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**CONCISE REVIEW PAPER**

## Numerical simulation of corner singularities: a paradox in Maxwell-like problems

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**Abstract**

This paper sums up some recent studies related to the numerical solution of boundary value problems deriving from Maxwell's equations. These studies bring to light the theoretical origins of the 'corner paradox' pointed out by numerical experiments for years: *In a domain surrounded by a perfect conductor, a 'nodal' discretization can approximate the electromagnetic field only if the domain has no reentrant corners or edges.* The explanation lies in a mathematical curiosity: two different interpretations of the same variational equation, which are both well-posed and lead either to the *physical* or a *spurious* solution! Two strategies which were recently proposed to remedy this flaw of nodal elements are described. To cite this article: C. Hazard, C. R. Mecanique 330 (2002) 57–68. © 2002 Académie des sciences/Éditions scientifiques et médicales Elsevier SAS

**computational fluid mechanics / Maxwell's equations / singularities of solutions / finite elements**

### Simulation numérique de singularités de coins: un paradoxe pour les équations de Maxwell

**Résumé**

Cet article résume des travaux récents concernant la résolution numérique de problèmes aux limites dérivant des équations de Maxwell. Ces travaux mettent en lumière les origines théoriques du « paradoxe des coins » constaté numériquement depuis des années : dans un domaine entouré par un conducteur parfait, une discrétisation par éléments finis « nodaux » ne permet d'approcher le champ électromagnétique que si le domaine ne possède pas de coins rentrants. L'explication réside dans une curiosité mathématique : deux interprétations distinctes d'une même équation variationnelle, qui mènent soit à la solution *physique*, soit à une solution *parasite* ! Deux stratégies proposées récemment pour parer à cet inconvénient des éléments nodaux sont décrites. Pour citer cet article : C. Hazard, C. R. Mecanique 330 (2002) 57–68. © 2002 Académie des sciences/Éditions scientifiques et médicales Elsevier SAS

**mécanique des fluides numérique / équations de Maxwell / singularités de solutions / éléments finis**

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## 1. Introduction

It may seem surprising to find a paper devoted to electromagnetism in a journal which is rather turned towards mechanics. Apart from a ‘politically correct’ argument of interdisciplinarity, one can motivate the reader by invoking the fact that the mathematical curiosity described here is probably not peculiar to electromagnetism (see Section 6). At first glance, it appears as a *warning* for the numerical simulation of partial differential systems involving the **curl** and div operators. Taking a closer look, it shows that choosing two different finite elements for discretizing the *same* variational equation can lead to approximate two different objects among which only one is ‘physical’. And the only way to distinguish between them is to identify the functional spaces they live in. These objects actually are the solutions of a *single* variational equation which is well-posed in *two* different spaces. In short the reader will find here a convincing illustration of the fact that sometimes only a deep mathematical understanding of the problem can lead to appropriate numerical schemes!

In the last 30 years, various finite element methods were developed for the simulation of electromagnetic phenomena, with more or less success. Roughly speaking, their defenders may be split in two families.

- On one hand, the ‘conservatives’ have decided to cling to the well-known *nodal finite elements*, widely used in mechanics for fluid or structure problems. Here the word *nodal* refers to the nature of the degrees of freedom: the unknowns are the values of the searched field at given points.
- On the other hand, the ‘progressives’ advocate the use of *edge elements*, sometimes called Nédélec’s elements, or Whitney’s, or . . . , depending on what community the ‘progressive’ belongs to. Here a degree of freedom may represent some flux across an edge of an element.

For the latter family, the present paper may appear as an acknowledgement of the failure of the former. Indeed one of its conclusions could be: *Conservatives have to be very careful near ‘reentrant’ corners or edges, since a purely nodal discretization cannot in general approximate the singular behaviour of the electromagnetic field near such geometrical singularities.* But the conservatives could retort that they have now a cure for this flaw. And the progressives could then object that *their* edge elements allow to capture the singular behaviour of the field, provided the mesh is refined enough near corners and edges. So why should they replace a simple refinement by a cure which is based on an intricate mathematical study and actually brings a higher numerical complexity? The conservatives could argue that the use of nodal elements is more appropriate in some situations. . . . Our aim is not to take part in the debate, but rather to adopt definitely a conservative point of view by presenting the recent theoretical and numerical studies which form the different ingredients of the above mentioned cure.

The flaw of nodal finite elements has been brought to the fore by numerical experiments for a long time: such a discretization ‘erases’ the physical ‘corner effect’ on the electromagnetic field. But the explanation of this flaw was understood far later thanks to the theoretical work of Costabel and Dauge [1]. The numerical remedies that have been proposed are based on a simple idea: the field is split into the sum of a *regular part* that is suited for a nodal approximation and a *singular part* whose description follows from an explicit knowledge of the corner effect.

One could be tempted to compare this strategy with the so-called *singular function methods* [2] used for instance in elasticity to simulate cracks, since they apparently derive from the same idea. By enriching the finite element space, they improve the quality of the numerical solution without using a mesh refinement. More precisely they improve the poor convergence of finite element schemes due to the singularities of the solution near the ends of the cracks. For Maxwell-like problems, the methods we present show a basic difference: the question is no longer to obtain a better convergence, but rather to obtain the ‘physical’ solution (the enrichment of the finite element space becomes *necessary* to attain this solution).

The paper is organized as follows. In Section 2, we present various formulations of a model ‘Maxwell problem’. We precise in Section 3 the proper functional framework in which these formulations are equivalent. In Section 4 we investigate the core of the *corner paradox*, which lies in the existence of *spurious* formulations of the model problem. Section 5 shortly describes two strategies for a cure, and refers to a more recent promising approach. Finally we mention in Section 6 some related studies.

## 2. A model problem

The whole paper is devoted to one of the simplest Maxwell-like problems, which describes magnetostatics in a bounded domain surrounded by a perfect conductor. Despite the quite restricted physical relevance of such a model, it contains the main features of the *corner paradox*, which is essentially related to the **curl curl** operator. Many other applications to more involved situations can be achieved following the same lines (see Section 6). The main advantage of this pedagogical model lies in its simplicity.

