and m -weakly sinusoidal. Providing a solution to this problem in its full generality exceeds the scope of this book, but what to do is intuitively obvious. Look at Fig. 5.8. To obtain all curl-free fields, one should add to the tree *one* (because there is one loop in this case) of the co-edges of the same class as c , the circuit of

which doesn't bound. The augmented tree we get this way can be called²² a "belted tree", the "belt" being this non-bounding circuit,²³ and the loop co-edge acting as the belt "fastener". Note that, thanks to this added edge, the circuits of all remaining co-edges do bound. (The circuits of other co-edges homologous to c pass by the belt fastener.)

5.3.3 Trees and graphs

If $p = 1$, and if Δ is empty, we may consider nodes and edges as forming a graph; a spanning tree then appears to be a maximal subgraph "without loops". (As one easily sees, maximality implies that such a tree must "visit" all nodes, hence "spanning".) But the distinction between closed chains and boundaries is lost in the graph-theoretic context, so there is no straightforward way to build a belted tree via graph-oriented algorithms, whereas this problem is easily solved in algebraic terms. In the case of edges, for example, the belted tree corresponds to a basis of $\text{cod}(\mathbf{R}^t)$, and the tree to a basis of $\text{ker}(\mathbf{G}^t)$, which both are found by the same kind of algebraic manipulations (extract a matrix of maximal rank).

The other case where graphs are relevant is when $p = d - 1$, where d is the dimension of space. For instance, if $d = 3$, a spanning tree of faces, in the sense of Def. 5.2, can be described as a spanning tree of the graph the nodes of which are tetrahedra (beware!), and the arrows, the faces of the mesh. This is easy to understand, by duality, for this graph is nothing else than the standard nodes-to-edges graph of the *dual* mesh, the incidence matrix of which is \mathbf{D}^t . Otherwise, the case $1 < p < d - 1$ is not explainable in terms of graphs.²⁴

However, $d = 2$ in many applications, which partly explains why the irrelevance of graph theory may have been overlooked. (The esthetic appeal of graphs also probably played a role.) In dimension 2, some problems about belted trees can even be solved in terms of graphs.

Figure 5.9 offers an example. Start from a spanning tree (in the graph-theoretic sense) on the surface of a torus. Form the *dual* subgraph, by

²²Of course this "belted tree" is no longer a tree in the strict sense, so this is doubtful terminology. But we face a dilemma here. The right concepts are those of homology, not of graph theory, but the vocabulary of the latter has already prevailed, and it's too late to go against the grain. The oxymoron "belted tree" is a compromise, trying at once to refer to the familiar concept of tree and to mark its inadequacy.

²³The received name for a belt is *homology cycle* of dimension 1.

²⁴Even if $p = 1$ or d , the (indispensable) notion of *relative* tree is quite awkward in a graph-theoretic framework.

joining all centers between adjacent triangles which are not separated by an edge of the primal graph. The dual subgraph is not a tree, only a “bounding-circuit free” maximal subgraph, that is, a belted tree, for it contains two circuits that do not bound, or belts. Now, the two co-edges of the “primal” spanning tree which are crossed by the dual belt-fasteners are special in that the circuits they close do not bound on the torus (they are representative of the two homology classes of cycles, i.e., classes of cycles that don’t bound, cf. Notes 20 and 23). So if we add them to the primal tree, as belt fasteners, we do have a belted tree.

