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Constructing exact sequences on non-conforming discrete spaces

Construction de suites exactes sur des espaces discrets non conformes

Martin Campos Pinto

CNRS, Sorbonne Universités, UPMC Université Paris-6, UMR 7598, Laboratoire Jacques-Louis-Lions, 4, place Jussieu, 75005 Paris, France

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ABSTRACT

In this note, we propose a general procedure to construct exact sequences involving a non-conforming function space and we show how this construction can be used to derive a proper discrete Gauss law for structure-preserving discontinuous Galerkin (DG) approximations to the time-dependent 2d Maxwell equations.

RÉSUMÉ

Dans cette note, nous proposons un procédé général pour construire des suites exactes autour d'un espace non conforme, et nous montrons comment ce procédé peut servir à écrire une loi de Gauss discrète convenable dans le cadre d'approximations Galerkin discontinues (DG) des équations de Maxwell temporelles en 2d.

Version française abrégée

Étant donné une suite exacte discrète $V_h^0 \xrightarrow{d_h^0} V_h^1 \xrightarrow{d_h^1} V_h^2$, qui sera composée en pratique d'espaces conformes (i.e. inclus dans des espaces de référence de dimension infinie), il est possible de construire une nouvelle suite exacte mettant en jeu un espace arbitraire $\tilde{V}_h^1$ par la procédure suivante.

- En s'appuyant sur un projecteur $\mathcal{P}_h^1$ vers l'espace conforme V_h^1, on pose $\tilde{d}_h^1 := d_h^1 \mathcal{P}_h^1$. Le noyau de ce nouvel opérateur est essentiellement composé de l'image de d_h^0 et du noyau de $\mathcal{P}_h^1$.
- Pour définir un bon opérateur $\tilde{d}_h^0$, on étend l'opérateur d_h^0 à un espace $\tilde{V}_h^0$ contenu dans $V_h^0 \times \tilde{V}_h^1$, de façon à atteindre tous les éléments de ce nouveau noyau. On montre alors que la suite ainsi construite,

E-mail address: campos@ljll.math.upmc.fr.

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$$\tilde V_h^0 \xrightarrow{\tilde d_h^0} \tilde V_h^1 \xrightarrow{\tilde d_h^1} V_h^2,$$

est exacte.

Cette construction est motivée par l'analyse et le développement de méthodes d'approximation non conformes (ou externes, suivant la terminologie classique [11]) préservant la structure. En particulier, on montre qu'il est possible de l'appliquer au cadre des schémas DG pour les équations de Maxwell en 2d. Lorsque l'opérateur $\mathcal{P}_h^1$ est obtenu par moyennisation locale des degrés de liberté d'arêtes dans une extension aux fonctions régulières par morceaux de l'interpolant canonique sur les éléments finis de Nédélec en 2d, la construction proposée ici permet en effet de retrouver l'opérateur rotationnel discret standard du schéma DG à flux centré.

La suite exacte ainsi construite fait alors intervenir un nouvel opérateur discret de type gradient dans un cadre Galerkin discontinu, qui par dualité définit un nouvel opérateur de divergence discrète. Conformément au programme de travail décrit dans [7–9] en vue d'obtenir des schémas généraux préservant la structure pour les équations de Maxwell temporelles, cet opérateur divergence a les propriétés requises pour définir une loi de Gauss discrète devant être vérifiée par un schéma DG préservant la charge.

1. Introduction

Exact sequences of function spaces with differential operators such as gradient, curl or divergence play a major role in the construction and analysis of mixed finite element approximations of physical problems. This is especially true in computational electromagnetics since the works of Bossavit [5,6], who has pointed out the importance of preserving at the discrete level the natural structure of Maxwell's equations in terms of de Rham diagrams of differential forms [16], and in the recent decades the study of structure-preserving schemes has become a field of its own with numerous developments, see, e.g., [2,15,12,3,18,13,1,4,10].

In the context of Hilbert spaces, de Rham diagrams take the form of sequences like

$$H^1(\Omega) \xrightarrow{\mathbf{grad}} H(\mathbf{curl};\Omega) \xrightarrow{\mathbf{curl}} H(\mathrm{div};\Omega) \xrightarrow{\mathrm{div}} L^2(\Omega) \tag{1}$$

which, under some smoothness and topological assumptions on the domain Ω, are *exact* in the sense that the range of each operator coincides with the kernel of the next one in the sequence. Many fundamental properties of finite-element discretizations, such as the spectral correctness of Maxwell's eigenvalue problem are then related to the question whether the underlying function spaces preserve this property.