Consider a bounded open *polyhedron*  $\Omega \subset \mathbb{R}^3$  with boundary  $\Gamma$ . We denote by  $\mathbf{n}$  the unit outer normal to  $\Gamma$ . For technical reasons, we assume that  $\Omega$  is connected and simply connected, i.e., it is made of a single piece without holes (this assumption could be removed: it slightly simplifies the presentation), and that  $\Gamma$  is a Lipschitz surface (which dismisses some very specific polyhedrons).

The question is to find a numerical approximation of a vector field  $\mathbf{u}$  (which represents the potential of the magnetic field in magnetostatics) satisfying the following equations referred to as ‘Maxwell problem’  $\mathcal{M}$  in the sequel:

$$\mathbf{curl curl} \mathbf{u} = \mathbf{f} \quad \text{in } \Omega \quad (1)$$

$$\text{div} \mathbf{u} = 0 \quad \text{in } \Omega \quad (2)$$

$$\mathbf{u} \times \mathbf{n} = 0 \quad \text{on } \Gamma \quad (3)$$

for some datum  $\mathbf{f}$  assumed divergence-free:

$$\text{div} \mathbf{f} = 0 \quad \text{in } \Omega \quad (4)$$

The finite element methods we are interested in are based on alternative formulations of this problem.

On one hand, we consider a *mixed* interpretation of the above system. It consists in introducing a supplementary scalar unknown  $p$  which plays the role of a *Lagrange multiplier* for the divergence-free constraint (2). For the same datum  $\mathbf{f}$ , the pair  $(\mathbf{u}, p)$  must satisfy the following equations that will be called ‘Lagrange problem’  $\mathcal{L}$ :

$$\mathbf{curl curl} \mathbf{u} - \mathbf{grad} p = \mathbf{f} \quad \text{in } \Omega \quad (5)$$

$$\text{div} \mathbf{u} = 0 \quad \text{in } \Omega \quad (6)$$

$$\mathbf{u} \times \mathbf{n} = 0 \quad \text{on } \Gamma \quad (7)$$

$$p = 0 \quad \text{on } \Gamma \quad (8)$$

On the other hand, we are concerned with another formulation which may be seen as an exact *penalty* of the divergence-free condition. Here, we search  $\mathbf{u}$  solution to

$$\mathbf{curl curl} \mathbf{u} - \mathbf{grad} \text{div} \mathbf{u} = \mathbf{f} \quad \text{in } \Omega \quad (9)$$

$$\text{div} \mathbf{u} = 0 \quad \text{on } \Gamma \quad (10)$$

$$\mathbf{u} \times \mathbf{n} = 0 \quad \text{on } \Gamma \quad (11)$$

where (9) is nothing but a vector Poisson equation since

$$\mathbf{curl curl} \mathbf{u} - \mathbf{grad} \text{div} \mathbf{u} = -\Delta \mathbf{u} \quad (12)$$

We thus call this system ‘Poisson problem’  $\mathcal{P}$ . Let us point out that the divergence-free constraint is replaced here by a simple boundary condition.

Someone who is not interested in functional details would claim

$$\mathcal{M} \iff \mathcal{L} \iff \mathcal{P} \tag{13}$$

Indeed it is clear that a solution to  $\mathcal{M}$  satisfies  $\mathcal{L}$  (with  $p = 0$ ) as well as  $\mathcal{P}$ . Conversely, assume first that  $(\mathbf{u}, p)$  is a solution to  $\mathcal{L}$ . Obviously  $\mathbf{u}$  satisfies  $\mathcal{M}$  if  $p \equiv 0$ . To prove this, it suffices to apply the divergence operator to (5): by virtue of the assumption (4), we see that  $p$  satisfies

$$\Delta p = 0 \quad \text{in } \Omega \tag{14}$$

$$p = 0 \quad \text{on } \Gamma \tag{15}$$

whose only solution is known to be 0. Similarly if  $\mathbf{u}$  is a solution to  $\mathcal{P}$ , it satisfies  $\mathcal{M}$  if  $\text{div } \mathbf{u} \equiv 0$ . Setting  $p := \text{div } \mathbf{u}$  and applying the div operator to (9) shows that  $p$  satisfies again (14)–(15), and the same conclusion follows.

A forewarned mathematician would temper the assertion claimed in (13), which can be *true* but also *false*: it depends on the functional space in which  $\mathbf{u}$  is searched! Indeed the uniqueness of the solution to (14)–(15) holds provided  $p$  is *regular* enough. We shall see that if  $\Omega$  is a nonconvex polyhedron, the set of  $L^2(\Omega)$ -solutions of this homogeneous problem even consists in a space of infinite dimension! Therefore it is necessary to precise the functional framework associated with these three problems, and the proper interpretation of the equations. The core of the *corner paradox* is that both problems  $\mathcal{L}$  and  $\mathcal{P}$  appear to be well-posed in two neighboring function spaces which differ as soon as the domain has reentrant corners or edges.

### 3. A first glance at the functional jumble

Let us introduce some notations. The space of infinitely differentiable functions with compact support in  $\Omega$  is referred to as  $\mathcal{D}(\Omega)$ . Its dual  $\mathcal{D}'(\Omega)$  is the space of distributions in  $\Omega$ . The space  $\mathcal{D}(\overline{\Omega})$  consists of the restrictions to  $\Omega$  of the functions of  $\mathcal{D}(\mathbb{R}^3)$ . Since there is no ambiguity on the domain of integration, we simply denote by  $L^2$  (respectively,  $\mathbf{L}^2$ ) the space of square integrable scalar functions in  $\Omega$  (respectively, vector fields), by  $H^1$  or  $\mathbf{H}^1$ , more generally  $H^n$ , the usual Sobolev spaces in  $\Omega$  (i.e.,  $L^2$  partial derivatives of order  $k \leq n$ ), and  $H_0^1 = \{\psi \in H^1; \psi|_\Gamma = 0\}$ . The usual scalar product and norm in  $L^2$  or  $\mathbf{L}^2$  are denoted  $(\cdot, \cdot)$  and  $\|\cdot\|$ .