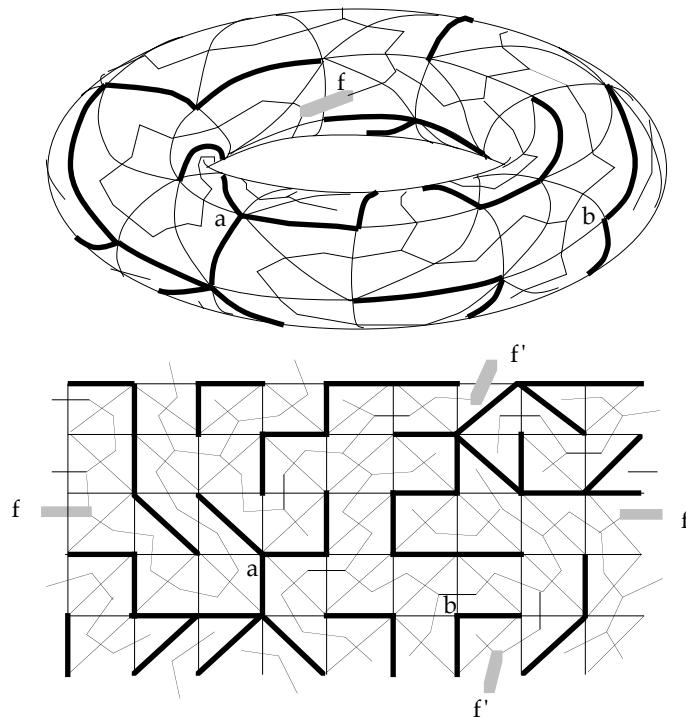


FIGURE 5.9. Spanning tree on the surface of a torus (in thick lines) and its dual, which is no more a genuine tree but a “belted tree” (co-edges not drawn). Points a and b should help make the correspondence between the spatial view and the plane diagram (which is an unfolding of the torus surface, after suitable cutting; nodes on opposite sides should be identified). The two “belt fasteners” f and f' are drawn in thick lines (f' can’t be seen in the top view).

Techniques of this kind are useful for problems of eddy-currents on thin conductive sheets [B2, T&]. But the nice illustrations by graphs should not hide their essentially algebraic nature: Tree and cotree methods really belong to *homology*.

EXERCISES

Exercises 5.1 and 5.2 are on p. 127, Exer. 5.3 on p. 131. Exercises 5.4 to 5.6 are on p. 141, Exer. 5.7 p. 143, Exer. 5.8 p. 148, and Exer. 5.9 p. 150.

Exercise 5.10. Compute all the terms of \mathbf{M}_p as defined in (16), when $\alpha = 1$, for all p .

Exercise 5.11. Inquire about the "Poincaré inequality" (and preferably, devise your own proof): *If D is a bounded domain of E_d , there exists a constant $c(D)$ such that*

$$\int_D |\varphi|^2 \leq c(D) \int_D |\text{grad } \varphi|^2$$

for all functions $\varphi \in C_0^\infty(D)$.

Exercise 5.12. In the previous exercise, the point of having φ vanish on the boundary is to provide a "reference value" for φ , to which one might otherwise add any constant (and hence, give an arbitrary large norm) without changing the gradient. This reference value may as well be the average of φ over the domain, that is, $\bar{\varphi} = (\int_D \varphi) / \text{vol}(D)$. So prove the existence of a constant $c(D)$ such that

$$(\int_D |\varphi - \bar{\varphi}|^2)^{1/2} \leq c(D) (\int_D |\text{grad } \varphi|^2)^{1/2}$$

for all functions $\varphi \in C^\infty(\bar{D})$. (This is the "Poincaré–Friedrichs (or Poincaré–Wirtinger) inequality".)

Exercise 5.13. Show that, for a smooth field $\mathbf{a} = \{a^1, a^2, a^3\}$,

$$\text{rot } \mathbf{a} = \text{grad } \text{div } \mathbf{a} - \Delta \mathbf{a},$$

where $\Delta \mathbf{a} = \{\Delta a^1, \Delta a^2, \Delta a^3\}$. Use this to prove that, if \mathbf{a} has bounded support,

$$(18) \quad \int (\text{div } \mathbf{a})^2 + \int |\text{rot } \mathbf{a}|^2 = \sum_{i=1,2,3} \int |\text{grad } a^i|^2.$$

where integrals are over all space.

HINTS

5.2. In dimension $d = 1$, for $D =]-1, 1[$, the function $x \rightarrow 1 - |x|$. For $d > 1$ and $D = \{x : |x| < 1\}$, aim at a function of $|x|$ with a singularity at 0, and not too fast growth there. Case $d = 2$ will appear special.

5.3. Of course the kernels are closed in the stronger norm, as pre-images of the closed set $\{0\}$, but one cannot employ this argument about the \mathbb{L}^2 norm, in which rot and div are not continuous, only closed. Use (2), and its analogue for rot .

5.4. See the cotangent formula of 3.3.4 and Lemma 4.1. The latter is especially useful (if applied with a measure of creative laziness).

