CHAPTER 2

The 'Scaler' Poincare Steklov Operator and the 'Vector' One: Algebraic Structures which Underlie Their Duality

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Abstract. The Poincaré-Steklov operator, which links the trace and the normal derivative of a harmonic function, is a standard tool in domain decomposition. From the point of view of differential geometry, this operator is one in a family, a family which has two members in dimension 3. The other P.-S. operator (the "vector" one, as opposed to the standard "scalar" one) is useful too. Their relationship is studied and numerical methods to compute them are suggested.

Introduction. Consider a regular bounded domain D of IR^3 (boundary S, unit normal field n, directed towards the interior of D). Let a function φ_S be given in $H^{1/2}(S)$. There exists a unique harmonic function φ in $IR^3 - D$, with finite Dirichlet norm $(\int_{IR^3 - D} |\text{grad } \varphi|^2)^{1/2}$, such that $\varphi_{|S} = \varphi_S$. Then, the normal derivative n . grad φ is a linear function of φ_S, say n . grad $\varphi = R\,\varphi_S$, and the operator R is an isomorphism between $H^{1/2}(S)$ and $H^{-1/2}(S)$ [8]. The inverse of R is known as the *Poincaré-Steklov operator* [2] of the outer region. (The name could fit R as well, and this is a matter of convention.) A similar operator can be defined (modulo some care about ker(R)) for the inner region D.

It is hardly necessary to recall how fundamental this operator is in domain decomposition methods. This is so because R can often be interpreted as a kind of impedance (or admittance, as the case may be) of the given region, and matching partial solutions in domain decomposition methods is akin to matching impedances in electrical engineering [3]. The existence of this powerful analogy may perhaps excuse the slight overuse in the present paper of a nomenclature which is borrowed from electromagnetism. The ideas, of course, apply to other fields of numerical engineering just as well.

The Poincaré-Steklov operator may also be conceived as a device to *transfer boundary conditions* from one boundary to another [1], and especially to pull-back conditions at infinity to an artificial boundary at finite distance. To give only one specific example, consider the basic problem of magnetostatics: given a "source" magnetic field h^s, such that $j^s = \text{curl } h^s$ (the "source" current) has its support within D, find in IR^3 a function φ (the magnetic potential), with finite Dirichlet norm, such that $\text{div}(\mu(h^s + \text{grad } \varphi)) = 0$. (The permeability μ is equal to a constant μ_0 out of D,

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and we'll forget it by assuming a unit system where $\mu_0 = 1$.) This amounts to solving the boundary value problem

$$(1) \qquad \mathrm{div}(\mu_0(h^s + \mathrm{grad}\ \varphi)) = 0 \quad \text{in } D, \qquad n \,.\, \mathrm{grad}\ \varphi = R\,\varphi \quad \text{on } S.$$

Problem (1) can be solved with finite elements, hence a *hybrid* method for the original problem in the whole space: finite elements in the inner region, and some kind of boundary elements procedure on S in order to get R.

Which procedure? There are many, starting from Trefftz's method and similar ones [7, 10], but the most natural one is probably what follows, which has a straightforward physical interpretation. Let $q \in H^{-1/2}(S)$ be given (a "single layer of magnetic charge"), and let

$$(2) \qquad \varphi(x) = (4\pi)^{-1} \int_S dy\ (|y - x|)^{-1}\ q(y)$$

be the associated magnetic potential. The corresponding magnetic field $h = \mathrm{grad}\ \varphi$ is not continuous across S. When one crosses S from outside, the decrease of the normal derivative of φ, or "jump", noted $[n \,.\, \mathrm{grad}\ \varphi]$, is precisely q, and the normal derivative (from outside) on S is

$$(3) \qquad (n \,.\, \mathrm{grad}\ \varphi)(x) = q(x)/2 + (4\pi)^{-1} \int_S dy\ (|y - x|)^{-3}\ n(x) \,.\, (y - x)\ q(y).$$

Let us rewrite (3) in compact form as $n \,.\, \mathrm{grad}\ \varphi = (1/2 + H)\ q$, with obvious notation. Let $\varphi_S = G\ q$ be the trace on S of the φ of (2). By eliminating q, one gets $n \,.\, \mathrm{grad}\ \varphi = R\ \varphi_S$, and therefore

$$(4) \qquad R \equiv (1/2 + H)\ G^{-1}.$$

Formula (3) thus appears as a device to *compute* the (inverse of) the Poincaré-Steklov operator, at the price of solving eq. 2, which is a Fredholm integral equation of the first kind for the unknown charge q. Of course, a suitable discretization of (4) must be done [5].