We then consider the following (Hilbert) spaces, where the index  $N$  means that the fields are normal to  $\Gamma$ :

$$\mathbf{H}_N(\mathbf{curl}) = \{ \mathbf{v} \in \mathbf{L}^2; \mathbf{curl } \mathbf{v} \in \mathbf{L}^2 \text{ and } (\mathbf{v} \times \mathbf{n})|_\Gamma = 0 \}$$

$$\mathbf{H}_N(\mathbf{curl}, \text{div}) = \{ \mathbf{v} \in \mathbf{H}_N(\mathbf{curl}); \text{div } \mathbf{v} \in L^2 \}$$

$$\mathbf{H}_N(\mathbf{curl}, \text{div } 0) = \{ \mathbf{v} \in \mathbf{H}_N(\mathbf{curl}); \text{div } \mathbf{v} = 0 \text{ in } \Omega \}$$

The latter two can be equipped with the scalar products obtained by removing the  $L^2$  contribution in the natural ones. This is the object of the following lemma which derives from the compactness of the embedding of  $\mathbf{H}_N(\mathbf{curl}, \text{div})$  in  $L^2$  (see [3,4]).

LEMMA 3.1. – *The bilinear form  $(\mathbf{curl } \cdot, \mathbf{curl } \cdot) + (\text{div } \cdot, \text{div } \cdot)$  defines a norm on  $\mathbf{H}_N(\mathbf{curl}, \text{div})$  equivalent to its natural norm (hence  $(\mathbf{curl } \cdot, \mathbf{curl } \cdot)$  defines a norm on  $\mathbf{H}_N(\mathbf{curl}, \text{div } 0)$ ).*

#### 3.1. The Maxwell problem

In the sequel we assume that the datum  $\mathbf{f}$  belongs to  $\mathbf{L}^2$ . Integrating by parts formally the scalar product of (1) by a test field  $\mathbf{v}$  such that  $(\mathbf{v} \times \mathbf{n})|_\Gamma = 0$  yields the ‘natural’ variational formulation of our initial

Maxwell-like problem  $\mathcal{M}$ :

$$(\mathcal{M}(\mathbf{curl})) \quad \begin{array}{l} \text{Find } \mathbf{u} \in \mathbf{H}_N(\mathbf{curl}, \text{div } 0) \text{ such that} \\ (\mathbf{curl } \mathbf{u}, \mathbf{curl } \mathbf{v}) = (\mathbf{f}, \mathbf{v}) \quad \forall \mathbf{v} \in \mathbf{H}_N(\mathbf{curl}) \end{array}$$

The existence and uniqueness of the solution to  $\mathcal{M}(\mathbf{curl})$  can be proved by restricting the space of test fields to  $\mathbf{H}_N(\mathbf{curl}, \text{div } 0)$ , which is allowed by the following lemma [5]:

LEMMA 3.2. – Every  $\mathbf{v} \in \mathbf{H}_N(\mathbf{curl})$  can be decomposed as

$$\mathbf{v} = \mathbf{v}_0 + \mathbf{grad } \varphi, \quad \text{where } \begin{cases} \mathbf{v}_0 \in \mathbf{H}_N(\mathbf{curl}, \text{div } 0) \text{ and } \mathbf{curl } \mathbf{v}_0 = \mathbf{curl } \mathbf{v} \\ \varphi \in H_0^1 \text{ and } \Delta \varphi = \text{div } \mathbf{v} \end{cases}$$

Noticing that for a test field  $\mathbf{v} = \mathbf{grad } \varphi$  with  $\varphi \in H_0^1$ , both terms of the above variational equation vanish (by virtue of (4)), this lemma shows that  $\mathcal{M}(\mathbf{curl})$  is equivalent to

$$(\mathcal{M}(\mathbf{curl}, \text{div } 0)) \quad \begin{array}{l} \text{Find } \mathbf{u} \in \mathbf{H}_N(\mathbf{curl}, \text{div } 0) \text{ such that} \\ (\mathbf{curl } \mathbf{u}, \mathbf{curl } \mathbf{v}) = (\mathbf{f}, \mathbf{v}) \quad \forall \mathbf{v} \in \mathbf{H}_N(\mathbf{curl}, \text{div } 0) \end{array}$$

PROPOSITION 3.3. –  $\mathcal{M}(\mathbf{curl})$  and  $\mathcal{M}(\mathbf{curl}, \text{div } 0)$  are equivalent and both well-posed. Their common solution is the unique field  $\mathbf{u} \in \mathbf{H}_N(\mathbf{curl}, \text{div } 0)$  which satisfies (1) in  $\mathcal{D}'(\Omega)^3$  (i.e., in the sense of distributions).

*Proof.* – For  $\mathcal{M}(\mathbf{curl}, \text{div } 0)$ , this is a direct consequence of Lemma 3.1 and Riesz lemma. The interpretation in  $\mathcal{D}'(\Omega)^3$  follows from  $\mathcal{M}(\mathbf{curl})$  thanks to the density [5] of  $\mathcal{D}(\Omega)^3$  in  $\mathbf{H}_N(\mathbf{curl})$ .  $\square$

### 3.2. The Lagrange problem

The variational interpretation of  $\mathcal{L}$ , deduced from (5)–(8) by Green’s formulas, involves now two test functions  $\mathbf{v}$  and  $q$ . Depending on the equation where the  $\mathbf{grad} \leftrightarrow \text{div}$  integration by parts is applied, we obtain two possible formulations:

$$(\mathcal{L}(\mathbf{curl})) \quad \begin{array}{l} \text{Find } \mathbf{u} \in \mathbf{H}_N(\mathbf{curl}) \text{ and } p \in H_0^1 \text{ such that} \\ (\mathbf{curl } \mathbf{u}, \mathbf{curl } \mathbf{v}) - (\mathbf{grad } p, \mathbf{v}) = (\mathbf{f}, \mathbf{v}) \quad \forall \mathbf{v} \in \mathbf{H}_N(\mathbf{curl}) \\ (\mathbf{grad } q, \mathbf{u}) = 0 \quad \forall q \in H_0^1 \end{array}$$

and

$$(\mathcal{L}(\mathbf{curl}, \text{div})) \quad \begin{array}{l} \text{Find } \mathbf{u} \in \mathbf{H}_N(\mathbf{curl}, \text{div}) \text{ and } p \in L^2 \text{ such that} \\ (\mathbf{curl } \mathbf{u}, \mathbf{curl } \mathbf{v}) + (p, \text{div } \mathbf{v}) = (\mathbf{f}, \mathbf{v}) \quad \forall \mathbf{v} \in \mathbf{H}_N(\mathbf{curl}, \text{div}) \\ (q, \text{div } \mathbf{u}) = 0 \quad \forall q \in L^2 \end{array}$$

In short, one can choose to exchange some regularity between  $\text{div } \mathbf{u}$  and  $\mathbf{grad } p$ . But fortunately these formulations are equivalent: the following proposition precises the proper functional framework in which the equivalence  $\mathcal{M} \iff \mathcal{L}$  claimed in (13) holds.