5.5. In terms of the nodes-to-edges incidence matrix elements, one has

$$w_e = G_{me} w_m \nabla w_n + G_{ne} w_n \nabla w_m.$$

Develop, and use Exer. 3.10. Set $g^{ij} = \nabla w_i \cdot \nabla w_j$. (The analogy with the metric coefficients g_{ij} of Riemannian geometry is not accidental.)

5.6. First show that $x \cdot \nabla w_n - w_n(x)$ is a constant inside each tetrahedron (Lemma 4.1). Then develop $(\nabla w_m \times \nabla w_n) \times x$.

5.8. Look at Fig. 4.3 and express the numbers N', E', F' relative to the refined mesh in terms of N, E, F .

5.9. Use Proposition 5.5, second part first, then first part.

5.11. Begin with $d = 1$. Then $D =]a, b[$, and $\varphi(x) = \int_a^x \partial \varphi(\xi) d\xi$. Use Cauchy-Schwarz, then sum with respect to x . For $d > 1$, note that, in the arrowed notation where " $X \rightarrow Y$ " means "all functions from X to Y ", the functional space $\mathbb{R} \times \dots [d \text{ times}] \dots \times \mathbb{R} \rightarrow \mathbb{R}$ can be identified with $\mathbb{R} \rightarrow (\mathbb{R} \times \dots [d - 1 \text{ times}] \dots \times \mathbb{R} \rightarrow \mathbb{R})$.

5.12. In dimension 1 first, $\varphi(y) - \varphi(x) = \int_x^y \partial \varphi(\xi) d\xi$, hence $\varphi(x) - \varphi(y) \leq C \|\partial \varphi\|$, for all pairs of points $\{x, y\}$ in $[a, b]$. Integrate with respect to y to get $\varphi(x) - \bar{\varphi} \leq C \|\partial \varphi\|$, then invoke Cauchy-Schwarz. Adapt this to d dimensions as in the previous case.

5.13. In Cartesian coordinates, $(\text{rot rot } a)^i = \sum_j \partial_j (\partial_i a^j - \partial_j a^i)$. For (18), integrate by parts.

SOLUTIONS

5.1. If $\{0, u\}$ is in the closure of GRAD , i.e., is the limit of some sequence $\{\psi_n, \text{grad } \psi_n\}$ the terms of which belong to GRAD , then $\int_D \psi_n \text{div } j' = -\int_D \text{grad } \psi_n \cdot j'$ for all j' in $C_0^\infty(D)$, hence $\int_D u \cdot j' = 0 \quad \forall j' \in C_0^\infty(D)$ at the limit, and hence $u = 0$. If $\{0, u\}$ is in the closure of ROT , i.e., the limit of some $\{a_n, \text{rot } a_n\}$ of ROT , then $\int_D a_n \cdot \text{rot } h' = -\int_D \text{rot } a_n \cdot h'$ for all h' in $C_0^\infty(D)$, hence $\int_D u \cdot h' = 0 \quad \forall h' \in C_0^\infty(D)$ at the limit, and $u = 0$.

5.2. On $D = \{x : |x| < 1\}$, functions of the form $x \rightarrow |x|^{-\alpha}$ foot the bill, if $\alpha > 0$ (in order to have a singularity at 0), $\int_0^1 r^{-2\alpha} dr < \infty$ (for the function to be square-summable) and $\int_0^1 r^{d-1-2(1+\alpha)} dr < \infty$ (for its gradient to be square-summable). This happens for $0 < \alpha < 1/2$ and $1 + \alpha < d/2$, the latter constraint being redundant if $d > 2$. For $d = 2$, look at the function $x \rightarrow |x| \log|x|$.

5.3. After (2), " $\int_D b \cdot \text{grad } \varphi' = 0 \quad \forall \varphi' \in C_0^\infty(D)$ " characterizes elements of $\ker(\text{div})$, and if a sequence of fields $\{b_n\}$ which all satisfy this predicate converges to some b in $L^2(D)$, this also holds for b , by continuity of the scalar product. Same argument for fields b such that $n \cdot b = 0$, since they are characterized by $\int_D \text{div } b \varphi' + \int_D b \cdot \text{grad } \varphi' = 0 \quad \forall \varphi' \in L^2_{\text{grad}}(D)$, and for fields such that $n \times b = 0$, by using the similar formula in rot .