Electrical engineering has us accustomed with a kind of duality between charges and currents. When something can be done with charges, it can often be done with currents as well (recall, for instance, the equivalence between current loops and double layers of magnetic charge in high-school physics). Let j be a tangent vector field defined on S (a "single layer of current"), and let

$$(5) \qquad a(x) = (4\pi)^{-1} \int_S dy\ (|y - x|)^{-1}\ j(y),$$

be the associated vector potential. The normal component $n \,.\, b$ of the corresponding magnetic induction $b = \mathrm{curl}\ a$ is continuous across S, but its tangential component, which is $n \times \mathrm{curl}\ a$ up to a $\pi/2$ rotation around the normal, is not: one has $[n \times \mathrm{curl}\ a] = j$, and

$$(6) \qquad (n \times \mathrm{curl}\ a)(x) = j(x)/2 + (4\pi)^{-1} \int_S dy\ (|y - x|)^{-3}\ n(x) \times ((y - x) \times j(y)),$$

and formulas (5) and (6) provide a link between the tangential part of a (call it a_S) and $n \times \mathrm{curl}\ a$ as determined from outside: $n \times \mathrm{curl}\ a = (1/2 + H)\ j$, $a_S = G\ j$. These are not the same operators H and G as above, of course, but it is useful to stress the analogy by this notational abuse (we shall be more rigorous below). Let us therefore set $R \equiv (1/2 + H)\ G^{-1}$ in accordance. We shall call this the (inverse of) the "vector" P.-S. operator, the previous R being the "scalar" one. Now $n \times h = R\ a_S$, with R as in (5), *also* can serve as boundary condition on S, as follows: solve

$$(7) \qquad \mathrm{curl}(h^s + \mathrm{curl}\ a) = 0 \quad \text{in } D, \quad n \times \mathrm{curl}\ a = R\ a_S \quad \text{on } S,$$

where R is obtained by solving the Fredholm's equation $R \equiv (1/2 + H)\ G^{-1}$ for the unknown surface current j. (Note that a is not unique in (7), but this hardly matters, since $h = h^s + \mathrm{curl}\ a$, the desired result, is unique.)

So the method first sketched was not the only conceivable hybrid one. There are at least two

such methods, corresponding to two different Poincaré-Steklov operators, the "scalar" and the "vector" one.

But now, if there are two ways of doing things, is that all? Are there other ways? The point of the present paper is to answer this question. Doing this will require a detour, a change of viewpoint. Our approach will consist in first trying to understand why formulas (3) and (6) look so much alike. We shall see that, from the correct perspective, they are in fact two versions of the same formula, and that no other variants exist in three dimensions. We shall also realize that besides (4), there exists another formula which can be used to compute R. Therefore, all in all, there are *four* basic algorithms, involving the two P.-S. operators, which can serve for the kind of transfer of boundary conditions we have been considering, and more generally for domain decomposition procedures.

The "correct perspective" is in our opinion the one given by considering vector fields like h, b, etc. (and, in other areas of interest, vector fields like the heat flux, the flow of fluid, etc.), as *differential forms* (DF). More to the point, we contend that physical entities which are usually represented with such vector fields are better represented by DF. We first make this point, while giving definitions (Section 1), then we investigate the algebraic structure of the theory of the potentials of forms (Section 2). This results in a classification of integral methods which can serve to compute Poincaré-Steklov-like operators (Section 3). Some indications about the discretization of these methods will then be given (Section 4).

1. Fields and their Potentials, as Differential Forms. Consider for instance j, the above surface current. Let v be a small vector tangent to S. Then, $(n \times j) \cdot v$ is the flux of electric charge which crosses the line element v during a unit of time. Thus, the real mathematical nature of j is that of the mapping $v \to (n \times j) \cdot v$, which tells about the current flux through any tangential line element (and, by integration, through any line drawn on S). A mapping of this kind is called a *differential form over* S. It may be *represented* via a vector field, as here j, but the vector field is no more than a representation, an auxiliary: if the dot- and cross-products were to change, for instance because of a change of units, the vector field j would change, but not the DF which it represents. This last mathematical object is therefore the most appropriate one to stand for the surface current density. Induction b is a DF, too (over $\mathbb{R}^3$): it is the mapping $\{v, w\} \to b \cdot (v \times w)$, which tells about the induction flux through a surface element $\{v, w\}$, and by integration, through any surface. Here, there are two vectors as arguments, so b is "a DF of degree 2", or "2-form", while j was of degree 1. It can be shown by similar arguments that h and a are 1-forms, and that q is a 2-form over S.