PROPOSITION 3.4. – Both problems  $\mathcal{L}(\mathbf{curl})$  and  $\mathcal{L}(\mathbf{curl}, \text{div})$  are well-posed. Their common solution is the pair  $(\mathbf{u}, 0)$  where  $\mathbf{u}$  is the solution to  $\mathcal{M}(\mathbf{curl})$  (or  $\mathcal{M}(\mathbf{curl}, \text{div } 0)$ ).

*Proof.* – The well-posedness follows from classical arguments of the theory of mixed problems [5,6]. Moreover, taking  $\mathbf{v} = \mathbf{grad } p \in \mathbf{H}_N(\mathbf{curl})$  in  $\mathcal{L}(\mathbf{curl})$  yields  $\|\mathbf{grad } p\| = 0$  by virtue of the assumption (4), hence  $p \equiv 0$ , which shows that  $\mathbf{u}$  satisfies  $\mathcal{M}(\mathbf{curl})$ . On the other hand, the solution  $\mathbf{u}$  to  $\mathcal{L}(\mathbf{curl}, \text{div})$  obviously satisfies  $\mathcal{M}(\mathbf{curl}, \text{div } 0)$  (take  $\mathbf{v}$  such that  $\text{div } \mathbf{v} = 0$ ), and  $p$  again vanishes: it suffices to choose  $\mathbf{v} = \mathbf{grad } \varphi$  where  $\varphi \in H_0^1$  is the solution to  $\Delta \varphi = p$  in  $\Omega$ .  $\square$

### 3.3. The Poisson problem

The case of the penalty formulation  $\mathcal{P}$  of our Maxwell problem can be dealt with similarly. Here only one variational interpretation is naturally obtained

$$(\mathcal{P}(\mathbf{curl}, \text{div})) \quad \text{Find } \mathbf{u} \in \mathbf{H}_N(\mathbf{curl}, \text{div}) \text{ such that} \\ (\mathbf{curl} \mathbf{u}, \mathbf{curl} \mathbf{v}) + (\text{div} \mathbf{u}, \text{div} \mathbf{v}) = (\mathbf{f}, \mathbf{v}) \quad \forall \mathbf{v} \in \mathbf{H}_N(\mathbf{curl}, \text{div})$$

PROPOSITION 3.5. – *Problem  $\mathcal{P}(\mathbf{curl}, \text{div})$  is well-posed, and its solution coincide with that to  $\mathcal{M}(\mathbf{curl})$ .*

*Proof.* – As for Proposition 3.3, the well-posedness follows from Lemma 3.1 and Riesz lemma. Moreover setting  $p = \text{div} \mathbf{u}$  and choosing as above  $\mathbf{v} = \mathbf{grad} \varphi$  where  $\varphi \in H_0^1$  is the solution to  $\Delta \varphi = p$ , yields again  $p \equiv 0$ .  $\square$

### 3.4. Which ones are well suited for a numerical approximation?

Neither  $\mathcal{M}(\mathbf{curl})$  nor  $\mathcal{M}(\mathbf{curl}, \text{div} 0)$  are appropriate for a finite element discretization. Indeed, the divergence-free condition is taken into account in a ‘strong sense’, since it is imposed directly on the solution, not in the variational equation. Hence a conforming approximation would require divergence-free discrete fields. The essential interest of the alternative problems  $\mathcal{L}$  and  $\mathcal{P}$  is to offer a weak interpretation of the divergence-free condition.

But  $\mathcal{L}(\mathbf{curl}, \text{div})$  and  $\mathcal{P}(\mathbf{curl}, \text{div})$  are in general no more appropriate. From the results of the next section, one will easily convince himself that if the domain has reentrant corners or edges, there is no piecewise polynomial discretization which is conforming in  $\mathbf{H}_N(\mathbf{curl}, \text{div})$ . This is a consequence of the *non-density* of regular fields (satisfying  $(\mathbf{u} \times \mathbf{n})|_\Gamma = 0$ ) in  $\mathbf{H}_N(\mathbf{curl}, \text{div})$ . More intuitively one can notice that a piecewise polynomial field  $\mathbf{u}$  is such that  $\mathbf{curl} \mathbf{u} \in L^2$  and  $\text{div} \mathbf{u} \in L^2$  if and only if it is continuous in  $\Omega$  (since both normal and tangential components must be continuous across elements). Hence this field belongs to  $\mathbf{H}^1$ . The core of the corner paradox is that such discrete fields can only approximate a genuine subspace of  $\mathbf{H}_N(\mathbf{curl}, \text{div})$ .

The sole remaining formulation is the ‘good’ one:  $\mathcal{L}(\mathbf{curl})$  is the starting point of a discretization by *edge* elements [7,8], which consists in a  $\mathbf{H}_N(\mathbf{curl})$ -conforming approximation (the tangential component of a discrete field is continuous across elements, not the normal one).