5.4. Let h be the height of node n above the plane of f (observe how "above" makes sense if space is oriented, as well as f). Then $\text{vol}(\tau) = h \cdot \text{area}(\{k, \ell, m\})/3 = \text{area}(\{k, \ell, m\})/(3|\nabla w_n|)$. There are many ways to derive these relations, but the most illuminating is to remark that 3×3 matrices such as $(\nabla w_k, \nabla w_\ell, \nabla w_m)$ and $(nk, n\ell, nm)$ are inverses, by Lemma 4.1, and that $\text{vol}(\tau) = \det(nk, n\ell, nm)/6$, that $\text{area}(\{k, \ell, m\}) = \det(k\ell, km)/2$, etc.

5.5. Up to obvious sign changes, there are only three cases:

- (a) $e = e' = \{m, n\}$: $(12 \text{ vol}(\tau)/5!) (g^{mn} + g^{mm} - g^{nn})$,
- (b) $e = \{m, n\}$, $e' = \{m, \ell\}$: $(6 \text{ vol}(\tau)/5!) (2g^{n\ell} - g^{m\ell} - g^{nm} + g^{mm})$,
- (c) $e = \{k, \ell\}$, $e' = \{m, n\}$: $(6 \text{ vol}(\tau)/5!) (g^{\ell n} - g^{kn} - g^{\ell m} + g^{km})$.

5.6. $(\nabla w_m \times \nabla w_n) \times x = x \cdot \nabla w_m \nabla w_n - x \cdot \nabla w_n \nabla w_m = w_m \nabla w_n - w_n \nabla w_m + b$, where b is some vector, hence $w_{\{m, n\}} = (\nabla w_m \times \nabla w_n) \times x + b$. Now, observe (cf. 3.3.4 and Lemma 4.1) that

$$\nabla w_m \times \nabla w_n = (kn \times k\ell) \times \nabla w_n / 6 \text{ vol}(\tau) = k\ell / 6 \text{ vol}(\tau).$$

Using this, one has the following alternative form for the face element:

$$w_f = 2(w_\ell k\ell + w_m km + w_n kn) / 6 \text{ vol}(\tau),$$

hence the desired result (place the origin at node k).

5.7. If $e = \{m, n\}$ and $R_{fe} \neq 0$, then $f = \{\ell, m, n\}$ or $\{\ell, n, m\}$, for some ℓ . In both cases,

$$R_{fe} w_f = w_f = 2(w_\ell \nabla w_m \times \nabla w_n + w_m \nabla w_n \times \nabla w_\ell + w_n \nabla w_\ell \times \nabla w_m).$$

Therefore, summing over all faces,

$$\sum_{f \in \mathcal{F}} R_{fe} w_f = 2 \sum_{\ell \in \mathcal{N}} (w_\ell \nabla w_m \times \nabla w_n + \dots) = 2 \nabla w_m \times \nabla w_n.$$

For the divergence, just notice that $\operatorname{div} w_f = 2(\nabla w_\ell \cdot \nabla w_m \times \nabla w_n + \dots) = 6 \det(\nabla w_\ell, \nabla w_m, \nabla w_n) = w_T$ if $T = \{k, \ell, m, n\}$. Two compensating changes of sign occur if $T = \{\ell, k, m, n\}$, the other orientation.

5.8. $F' = 4F$, $E' = 2E + 3F$, $N' = N + E$, hence $N' - E' + F' = N + E - (2E + 3F) + 4F = N - E + F$.

5.9. Since $\ker(\operatorname{div}; W^2) = \operatorname{rot} W^1$, its dimension is the dimension of W^1 , which is E , minus the dimension of $\ker(\operatorname{rot}; W^1) = \operatorname{grad} W^0$. The latter is the dimension of W^0 , i.e., N , minus the dimension of $\ker(\operatorname{grad}; W^0)$, which is 1. Project: Practice with this in the general case, to see how the Betti numbers come to slightly modify these dimensions (but not their asymptotic behavior when the mesh is refined).