Let us now give definitions. (One may refer to [6] or [9] for serious study.) In dimension n, a p-covector ($0 \le p \le n$) is a mapping $\{v_1, \ldots, v_p\} \to \mathbb{R}$, multilinear, and alternating (meaning that to permute two v_i's will invert the sign of the result). A p-form is a (smooth) field of covectors. If $n = 3$, and for a given metric with dot-product "." and volume-element "det" (the determinant of a triplet of vectors), a vector field h (**resp.** b) generates a 1-form $v \to h(x) \cdot v$ (**resp.** a 2-form $\{v, w\} \to \det(b(x), v, w)$). A scalar field φ yields a 0-form (the function itself, by convention), or a 3-form $\{u, v, w\} \to \varphi(x) \det(u, v, w)$. Differential geometry defines an operator d, the exterior differential, which maps p-forms into (p+1)-forms, and appears as generalizing the classical grad, curl, div, because the d of the 1-form h is the 2-form generated by curl h, the d of the 2-form b is the 3-form coming from div b, etc. It also features the *Hodge operator* $*$, which transforms p-forms into (n−p)-forms. Its definition is as follows. Let ω be a p-form, let ω_x be its value at point x. If $\{v_1, \ldots, v_n\}$ is a direct orthonormal basis at point x, $*\omega(x)$ is the mapping $\{v_{p+1}, \ldots, v_n\} \to \omega(x)(v_1, \ldots, v_n)$, which can be extended to non-orthonormal (n−p)-uples of vectors by linearity. Remark that $*^1h = {}^2h$, and $*^2b = {}^1b$. In dimension 2, starring a 1-form amounts to rotate the vector field it comes from, 90° around the normal. (Hence $** = -1$ in this case. There are unavoidable minus signs all around the place in this theory.) Besides d, there is a *codifferential* $\delta = *d*$ (again, up to sign). Last, we need a notion of *trace* of a DF on S: the trace $t\omega$ of ω is the field of mappings $\{v_1, \ldots, v_p\} \to \omega(x)(v_1, \ldots, v_p)$, for all x in S and all vectors v_i tangent to S. Nothing more natural, but there are surprises when we come back to the representative vector- or scalar-fields: th is represented by the *tangential* part of h (noted h_S), but tb (a surface 2-form) is represented by the scalar field $n \cdot b$, the *normal* part of b. One has $td = dt$.

2. Algebraic structures of the theory. Now let us look at Fig. 1. It displays familiar entities in this new notation. For instance, b = da and dta = tb would read as b = curl a and $\mathrm{curl}_S a_S$ = n . b in conventional notation. It also features both operators called R above, which here are more properly labeled R_0 and R_1.

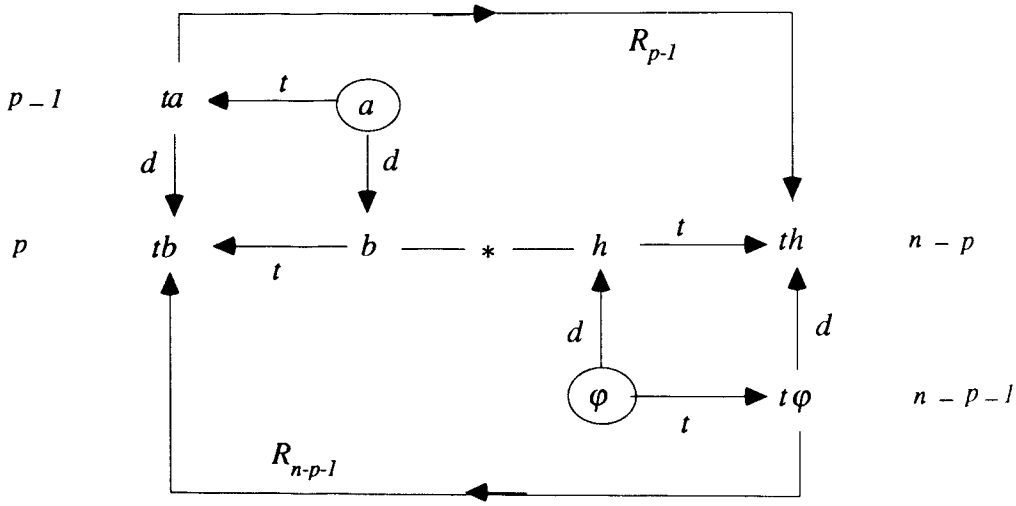

Figure 1. The interplay of forms h, b, their potentials, their traces, and the two Poincaré-Steklov operators. The notation corresponds to the case n = 3, p = 2.