## 4. A mathematical curiosity

The trouble originates from the following relation which derives immediately from (12) by Green’s formulas:

$$\int_{\mathbb{R}^3} (\mathbf{curl} \mathbf{u} \cdot \mathbf{curl} \mathbf{v} + \text{div} \mathbf{u} \text{div} \mathbf{v}) \, dx = \int_{\mathbb{R}^3} \mathbf{grad} \mathbf{u} \cdot \mathbf{grad} \mathbf{v} \, dx \quad \forall \mathbf{u}, \mathbf{v} \in \mathcal{D}(\mathbb{R}^3)^3$$

It actually shows that

$$\mathbf{H}^1(\mathbb{R}^3) = \mathbf{H}(\mathbf{curl}, \text{div}; \mathbb{R}^3) := \{ \mathbf{u} \in L^2(\mathbb{R}^3); \mathbf{curl} \mathbf{u} \in L^2(\mathbb{R}^3) \text{ and } \text{div} \mathbf{u} \in L^2(\mathbb{R}^3) \}$$

since  $\mathcal{D}(\mathbb{R}^3)^3$  is *dense* in both spaces [5]. Such an identity is unlikely to hold for a subset  $\Omega$  of  $\mathbb{R}^3$ : boundary integrals appear in the above relation when applying Green’s formulas. However these boundary terms vanish if  $\mathbf{u}$  and  $\mathbf{v}$  are normal to  $\Gamma$ . More precisely one has [9]:

LEMMA 4.1. – *Let  $\mathbf{D}_N$  be the subspace of  $\mathcal{D}(\overline{\Omega})^3$  consisting of the fields  $\mathbf{u}$  such that  $(\mathbf{u} \times \mathbf{n})|_\Gamma = 0$  and  $\mathbf{u}$  vanishes in a (volumic) vicinity of the edges and corners of the polyhedron  $\Omega$ . Then*

$$(\mathbf{curl} \mathbf{u}, \mathbf{curl} \mathbf{v}) + (\text{div} \mathbf{u}, \text{div} \mathbf{v}) = (\mathbf{grad} \mathbf{u}, \mathbf{grad} \mathbf{v}) \quad \forall \mathbf{u}, \mathbf{v} \in \mathbf{D}_N \quad (16)$$

Noticing in addition that  $\mathbf{D}_N$  is *dense* [10] in

$$\mathbf{H}_N(\mathbf{grad}) := \{ \mathbf{v} \in \mathbf{H}^1; (\mathbf{v} \times \mathbf{n})|_{\Gamma} = 0 \} \quad (17)$$

this formula shows that  $\mathbf{H}_N(\mathbf{grad})$  is a *closed subspace* of  $\mathbf{H}_N(\mathbf{curl}, \text{div})$ . A hasty conclusion would be the assertion of their equality, as in the case of  $\mathbb{R}^3$ . This actually is true if  $\Omega$  is *convex* or has a *regular boundary* [5]. But for a nonconvex polyhedron,  $\mathbf{H}_N(\mathbf{grad})$  is a *genuine* subspace of  $\mathbf{H}_N(\mathbf{curl}, \text{div})$ : there exists a non-trivial subspace  $\mathbf{H}_{\text{sing}}$  of  $\mathbf{H}_N(\mathbf{curl}, \text{div})$  such that the latter has the *direct* decomposition

$$\mathbf{H}_N(\mathbf{curl}, \text{div}) = \mathbf{H}_N(\mathbf{grad}) \oplus \mathbf{H}_{\text{sing}} \quad (18)$$

The physical meaning of the *singular fields* contained in  $\mathbf{H}_{\text{sing}}$  is nothing but the well-known ‘corner effect’ in electromagnetism, i.e., the high intensity of the electromagnetic field near *reentrant* corners: a metallic knife in a microwave oven yields a convincing demonstration of this effect!

#### 4.1. About the theory of ‘singularities’ for the scalar Laplace operator

In order to obtain a precise characterization of  $\mathbf{H}_{\text{sing}}$ , we recall some essential results concerning the *singularities* of the scalar Laplace operator in a *nonconvex* polyhedral domain  $\Omega$  (see [11–13] for details). Their definition is based on a technical result which asserts that *the image of  $H_0^1 \cap H^2$  by the operator  $\Delta$  is a closed subspace of  $L^2$  whose codimension is infinite*. Let  $\mathcal{N}$  denote its orthogonal complement in  $L^2$ : a function  $p \in L^2$  belongs to  $\mathcal{N}$  if and only if

$$(p, \Delta\psi) = 0 \quad \forall \psi \in H_0^1 \cap H^2 \quad (19)$$

This property actually furnishes the proper interpretation of *very weak* solutions to the homogeneous problem (14)–(15). To see this, first choose  $\psi \in \mathcal{D}(\Omega)$ , which yields  $\Delta p = 0$  in the sense of distributions. The difficulty lies in the Dirichlet boundary condition (15) which cannot be understood as the *trace* of a  $H^1$  function. Indeed if  $p$  belonged to  $H^1$ , Green’s formula would give

$$\int_{\Gamma} p \partial_n \psi \, d\gamma = 0 \quad \forall \psi \in H_0^1 \cap H^2$$

which is enough to conclude that  $p|_{\Gamma} = 0$  (since  $\partial_n \psi$  can spread over a dense subset of  $L^2(\Gamma)$ ), thus  $p \equiv 0$ . However it may be seen (by a simple symmetry argument, often called the *image principle*) that  $p$  is regular up to the boundary except near corners and edges. Hence one can apply Green’s formula for  $\psi$  vanishing near these geometric singularities, which shows that the *trace* of  $p$  on  $\Gamma$  exists and vanishes outside corners and edges. This idea is related to a ‘very weak’ notion of trace, which can be more generally defined by a duality technique. For our purposes, we may content ourselves with the following definition (see [12] in 2D, and [14] in 3D).

**DEFINITION 4.2.** – A function  $p \in L^2 \setminus H^1$  is said to be a *very weak solution* to the homogeneous Dirichlet problem (14)–(15) if it satisfies (19) (i.e.,  $p \in \mathcal{N}$ ).

These functions play a fundamental role in the regularity of the variational solution  $\varphi \in H_0^1$  to the scalar Poisson equation  $\Delta\varphi = g \in L^2$ , i.e.,

$$-(\mathbf{grad} \varphi, \mathbf{grad} \psi) = (g, \psi) \quad \forall \psi \in H_0^1 \quad (20)$$

which will be denoted for simplicity  $\varphi = \Delta^{-1}g$ . Projecting  $g$  along the orthogonal decomposition  $L^2 = \Delta(H_0^1 \cap H^2) \oplus \mathcal{N}$  shows that  $\varphi$  can be split into a *regular* part and a *singular* part:

$$\varphi = \varphi_R + \varphi_S, \quad \text{where } \varphi_R \in H_0^1 \cap H^2 \text{ and } \varphi_S \in \mathcal{S} := \Delta^{-1}(\mathcal{N}). \quad (21)$$

Note that by construction  $\mathcal{S} \subset H_0^1 \setminus H^2$ : this justifies the word *singular*.