To our knowledge, most of the available work in the field is concerned with *conforming* methods where the finite-dimensional function spaces are embedded in the above sequence (1). In this note, we address the case of non-conforming methods (or exterior, following the classical terminology of [11]) and propose a general procedure to construct an exact sequence involving an arbitrary function space. We then show how it can be used to derive a proper discrete Gauss law in the context of structure-preserving discontinuous Galerkin (DG) approximations of the time-dependent Maxwell equations in 2d, following the approach proposed in [7].

2. Abstract construction of exact sequences on arbitrary spaces

In this section, we provide a general procedure to build an exact sequence on an arbitrary discrete space, starting from a known exact sequence. To this end, we consider an abstract sequence of the form

$$V_h^0 \xrightarrow{d_h^0} V_h^1 \xrightarrow{d_h^1} V_h^2 \tag{2}$$

which is assumed exact in the sense that

$$\ker d_h^1 = d_h^0 V_h^0. \tag{3}$$

The typical situation that we have in mind is that of conforming spaces V_h^k (i.e. embedded in a sequence of Hilbert spaces such as (1)) and operators d_h^k defined as the restriction of the corresponding differential operators. Now, if $\tilde V_h^1$ is a finite-dimensional space that is a subset of neither V_h^1 nor the Hilbert space associated with the differential operator d_h^1 in the continuous sequence (1), we can build a new operator $\tilde d_h^1$ approximating d_h^1 on $\tilde V_h^1$ by considering a projection on V_h^1,

$$\mathcal{P}_h^1 : \hat V_h^1 \to V_h^1 \qquad \text{where} \qquad \hat V_h^1 := V_h^1 + \tilde V_h^1 \tag{4}$$

(here the sum is necessary since $\mathcal{P}_h^1$ must be defined on V_h^1), and by setting

$$\tilde d_h^1 := d_h^1 \mathcal{P}_h^1|_{\tilde V_h^1} : \tilde V_h^1 \to V_h^2. \tag{5}$$

In order to build an exact sequence involving $\tilde V_h^1$, we need to characterize the kernel of the latter operator.

Lemma 2.1. *It holds*

$$\ker \tilde{d}_h^1 = \left(d_h^0 V_h^0 \oplus (I - \mathcal{P}_h^1)\tilde{V}_h^1\right) \cap \tilde{V}_h^1.$$

Proof. The inclusion $\supset$ is easily verified by applying $\tilde{d}_h^1$; indeed this operator coincides with d_h^1 on $d_h^0 V_h^0$, since the latter is in V_h^1. To verify next the inclusion $\subset$, we take $u \in \ker \tilde{d}_h^1$. Then $\mathcal{P}_h^1 u$ is in V_h^1 and also in $\ker d_h^1$, hence in $d_h^0 V_h^0$ according to the exact sequence property (3). In particular, we have

$$u = \mathcal{P}_h^1 u + (I - \mathcal{P}_h^1)u \in d_h^0 V_h^0 \oplus (I - \mathcal{P}_h^1)\tilde{V}_h^1$$

where we have used that $u \in \tilde{V}_h^1$, and the inclusion follows. Here the direct sum is verified by applying $\mathcal{P}_h^1$ to some $u \in d_h^0 V_h^0 \cap (I - \mathcal{P}_h^1)\tilde{V}_h^1$: clearly $\mathcal{P}_h^1 u = 0$, and since $d_h^0 V_h^0 \subset V_h^1$ we also have $u = \mathcal{P}_h^1 u$. □

Now that the kernel of $\tilde{d}_h^1$ is characterized, we may define an approximation of d_h^0 on the product space $V_h^0 \times \tilde{V}_h^1$. Specifically, we set

$$\hat{d}_h^0 : \quad \hat{V}_h^0 \to \hat{V}_h^1, \quad (\varphi, u) \mapsto d_h^0 \varphi + (I - \mathcal{P}_h^1)u, \qquad \text{where} \qquad \hat{V}_h^0 := V_h^0 \times \tilde{V}_h^1. \tag{6}$$

The proper operator on $\tilde{V}_h^1$ is then obtained by a simple restriction

$$\tilde{d}_h^0 := \hat{d}_h^0|_{\tilde{V}_h^0} : \tilde{V}_h^0 \to \tilde{V}_h^1 \qquad \text{where} \qquad \tilde{V}_h^0 := (\hat{d}_h^0)^{-1}(\tilde{V}_h^1) = \left\{(\varphi, u) \in \hat{V}_h^0 : \hat{d}_h^0(\varphi, u) \in \tilde{V}_h^1\right\}, \tag{7}$$

indeed this yields the following result.