It is well known that φ and a, in Fig. 1, can respectively be obtained as the potential of a charge q, as in (2), and of a current density j, as in (5). This applies also to DFs. Let α be a p-form on S. Its potential is by definition the p-form ω whose value ω_x at point x (not necessarily in S) is given by the mapping

$$(8) \qquad \{v_1, \ldots, v_p\} \to (4\pi)^{-1} \int_S dy\, (|y - x|)^{-1}\, \alpha(y)(v_1, \ldots, v_p).$$

We shall note this $\omega = \mathbf{G}_p \alpha$, where p is the degree of α (to be omitted when there is no ambiguity). Formulas (2) and (5) correspond to the cases p = 0 and p = 1. If p = 2, and if α is represented by the function ψ, ω is represented by a vector field u the values of which are

$$u(x) = (4\pi)^{-1} \int_S dy\, (|y - x|)^{-1}\, \psi(y)\, n(y).$$

This is sometimes called a "curl-potential".

There is again a complex interplay between charges, the potentials of their Hodge duals, and the traces of these potentials (Fig. 2). The nomenclature in this figure (j, a, etc.) corresponds to the case p = 2. Note that j = δψ corresponds to j = − n x grad ψ, in standard notation (ψ is the so-called "stream-function" of the surface current j), and δj = 0 to div j = 0. The algebraic content of Fig. 2 is the simple formula $\mathbf{G}\delta = \delta\mathbf{G}$, which is easily derived from (8) and from the definitions of δ and *. (Note that δj = 0 thus implies δa = 0, i.e. a is divergence-free, as a vector field.)

But there is more, because the two diagrams are separately displayed only for readability. In fact, they merge into a single structure: the two circles in Fig. 2 are supposed to correspond to the ones similarly placed on Fig. 1, and serve as bridges between the two diagrams.

The algebraic justification for this merger is the formula $d*d\mathbf{G} = (-)^p *d\mathbf{G}\delta$, also provable from first principles. Fig. 3 is an attempt to display the two interconnected diagrams as a whole.

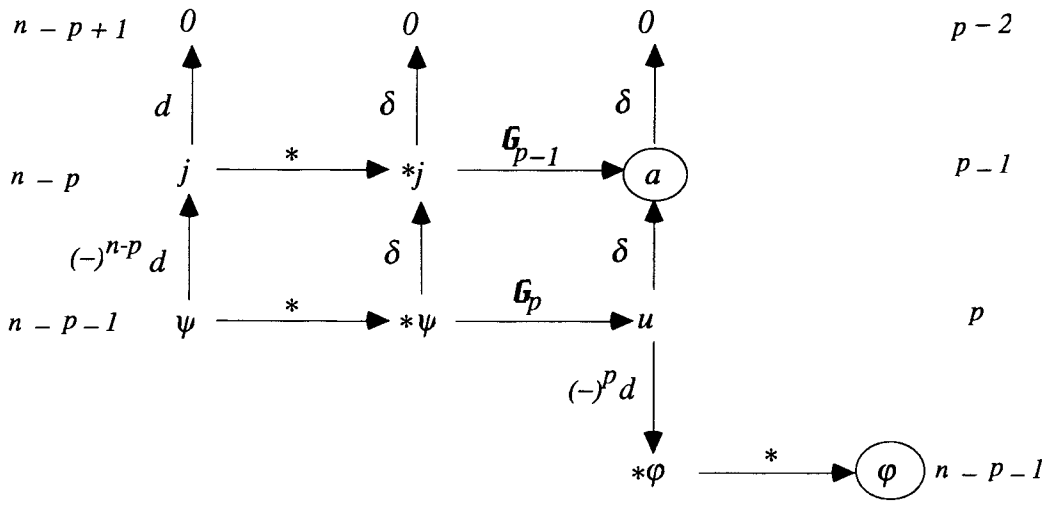

Figure 2. The interplay of charges and their potentials. The diagram is "commutative", as was that of Fig. 1: if two nodes can be joined by two different chains of arrows, each of which corresponds to an operator, the two operators obtained by composition along the way are equal. For instance, $\mathbf{G}_{p-1}\delta = \delta\mathbf{G}_p$. (The notation fits the case n = 3, p = 2.)