5.11. Since D is bounded, it is contained in a set of the form $P =]a, b[\times \mathbb{R} \times \dots \times \mathbb{R}$. Extending by 0, outside D , the functions of $C_0^\infty(D)$, one identifies the latter space with $C_0^\infty(P)$, which is isomorphic to $C_0^\infty([a, b]; C_0^\infty(\mathbb{R}^{d-1}))$. Then, if $x = \{x^1, \dots, x^d\} \in P$, one has

$$\varphi(x) = \int_a^{x^1} \partial_1 \varphi(\xi, x^2, \dots, x^d) d\xi,$$

where $\partial_1 \varphi$ is the partial derivative with respect to the variable x^1 . By the Cauchy-Schwarz inequality,

$$|\varphi(x)|^2 \leq (x - a)^{1/2} \int_a^{x^1} |\partial_1 \varphi(\xi, \dots)|^2 d\xi \leq (b - a)^{1/2} \int_a^b |\nabla \varphi(\xi, \dots)|^2 d\xi,$$

and hence, by Fubini,

$$\begin{aligned} \int_P |\varphi(x)|^2 dx &\leq (b - a)^{1/2} \int_P dx^1 \dots dx^d \int_a^b |\nabla \varphi(\xi, \dots)|^2 d\xi \\ &= (b - a)^{1/2} \int_a^b dx^1 \int_P |\nabla \varphi(\xi, \dots)|^2 d\xi dx^2 \dots dx^d, \end{aligned}$$

hence $c(D) \leq (b - a)^{3/2}$. Of course, this is an upper bound, not the “best” value of $c(D)$, which can be obtained, but by very different methods.

5.13. First,

$$\begin{aligned} (\operatorname{rot} \operatorname{rot} a - \operatorname{grad} \operatorname{div} a)^i &= \sum_j [\partial_j (\partial_i a^j - \partial_j a^i) - \partial_i (\partial_j a^j)] \\ &= \sum_j [\partial_j (\partial_i a^j - \partial_j a^i) - \partial_j (\partial_i a^j)] = -\sum_j \partial_{jj} a^i. \end{aligned}$$

Then $\int (\operatorname{div} a)^2 + \int |\operatorname{rot} a|^2 = \sum_i \int -\Delta a^i a^i = \sum_i \int |\operatorname{grad} a^i|^2$. (Further study: What of a domain D with surface S ? Try to cast the surface terms that then appear in coordinate-free form, by using adequate curvature operators.)

REFERENCES and Bibliographical Comments

Whitney elements were rediscovered by numerical analysts beginning in 1975 in relation to the search for “mixed” finite elements. In particular, the edge element (9) appeared in [Nd], where it was described in terms of its “shape functions” $x \rightarrow a(T) \times x + b(T)$ in the tetrahedron T (cf. Exer. 5.6), where $a(T)$ and $b(T)$ are three-dimensional vectors. (There are thus six degrees of freedom per tetrahedron, in linear invertible correspondence with the six edge circulations.) Similarly [RT], the face element’s shape functions (the 2D version of which first appeared in [RT]) are $x \rightarrow \alpha(T)x + b(T)$, with $\alpha(T) \in \mathbb{R}$ (Exer. 5.6). The obvious advantage of representations such as (9) or (10) over shape functions is to explicitly provide a *basis* for W^1 or W^2 . The presentation by shape functions, however, seems preferable for vector-valued elements of polynomial degree higher than one (cf. [Ne]), whose description in Whitney’s style, with basis functions clearly related to geometrical elements of the simplicial complex, is still an open problem, as is, for that matter, the classification of “tangentially²⁵ continuous” vectorial elements proposed up to now by various authors [Cr, MH, vW, WC, . . .]. See [YT] for a recent attack on the problem. Face elements also were independently rediscovered, in relation with diffraction modelling [SW]. (The latter authors have the face flux *density* equal to 1, instead of the total flux.)

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²⁵I don’t mean to condone this dubious terminology, for it’s “*only* tangentially continuous” that one is supposed to understand: IP^1 elements *are* “tangentially continuous”, and don’t qualify, precisely because they are *also* “normally continuous”. Anyway, this misses the point: The point is the structural property $\text{grad } W^0 = \ker(\text{rot}; W^1)$, for simply-connected domains. This is the rule of the game, for whoever wants to propose new elements. Substitutes for the simple but too coarse tetrahedral first-degree edge-elements should be looked for, but *in conjunction with companion scalar-valued nodal elements*, in order to satisfy this structural rule. The discussion of spurious modes at the end of Chapter 9 should make that clear. (A more general and more complex compatibility condition between elements, the “Ladyzhenskaya-Babuska-Brezzi (LBB) condition”, or “inf-sup condition”, invented by mixed elements researchers [Ba, Br], happens to be implied by the above structural rule.)

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