Theorem 2.2. *The sequence*

$$\tilde{V}_h^0 \xrightarrow{\ \tilde{d}_h^0\ } \tilde{V}_h^1 \xrightarrow{\ \tilde{d}_h^1\ } V_h^2 \tag{8}$$

is exact, in the sense that $\tilde{d}_h^0 \tilde{V}_h^0 = \ker \tilde{d}_h^1$.

Proof. The claimed relation is straightforward to verify, using the definition of $\tilde{d}_h^0$ and Lemma 2.1. □

Remark 1. If we let $\hat{d}_h^1 := d_h^1 \mathcal{P}_h^1$ then the sequence

$$\hat{V}_h^0 \xrightarrow{\ \hat{d}_h^0\ } \hat{V}_h^1 \xrightarrow{\ \hat{d}_h^1\ } V_h^2 \tag{9}$$

is also exact, and it remains so if we set $\hat{V}_h^0 := V_h^0 \times \hat{V}_h^1$ in (6), since $(I - \mathcal{P}_h^1)\hat{V}_h^1 = (I - \mathcal{P}_h^1)\tilde{V}_h^1$.

Remark 2. If $V_h^1 \subset \tilde{V}_h^1$, the above construction simplifies, as the sequences (8) and (9) coincide.

3. Application to the centered DG discretization of the 2d Maxwell system

The abstract construction described above can be applied to the design of structure-preserving Maxwell schemes based on fully discontinuous finite-element spaces, following the program outlined in [7, Sec. 4]. In this short note, we illustrate this construction in the case of a discontinuous Galerkin (DG) discretization of the normalized 2d Maxwell system

$$\begin{cases} \partial_t B + \operatorname{curl} \boldsymbol{E} = 0 \\ \partial_t \boldsymbol{E} - \mathbf{curl}\, B = -\boldsymbol{J} \end{cases} \tag{10}$$

on some bounded domain Ω of $\mathbb{R}^2$. Here we assume that Ω is simply connected, Lipschitz and partitioned by a geometrically conforming triangulation $\mathcal{T}_h$ with set of edges denoted by $\mathcal{E}_h$.

3.1. A reference exact sequence with conforming spaces

To begin with we consider the conforming sequence

$$V_h^0 := \mathcal{L}_p(\Omega, \mathcal{T}_h) \xrightarrow{\ \mathbf{grad}\ } V_h^1 := \mathcal{N}_{p-1}(\Omega, \mathcal{T}_h) \xrightarrow{\ \operatorname{curl}\ } V_h^2 := \mathbb{P}_{p-1}(\mathcal{T}_h) \tag{11}$$

where

$$\mathcal{L}_p(\Omega, \mathcal{T}_h) := \mathbb{P}_p(\mathcal{T}_h) \cap H^1(\Omega) \tag{12}$$

denotes the continuous "Lagrange" elements of total degree $\le p$,

$$\mathcal{N}_{p-1}(\Omega, \mathcal{T}_h) := \mathcal{N}_{p-1}(\mathcal{T}_h) \cap H(\mathrm{curl};\Omega) \quad \text{with} \quad \mathcal{N}_{p-1}(T) := \mathbb{P}_{p-1}(T)^2 \oplus \begin{pmatrix} -y \\ x \end{pmatrix} \mathbb{P}^{\mathrm{hom}}_{p-1}(T) \tag{13}$$

is the first-kind Nédélec space of order p (introduced in [17] for the 3d case, see also [4, Sec. 2.3]), and

$$\mathbb{P}_{p-1}(\mathcal{T}_h) := \{v \in L^2(\Omega) : v|_T \in \mathbb{P}_{p-1}(T),\ T \in \mathcal{T}_h\} \tag{14}$$

are the discontinuous elements of degree $\le p-1$. As is well known, (11) is indeed exact in the sense that

$$\mathrm{Im}\,\mathbf{grad}_h = \ker \mathrm{curl}_h \tag{15}$$

holds with $\mathbf{grad}_h := \mathbf{grad}\,|_{V_h^0}$ and $\mathrm{curl}_h := \mathrm{curl}\,|_{V_h^1}$, which correspond to d_h^0 and d_h^1 in our abstract construction. Relation (15) is usually derived from the continuous exact sequence