There is a third basic formula: $[t*d\mathbf{G}] = *$. It connects together the charge density α and the jump through S of a quantity, namely $t*d\mathbf{G}\alpha$, which can be called the "normal derivative" of the potential $\omega = \mathbf{G}\alpha$. There are two paths in the combination of Figs. 1 and 2 along which one encounters operators $\mathbf{G}$, d, *, t, in this order (cf. Fig. 4), so there are two possible applications of this formula. One yields [n x curl a] = − j, and the other one, $[\varphi] = \psi$. For p = 1, these relations are [n . grad φ] = q and [n x a_S] = k.

The reader is invited to redraw Fig. 2 for p = 1. This will simply consist in a change of labels, according to the following substitutions: q for j, k for ψ, φ for a, a for φ. The 1-form k has a physical interpretation as a "surface magnetic current", and $q = -\mathrm{div}_S k$ is a magnetic charge. The corresponding substitutions in Fig. 1 should be: h for b, b for h, etc. (that is, a simple central symmetry). Note however that contrary to h and b, a and φ are *not* the same in both sets of diagrams: they differ by something whose d is zero. In Figs. 1--2, or Fig. 3, a was the potential of a "single layer" of currents, j, and φ that of the "double layer" ψ of electric charge. In the new drawing, φ will appear as the single-layer potential of q, and a as the (vector) potential of the double-layer k.

We have enough to grasp the generality of the situation: for each value of p, there is a couple of Hodge dual forms of degrees p and n − p, which are the potentials of a single layer of degree n − p and of a double layer of degree n − p − 1 respectively. The relations between them are summarized in the formulas $\mathbf{G}\delta = \delta\mathbf{G}$ and $d*d\mathbf{G} = (-)^p *d\mathbf{G}\delta$, and are graphically displayed, in the case p = 2, by Fig. 3. Aside from p = 1, there are no other non-trivial possibilities in dimension 3. Now, by looking at relations between traces on S of the various forms displayed above, we shall obtain equations which will enable us to compute R_{p-1} for p = 1 and 2. Since there are two

possible potential representations (single and double layer) and two interesting values of p, we may expect to find *four* feasible integral methods, as announced in the Introduction.

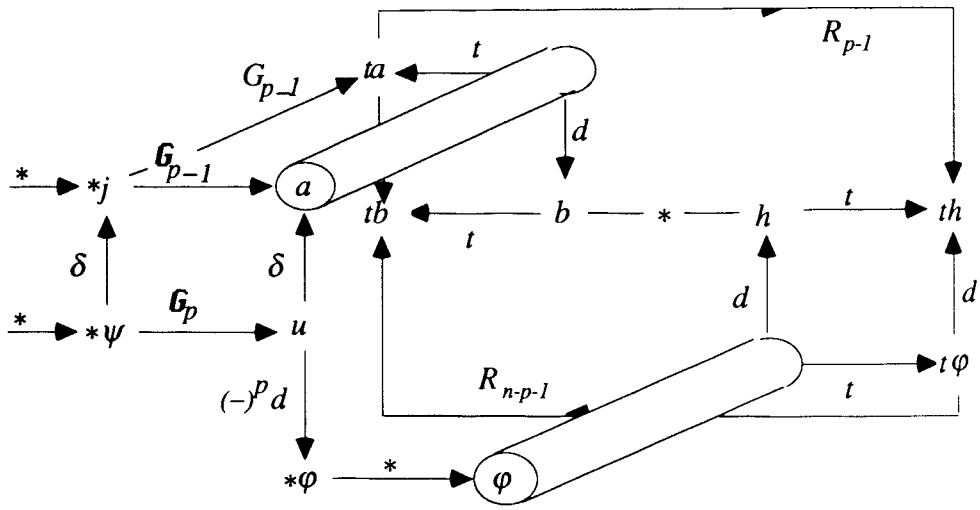

Figure 3. The two diagrams of Figs. 1 and 2, as a whole. (G_{p-1} is $t\mathfrak{G}_{p-1}$.)