#### 4.2. Description of the singular fields

The latter inclusion and the definition of  $\mathcal{S}$  clearly show that

$$\mathbf{grad} \mathcal{S} \subset \mathbf{H}_N(\mathbf{curl}, \text{div}) \setminus \mathbf{H}_N(\mathbf{grad})$$

But do these gradients cover all possible singular fields? The first (positive) answer seems to be due to Birman and Solomyak [15] (see also [10,16]):

THEOREM 4.3. – *The space  $\mathbf{H}_N(\mathbf{curl}, \text{div})$  has the following direct decomposition:*

$$\mathbf{H}_N(\mathbf{curl}, \text{div}) = \mathbf{H}_N(\mathbf{grad}) \oplus \mathbf{grad} \mathcal{S} \quad (22)$$

Hence  $\mathbf{grad} \mathcal{S}$  is a good candidate to play the role of the *singular space*  $\mathbf{H}_{\text{sing}}$  in (18). Obviously this is not the only one: the same results hold if we replace  $\mathcal{N}$  by any supplementary (but non orthogonal) subspace  $\mathcal{N}'$  to  $\Delta(H_0^1 \cap H^2)$  in  $L^2$ .

#### 4.3. Spurious interpretations of $\mathcal{L}$ and $\mathcal{P}$

The practical consequence of the above results is the existence of *spurious* variational problems  $\mathcal{L}(\mathbf{grad})$  and  $\mathcal{P}(\mathbf{grad})$  deduced from the  $(\mathbf{curl}, \text{div})$  interpretations of  $\mathcal{L}$  and  $\mathcal{P}$  by replacing  $\mathbf{H}_N(\mathbf{curl}, \text{div})$  by  $\mathbf{H}_N(\mathbf{grad})$ , i.e.,

$$\begin{aligned} (\mathcal{L}(\mathbf{grad})) \quad & \text{Find } \mathbf{u} \in \mathbf{H}_N(\mathbf{grad}) \text{ and } p \in L^2 \text{ such that} \\ & (\mathbf{curl} \mathbf{u}, \mathbf{curl} \mathbf{v}) + (p, \text{div} \mathbf{v}) = (\mathbf{f}, \mathbf{v}) \quad \forall \mathbf{v} \in \mathbf{H}_N(\mathbf{grad}) \\ & (q, \text{div} \mathbf{u}) = 0 \quad \forall q \in L^2 \end{aligned}$$

and

$$\begin{aligned} (\mathcal{P}(\mathbf{grad})) \quad & \text{Find } \mathbf{u} \in \mathbf{H}_N(\mathbf{grad}) \text{ such that} \\ & (\mathbf{curl} \mathbf{u}, \mathbf{curl} \mathbf{v}) + (\text{div} \mathbf{u}, \text{div} \mathbf{v}) = (\mathbf{f}, \mathbf{v}) \quad \forall \mathbf{v} \in \mathbf{H}_N(\mathbf{grad}) \end{aligned}$$

PROPOSITION 4.4. – *Problems  $\mathcal{L}(\mathbf{grad})$  and  $\mathcal{P}(\mathbf{grad})$  are both well-posed.*

*Proof.* – For  $\mathcal{P}(\mathbf{grad})$ , this follows from Lemma 4.1 and Riesz lemma. For  $\mathcal{L}(\mathbf{grad})$ , this can be proved by establishing the associated *inf-sup* condition [17].  $\square$

Obviously, the respective solutions to  $\mathcal{L}(\mathbf{grad})$  and  $\mathcal{P}(\mathbf{grad})$  are unlikely to coincide with the common ‘physical’ solution to the  $(\mathbf{curl}, \text{div})$  formulations since the functional spaces differ. Roughly speaking,  $\mathbf{H}_N(\mathbf{curl}, \text{div})$  plays the role of the *physical* space, whereas  $\mathbf{H}_N(\mathbf{grad})$  is the *spurious* one. Both *physical* and *spurious* solutions can be approximated by finite elements. And it may be proved that *edge* elements capture the physical one: they leave the spurious solution to *nodal* elements. Here the ‘progressives’ are a few points up on the ‘conservatives’!

Going back to the ‘strong’ formulations (5)–(8) and (9)–(11) of  $\mathcal{L}$  and  $\mathcal{P}$ , it is now clear that the only difference between the  $(\mathbf{curl}, \text{div})$  and the  $(\mathbf{grad})$  formulations lies in the interpretation of the boundary condition satisfied by  $p$  in  $\mathcal{L}$  or  $\text{div} \mathbf{u}$  in  $\mathcal{P}$ . For the spurious formulations it has to be taken in the ‘very weak’ sense of Definition 4.2 (see [10,18]): taking  $\mathbf{v} = \mathbf{grad} \psi$  with  $\psi \in H_0^1 \cap H^2$  in  $\mathcal{L}(\mathbf{grad})$  or  $\mathcal{P}(\mathbf{grad})$  clearly shows that  $p$  or  $\text{div} \mathbf{u}$  belongs to  $\mathcal{N}$ .

#### 5. Numerical remedies: two strategies

For the ‘conservatives’, a natural way to save their *nodal* elements was to take advantage of the results of the previous section to find a cure for the spurious formulations. Two different approaches were independently developed in the last... say 6 years. The general ideas can be explained for our 3D model,



but we describe the numerical implementation only for the 2D situation. In this case, the space  $\mathcal{S}$  has a *finite dimension* which is exactly the number of reentrant corners [11,12]. Near each of them, the behaviour of a function  $\varphi \in \mathcal{S}$  is given by

$$\varphi(r, \theta) = \alpha s(r, \theta) + \varphi_R(r, \theta), \quad \text{where } s(r, \theta) = r^{\pi/\omega} \sin\left(\frac{\pi}{\omega}\theta\right) \quad (23)$$

and  $(r, \theta)$  denote local polar coordinates with respect to the vertex of the corner, with  $\theta \in [0, \omega]$  and  $\omega$  is the opening angle. The coefficient  $\alpha$  plays the role of a ‘stress intensity factor’ whereas  $\varphi_R \in H_0^1 \cap H^2$  is the *regular* part of  $\varphi$  (the first *singular* part belongs to  $H_0^1 \setminus H^2$  near the corner). This very simple description of  $\mathcal{S}$  is the very difference from 3D situations.