$$H^1(\Omega) \xrightarrow{\ \mathbf{grad}\ } H(\mathrm{curl};\Omega) \xrightarrow{\ \mathrm{curl}\ } L^2(\Omega) \tag{16}$$

by using commuting diagrams of projection operators (see, e.g., [4]) but a direct argument can be given here: if $\boldsymbol{u} = \boldsymbol{v} + \binom{-y}{x} v \in \mathcal{N}_{p-1}$ with $\boldsymbol{v} \in \mathbb{P}^2_{p-1}$ and $v \in \mathbb{P}^{\mathrm{hom}}_{p-1}$, then $\mathrm{curl}\,\boldsymbol{u} = \mathrm{curl}\,\boldsymbol{v} + (p+1)v$. Now assume $\mathrm{curl}\,\boldsymbol{u} = 0$. Since $\mathrm{curl}\,\boldsymbol{v}$ clearly belongs to $\mathbb{P}_{p-2}$, this yields $v = 0$ and hence $\boldsymbol{u} \in \mathbb{P}^2_{p-1}$. Using this and the exact sequence (16), we find $\boldsymbol{u} = \mathbf{grad}\,\varphi$ for some φ that must belong to $\mathbb{P}_p$, hence (15).

3.2. A new exact sequence with discontinuous Galerkin spaces

We next consider replacing the Nédélec space V_h^1 by a fully discontinuous piecewise polynomial space

$$\tilde{V}_h^1 := \mathbb{P}_{p-1}(\mathcal{T}_h)^2 \not\subset H(\mathrm{curl};\Omega).$$

To construct an exact sequence based on this discontinuous space, following Section 2 we need a projection operator $\mathcal{P}_h^1$ on V_h^1. Here a natural choice is to extend the standard finite element interpolation based on the 2d Nédélec degrees of freedom, which correspond to (see, e.g., [4, Sec. 2.3])

$$\begin{cases} \mathcal{M}_T^1 = \{\boldsymbol{u} \mapsto \int_T \boldsymbol{u} \cdot \boldsymbol{v} : \boldsymbol{v} \in \mathcal{P}_{p-2}(T)^2\}, & T \in \mathcal{T}_h \\ \mathcal{M}_e^1 = \{\boldsymbol{u} \mapsto \int_e (\boldsymbol{n}_e \times \boldsymbol{u}) v : v \in \mathcal{P}_{p-1}(e)\}, & e \in \mathcal{E}_h \end{cases} \tag{17}$$

by using local averages on the edges. Specifically, we define

$$\mathcal{P}_h^1 : \hat{V}_h^1 \to V_h^1 = \mathcal{N}_{p-1}(\Omega, \mathcal{T}_h) \qquad \text{where} \qquad \hat{V}_h^1 := \tilde{V}_h^1 + V_h^1 \tag{18}$$

by the relations

$$\begin{cases} \mathcal{M}_T^1(\mathcal{P}_h^1 \boldsymbol{u}) = \mathcal{M}_T^1(\boldsymbol{u}), & T \in \mathcal{T}_h \\ \mathcal{M}_e^1(\mathcal{P}_h^1 \boldsymbol{u}) = \mathcal{M}_e^1(\{\boldsymbol{u}\}_e), & e \in \mathcal{E}_h. \end{cases} \tag{19}$$

Here we have used the standard notation for the averages on interior and boundary edges, namely

$$\{\boldsymbol{u}\}_e := \frac{1}{2}(\boldsymbol{u}|_{T_e^-} + \boldsymbol{u}|_{T_e^+})|_e \quad \text{and} \quad \{\boldsymbol{u}\}_e := (\boldsymbol{u}|_{T_e})|_e \quad \text{respectively.} \tag{20}$$

This projection operator has several interesting properties. First it is local, in the sense that the degrees of freedom of $\mathcal{P}_h^1 \boldsymbol{u}$ associated with some mesh element (i.e. edge or triangle) only depend on the values of $\boldsymbol{u}$ on the neighboring mesh elements. In particular, $\mathcal{P}_h^1$ can be implemented with a sparse matrix. Second, the non-conforming curl operator $\tilde{d}_h^1$ corresponding to (5), that we shall now denote

$$\mathrm{curl}_h^{\mathrm{dg}} := \mathrm{curl}\,\mathcal{P}_h^1|_{\tilde{V}_h^1} \tag{21}$$

coincides with the standard DG curl with centered fluxes [14]. Indeed, a straightforward computation using Green formulas and the form of the degrees of freedom (17) yields the following result.