3. Integral Methods. Let us set $G_p = t\mathfrak{G}_p$, and $H_p = t*d\mathfrak{G}_p - */2$. (The indexing is such that the subscript refer to the degree of the form the operator is applied to.) The introduction of a factor 1/2 should not surprise those accustomed to boundary integral methods. Thanks to it, H_p has an integral representation. This representation is the one which appears as the last term on the right in (3) for $p = 2$ and in (6) for $p = 1$, when the forms are represented in terms of functions or vector fields. Seen from the present viewpoint, (3) and (6) are the same formula.

The next step consists in deriving the following formulas:

$$R_{p-1}\, G_{p-1} = */2 + H_{p-1}, \quad R_{n-p-1}(*/2 + H_p) = (-)^p\, d\, G_{p-1}\, \delta.$$

These are literally read off Fig. 3, by following appropriate paths of arrows (cf. Fig. 4). Rearranging the indices for the case $n = 3$, we find the four formulas by which R_0 and R_1 can in principle be computed:

(9) $$R_0 = (*/2 + H_0)\, G_0^{-1}, \qquad R_1 = (*/2 + H_1)\, G_1^{-1},$$

(10) $$R_0 = d\, G_1\, \delta\, (*/2 + H_2)^{-1}, \qquad R_1 = -\, d\, G_0\, \delta\, (*/2 + H_1)^{-1}.$$

Those in (9) were recalled in the Introduction (cf. (4)). Those in (10), which imply the resolution of Fredholm *second kind* problems, may be interesting alternatives. To get a feeling for these problems, which respectively consist in finding ψ such that $(*/2 + H_2)\psi = \varphi_S$ and k such that $(*/2 + H_1)k = a_S$, better revert to conventional notation, which results in

(11) $$\psi(x)/2 + (4\pi)^{-1} \int_S dy\, (|y - x|)^{-3}\, n(y) \,.\, (y - x)\ \psi(y) = \varphi(x),$$

(12) $$k(x)/2 + (4\pi)^{-1} \int_S dy\, (|y - x|)^{-3}\, n(x) \times ((y - x) \times k(y)) = (n \times a)(x).$$

(Compare with (3) and (6). The change to n(y) in (11) is not a misprint.) Solving eq. 11 for the electric double layer ψ [**resp.** eq. 12 for the magnetic double layer k] will allow one to get the P.-S. operator R_0 [**resp.** R_1].

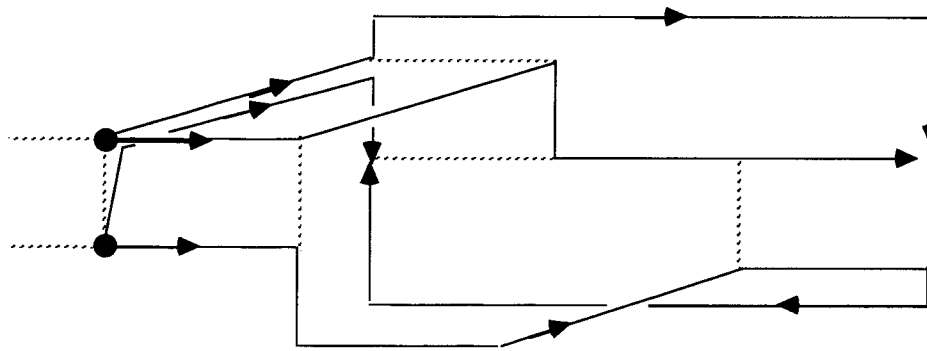

Figure 4. Paths across Fig. 3, which yield formulas (9) and (10).

4. Finite elements implementation. Still within the standard framework of vector fields and functions, we now hint at the way to obtain discretizations, associated with variational formulations, for the four methods. It will be enough to give the procedure in detail for (3), which corresponds to the first formula in (9), and is well known. Let us call Q and Φ the finite dimensional approximation spaces (not yet specified) for q and φ_S. Primes denote test-functions. The variational form of (2)(3) is

$$\int_S dx\ \varphi(x)\ q'(x) = (4\pi)^{-1} \iint_S dx\ dy\ (|y - x|)^{-1}\ q(y)\ q'(x) \qquad \forall\ q' \in Q,$$

$$\int_S dx\ (R_0\varphi)(x)\ \varphi'(x) = (\int_S dx\ q(x)\ \varphi'(x))/2 + \ ...$$

$$... + (4\pi)^{-1} \iint_S dx\ dy\ (|y - x|)^{-3}\ n(x) \,.\, (y - x)\ q(y)\ \varphi'(x) \quad \forall\ \varphi' \in \Phi.$$