### 5.1. The mixed approach

The method proposed by Assous, Ciarlet et al. [17,19,20] is related to the following proposition [17] which asserts that the solution to the *spurious* problem  $\mathcal{L}(\mathbf{grad})$  contains all the information required to recover the *physical* solution.

PROPOSITION 5.1. – *If  $(\mathbf{u}, p) \in \mathbf{H}_N(\mathbf{grad}) \times L^2$  satisfies  $\mathcal{L}(\mathbf{grad})$ , then the solution to  $\mathcal{M}(\mathbf{curl})$  is given by  $\mathbf{u}_{\mathcal{M}} = \mathbf{u} + \mathbf{u}_S(p)$  where  $\mathbf{u}_S(p) \in \mathbf{H}_N(\mathbf{curl}, \text{div } 0)$  is the solution to*

$$(\mathbf{curl} \mathbf{u}_S(p), \mathbf{curl} \mathbf{v}) + (p, \text{div } \mathbf{v}) = 0 \quad \forall \mathbf{v} \in \mathbf{H}_N(\mathbf{grad}) \quad (24)$$

This is the representation of  $\mathbf{u}_{\mathcal{M}}$  in the decomposition

$$\mathbf{H}_N(\mathbf{curl}, \text{div } 0) = \mathbf{H}_N(\mathbf{grad}, \text{div } 0) \oplus^\perp \{\mathbf{u}_S(p); p \in \mathcal{N}\} \quad (25)$$

where  $\mathbf{H}_N(\mathbf{grad}, \text{div } 0) = \{\mathbf{v} \in \mathbf{H}_N(\mathbf{grad}); \text{div } \mathbf{v} = 0 \text{ in } \Omega\}$ . This decomposition is orthogonal for the scalar product  $(\mathbf{curl} \cdot, \mathbf{curl} \cdot)$  (see Lemma 3.1).

Equation (24) signifies that  $\mathbf{curl} \mathbf{curl} \mathbf{u}_S(p) = \mathbf{grad} p$ , which is not an ‘optical illusion’: a **curl** can also be a **grad** if they both live near reentrant corners! But solving such an equation actually raises higher numerical difficulties as for our initial Maxwell problem ( $\mathbf{grad} p \notin L^2$  in general).

In 2D (but only in this case), we can get out of trouble thanks to an alternative characterization of the orthogonal complement of  $\mathbf{H}_N(\mathbf{grad}, \text{div } 0)$ , related to the singularities of the *Neumann* Laplace operator. Their definition is similar to the Dirichlet case recalled in Section 4, starting from the following decomposition of  $L_0^2 := \{p \in L^2; (p, 1) = 0\}$  (the index 0 stands for zero mean value):

$$L_0^2 = \Delta(H_{\text{neu}}^2) \oplus^\perp \mathcal{N}_{\text{neu}}, \quad \text{where } H_{\text{neu}}^2 := \{\psi \in H^2/\mathbb{R}; \partial_n \psi|_\Gamma = 0\}$$

The idea is to introduce this orthogonal sum in the following diagram [19] which involves the scalar and vector curl operators and gives a precise functional context for the formula  $\mathbf{curl} \mathbf{curl} = -\Delta$  (all arrows denote isomorphisms):

$$\begin{array}{ccc} \mathbf{H}_N(\mathbf{curl}, \text{div } 0) & \xrightarrow{\mathbf{curl}} & L_0^2 \\ \uparrow \mathbf{curl} & & \uparrow -\Delta_{\text{neu}} \\ H_{\text{neu}}^1 := \{\psi \in H^1/\mathbb{R}; \Delta \psi \in L^2 \text{ and } \partial_n \psi|_\Gamma = 0\} & & \end{array}$$

We obtain

$$\mathbf{H}_N(\mathbf{curl}, \text{div } 0) = \mathbf{H}_N(\mathbf{grad}, \text{div } 0) \oplus^\perp \mathbf{curl}^{-1}(\mathcal{N}_{\text{neu}}) \quad \text{with } \mathbf{curl}^{-1} = -\mathbf{curl} \circ \Delta_{\text{neu}}^{-1}$$

Hence setting  $\mathbf{u}_S(p) = \text{curl}^{-1} \varphi$  with  $\varphi \in \mathcal{N}_{\text{neu}}$  in (24) shows that  $\mathbf{curl} \varphi = \mathbf{grad} p$ . As a consequence a possible algorithm for computing  $\mathbf{u}_{\mathcal{M}}$  is: first compute a basis of  $\mathcal{N}$  and  $\mathcal{N}_{\text{neu}}$ , then solve  $\mathcal{L}(\mathbf{grad})$  by nodal elements, and finally find the singular part  $\mathbf{u}_S$  using the above trick. The numerical procedures proposed in [19,20] consist in a slight variation of this scheme. The computation of a basis of  $\mathcal{N}$  or  $\mathcal{N}_{\text{neu}}$  is achieved by a ‘Dirichlet-to-Neumann’ technique (based on separation of local polar coordinates near a corner, which yields an explicit series expansion).

## 5.2. The penalty approach

The method adopted by the CNRS/ENSTA team [10,21–23] consists in solving  $\mathcal{P}(\mathbf{curl}, \text{div})$  using a direct decomposition of type (18). Since  $\mathbf{H}_N(\mathbf{grad})$  can be approximated by nodal elements, it suffices to enrich such a discretization by a basis of  $\mathbf{H}_{\text{sing}}$ . The only question is: how to choose  $\mathbf{H}_{\text{sing}}$  to make the implementation easy?