Lemma 3.1. *The non-conforming curl operator defined on* $\tilde{V}_h^1 = \mathbb{P}_{p-1}(\mathcal{T}_h)^2$ *by* (18)–(21) *satisfies*

$$\langle \operatorname{curl} \mathcal{P}_h^1 \boldsymbol{u}, v\rangle = \sum_{T\in\mathcal{T}_h} \langle \boldsymbol{u}, \mathbf{curl}\, v\rangle_T - \sum_{e\in\mathcal{E}_h} \langle\{\boldsymbol{u}\}, [v]\rangle_e \quad \text{for all} \quad v \in \mathbb{P}_{p-1}(\mathcal{T}_h) \tag{22}$$

with a standard notation for the averages (20) *and tangential jumps on interior and boundary edges, i.e.*

$$[v]_e := (\boldsymbol{n}_e^- \times v|_{T_e^-} + \boldsymbol{n}_e^+ \times v|_{T_e^+})|_e \quad \text{and} \quad [v]_e := (\boldsymbol{n}_e \times v|_{T_e})|_e \quad \text{respectively}. \tag{23}$$

An exact sequence is then provided by the abstract construction from Section 2. Specifically, setting

$$\mathbf{grad}_h^{\mathrm{dg}}: \quad \tilde{V}_h^0 \to \tilde{V}_h^1, \quad (\varphi, \boldsymbol{u}) \mapsto \mathbf{grad}\,\varphi + (I - \mathcal{P}_h^1)\boldsymbol{u}, \tag{24}$$

with

$$\tilde{V}_h^0 := \left\{(\varphi, \boldsymbol{u}) \in V_h^0 \times \tilde{V}_h^1 : \mathbf{grad}\,\varphi + (I - \mathcal{P}_h^1)\boldsymbol{u} \in \tilde{V}_h^1\right\} \tag{25}$$

we find that the sequence

$$\tilde{V}_h^0 \xrightarrow{\ \mathbf{grad}_h^{\mathrm{dg}}\ } \tilde{V}_h^1 \xrightarrow{\ \operatorname{curl}_h^{\mathrm{dg}}\ } V_h^2 \tag{26}$$

is exact in the sense that

$$\operatorname{Im} \mathbf{grad}_h^{\mathrm{dg}} = \ker \operatorname{curl}_h^{\mathrm{dg}}. \tag{27}$$

3.3. A proper discrete Gauss law for the DG discretization of the 2d Maxwell system

Following [7, Sec. 4], the above construction can be used to derive a proper discrete Gauss law of the form

$$\operatorname{div}_h^{\mathrm{dg}} \tilde{\boldsymbol{E}}_h = \tilde{\rho}_h \tag{28}$$

(involving some approximation $\tilde{\rho}_h$ to the exact charge density ρ) that should be preserved by a structure-preserving DG scheme for the time-dependent problem (10). To do so, we define as a discrete divergence operator the adjoint of the above gradient operator (24) with a minus sign, namely

$$\operatorname{div}_h^{\mathrm{dg}} := -(\mathbf{grad}_h^{\mathrm{dg}})^* : \tilde{V}_h^1 \to \tilde{V}_h^0. \tag{29}$$

In particular, if ρ_h is an approximation to ρ in the continuous finite-element space $V_h^0 = \mathcal{L}_p(\Omega, \mathcal{T}_h)$, then setting $\tilde{\rho}_h := (\rho_h, 0) \in \tilde{V}_h^0$ allows us to rewrite the discrete Gauss law (28) with test functions in $\tilde{V}_h^0$, as

$$\langle \tilde{\boldsymbol{E}}_h, -\mathbf{grad}\,\varphi\rangle + \langle \tilde{\boldsymbol{E}}_h, (\mathcal{P}_h^1 - I)\boldsymbol{u}\rangle = \langle \rho_h, \varphi\rangle \qquad \text{for all} \quad (\varphi, \boldsymbol{u}) \in \tilde{V}_h^0. \tag{30}$$

Finally, we point out that such a discrete Gauss law is well suited to the design of charge-conserving DG-particle schemes, and we refer to the forthcoming articles [8,9] for more details.

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