To make this manageable, let us introduce matrices which express these various integrals in terms of the degrees of freedom (whatever they will be) of q, q', φ, φ'. Brackets $\langle\ ,\ \rangle$ will stand for the scalar product in a space of degrees of freedom. Vectors of freedoms and matrices will be underlined. With these conventions, what we just wrote is

$$\langle \underline{R}_0\ \underline{\varphi},\ \underline{\varphi}' \rangle = \langle \underline{B}\ \underline{q},\ \underline{\varphi}' \rangle/2 + \langle \underline{H}_0 \underline{q},\ \underline{\varphi}' \rangle \qquad \forall\ \underline{\varphi}' \in \underline{\Phi},$$

$$\langle \underline{B}^t\ \underline{\varphi},\ \underline{q}' \rangle = \langle \underline{G}_0\ \underline{q},\ \underline{q}' \rangle \qquad \forall\ \underline{q}' \in \underline{Q}$$

(where $\underline{\Phi}$ and $\underline{Q}$ stand for the spaces of degrees of freedom), whence

$$\underline{R}_0 = \mathrm{sym}((\underline{B}/2 + \underline{H}_0)\ \underline{G}_0^{-1}\ \underline{B}^t),$$

(where t stands for "transpose" and sym for "symmetric part").

From this example, how to implement the three other methods should be clear. The only difficulty lies in the choice of finite-element bases. For this, we shall follow a heuristic approach which has been proved efficient in numerical electromagnetism [5]. There are, according to concepts of differential geometry which date back to Whitney [11], specific finite elements for functions and vector fields, depending on the degree of the forms they are supposed to represent: "edge"-elements for fields e, h or a, "face"-elements for b and j, etc. (Cf. [4].) Something

similar exists in dimension 2, from which the right choice of finite elements for the entities introduced above as q, j, k, ψ, φ, a, has been inferred. Here follows a brief account of this.

Assume a triangulation of S. To a node n, assign the standard hat-function of finite-elements theory (continuous, piecewise affine, equal to 1 at node n, to 0 at other nodes), which we denote by w_n. To an edge e connecting nodes n and m, assign the "edge-element" basis (a tangential vector field) $w_e = w_n \, \mathrm{grad}_S w_m - w_m \, \mathrm{grad}_S w_n$, and also what we shall call a "twisted" edge-element, $w\hat{}_e = n \times w_e$. To a triangle t, assign the function w_t obtained by dividing the characteristic function of t by its area. Call W_0, W_1, W_2 the finite-dimensional spaces spanned by the w_n, w_e, w_t respectively, and ${}^tW_1$ the one spanned by the twisted edge-elements.

Now, we propose the following implementation principle. The approximation spaces for the above entities will be as indicated below:

Name of the function or vector-field:	ψ	φ_S	j	k	a_S	q
Approximation space:	W_0	W_0	${}^tW_1$	${}^tW_1$	W_1	W_2

For example, the entries of the matrix analog of H_1 in (9) will be, for all edges e and e',

$$\underline{H}_1^{e,e'} = \int\int_S dx\, dy \;\; (|y - x|)^{-3} \;\; n(x) \times ((x - y) \times w\hat{}_{e'}(y)) \cdot w_e(x).$$

Conclusion. Poincaré-Steklov operators should be studied within the framework provided by differential geometry. They operate on forms of degree p - 1 over a hypersurface, giving forms of degree n - p as images (cf. Fig. 1). In three dimensions, p = 0 and 1 are the only relevant values, so there are two such operators, the "scalar" and the "vector" one, respectively called R_0 and R_1 above. (The standard P.-S. operator of, for instance, ref. [2], is R_0^{-1}.) It has been shown that each can be obtained in two different ways, by solving a Fredholm's equation of either the first or the second kind, and that there are essentially no other possibilities. Poincaré-Steklov operators are useful to set artificial boundary conditions at finite distance in the case of PDE problems in unbounded domains. There are thus four ways to do this in dimension 3, at the price of solving a boundary integral equation. Finite elements for the discretization of these equations have been suggested.

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