In 2D, the simplest choice for  $\mathbf{H}_{\text{sing}}$  follows from (23) by introducing for each corner a smooth cut-off functions  $\eta(r)$  whose support is localized near the vertex. One can choose instead of  $\mathcal{S}$  the space  $\mathcal{S}_0$  spanned by the functions  $\eta(r) s(r, \theta)$  corresponding to all corners (where the supports of the different cut-off functions do not intersect). This leads to consider  $\mathbf{H}_{\text{sing}} = \mathbf{grad} \mathcal{S}_0$ . In this case, the solution  $\mathbf{u}$  to the *physical* problem  $\mathcal{P}(\mathbf{curl}, \text{div})$  can be rewritten  $\mathbf{u} = \mathbf{u}_R + \mathbf{grad} \varphi_S$  where the pair  $(\mathbf{u}_R, \varphi_S) \in \mathbf{H}_N(\mathbf{grad}) \times \mathcal{S}_0$  satisfies

$$\begin{aligned} (\mathbf{curl} \mathbf{u}_R, \mathbf{curl} \mathbf{v}_R) + (\text{div} \mathbf{u}_R, \text{div} \mathbf{v}_R) + (\Delta \varphi_S, \text{div} \mathbf{v}_R) &= (\mathbf{f}, \text{div} \mathbf{v}_R) \quad \forall \mathbf{v}_R \in \mathbf{H}_N(\mathbf{grad}) \\ (\text{div} \mathbf{u}_R, \Delta \psi_S) + (\Delta \varphi_S, \Delta \psi_S) &= (\mathbf{f}, \Delta \psi_S) \quad \forall \psi_S \in \mathcal{S}_0 \end{aligned}$$

Using a nodal discretization of  $\mathbf{H}_N(\mathbf{grad})$  and the basis of  $\mathcal{S}_0$  formed by the localized singular functions  $\eta s$ , we are led to a coupled problem between the discrete regular part and the ‘stress intensity factors’. The latter can be solved by a *block* method involving a solver of the discrete problem  $\mathcal{P}(\mathbf{grad})$ .

The flaw of this method is... its inaccuracy! Indeed the use of cut-off functions introduces high variations of the regular part (in the region where these functions vary from 0 to 1), hence a poor convergence of the finite element scheme. In order to get rid of these undesirable functions, the idea [23] is to construct an *orthogonal* decomposition (18) by solving a problem of type  $\mathcal{P}(\mathbf{grad})$  with *non-homogeneous* boundary conditions. It may be seen that for each corner (to which corresponds the singular function  $s$  given in (23)), the field  $\mathbf{u} + \mathbf{grad} s$  is orthogonal to  $\mathbf{H}_N(\mathbf{grad})$  (for the scalar product of Lemma 3.1) if  $\mathbf{u} \in \mathbf{H}^1$  satisfies

$$\begin{aligned} (\mathbf{curl} \mathbf{u}, \mathbf{curl} \mathbf{v}) + (\text{div} \mathbf{u}, \text{div} \mathbf{v}) &= 0 \quad \forall \mathbf{v} \in \mathbf{H}_N(\mathbf{grad}) \\ \mathbf{u} \times \mathbf{n} &= -\mathbf{grad} s \times \mathbf{n} \quad \text{on } \Gamma \end{aligned}$$

This problem is well suited for a nodal finite element scheme, which yields an approximation of  $\mathbf{H}_{\text{sing}}^\perp$ . In this case, the physical problem  $\mathcal{P}(\mathbf{curl}, \text{div})$  turns into the uncoupled computations of the regular part (by solving  $\mathcal{P}(\mathbf{grad})$ ) and the ‘stress intensity factors’. This version of the *singular field method* is easy to implement, and... accurate!

The recent work by Assous et al. [24,25] consists in an extension of this approach for the time-dependent Maxwell’s equations in the presence of charges, i.e., for a non-homogeneous divergence condition  $\text{div} \mathbf{u} = g$  instead of (2). The latter is taken into account by introducing a Lagrange multiplier in the *penalty* formulation, which may be seen as an augmented lagrangian technique. But this multiplier plays a different role from the *mixed* approach: here we are interested in the multiplier of the *physical* formulation, not of the *spurious* one.

## 5.3. What about 3D problems?

The  $\mathcal{L}$ -approach does not seem adapted to the treatment of 3D problems since it involves the solution of the ‘stiff’ problem (24). On the other hand, the first 3D implementation of the  $\mathcal{P}$ -approach has been carried

out very recently for an axisymmetric conical point [26]: in this case, the singular fields still live in a space of finite dimension. This does not hold for a polyhedral corner: the implementation seems possible, but at what price?

Can we conclude by the defeat of the ‘conservatives’ in 3D? Not yet: Costabel and Dauge [27] proposed an alternative cure for the failure of nodal elements, whose implementation in 3D seems easy. Apparently close to the  $\mathcal{P}$ -approach, it actually involves special weights inside the divergence integral, depending only on the distance from reentrant singularities. By a simple refinement of the mesh near the latter, nodal elements become capable of capturing the singular behaviour of the field. This ‘weighted regularization’ is justified by density arguments which go beyond the framework of the present paper.

## 6. Possible extensions and related topics

The *corner paradox* described here for a ‘schoolish’ model occurs for most problems deriving from Maxwell’s equations, either for electric or magnetic boundary conditions near a perfect conductor, or transmission conditions across discontinuities of the medium [10,16,28], as well as for time-dependent problems [24,25,20] (see also [29,30]). The situation is quite different if an *impedance* boundary condition is used: in theory, the addition of singular fields is no longer required (which follows from the density of smooth fields in the involved function space [31,32]). But in practice [33], a poor convergence of the numerical scheme can be observed.

One could be tempted to compare the *corner paradox* with the *plate paradox* [34] which is known to occur in the Kirchhoff model of the plate-bending problem, when a *hard* support is used: on a sequence of *convex* polygonal domains converging to a regular one, the solutions to the polygonal plate-bending problem do not converge to the solution to the limit problem! However the explanation of this paradox is quite different (although a similar phenomenon exists for Maxwell’s equations [35]): the limit problem has two possible interpretations again related to boundary conditions, whereas for a polygonal domain, both coincide.

On the other hand, in the context of linear aeroacoustics, Galbrun’s equation is dealt with in [36] by a penalty technique similar to our  $\mathcal{P}$ -approach, but where the roles of the operators **curl curl** and **grad div** are exchanged. As for Maxwell’s equations, the presence of reentrant corners can break the equivalence between the penalty problem and the initial *physical* problem, but the influence of singularities has not been studied yet.

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