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Boris Andreianov, Mostafa Bendahmane

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ON DISCRETE DUALITY FINITE VOLUME DISCRETIZATION OF GRADIENT AND DIVERGENCE OPERATORS IN 3D

BORIS ANDREIANOV AND MOSTAFA BENDAHDANE

ABSTRACT. This work is intended to provide a convenient tool for the mathematical analysis of a particular kind of finite volume approximations which can be used, for instance, in the context of nonlinear and/or anisotropic diffusion operators. Following the approach developed by F. Hermeline and by K. Domelevo and P. Omnès, we consider a “double” covering \mathfrak{T} of a three-dimensional domain by a rather general primal mesh and by a well-chosen “dual” mesh. The associated discrete divergence operator $\operatorname{div}^{\mathfrak{T}}$ is obtained by the standard finite volume approach. Then a consistent discrete gradient operator $\nabla^{\mathfrak{T}}$ is defined in such a way that $-\operatorname{div}^{\mathfrak{T}}, \nabla^{\mathfrak{T}}$ enjoy an analogue of the integration-by-parts formula known as the “discrete duality property”. We discuss the implications of these properties and give a brief survey of other “discrete calculus” tools for “double” finite volume schemes.

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1. INTRODUCTION

“Discrete duality” finite volume (DDFV) discretization of linear and nonlinear diffusion operators, introduced in papers [15, 26] (cf. also [30, 31]), is one of possible discretization strategies which applies to a large variety of PDEs including the Stokes problem, Maxwell equations, nonlinear and linear anisotropic diffusion and convection-diffusion problems (see e.g. [6, 3, 8, 10, 13, 14, 15, 25, 26, 27, 28, 30, 31] and references therein). Among different finite volume approaches intended to resolve the difficulties coming from anisotropy/nonlinearity of the PDE under consideration or from the need of working on non-orthogonal, non-conformal, locally refined meshes, let us mention those of [1, 5, 12, 17, 16, 29, 19, 20, 21, 22]. The closest to the DDFV strategy is the “complementary volumes” strategy as described by Handlovičová, Mikula and Sgallari in [23]. The same idea was used, in slightly different ways, in [2] and in [7] (see also [4, Sec.2.1], where the discrete duality formulas in 2D are shown for a typical complementary finite volume scheme). For extensive references on related works, we refer to Eymard, Gallouët and Herbin [18, 22] and Hermeline [28]. Benchmarks that reflect the behaviour of some of the above methods were presented by Herbin and Hubert in [24].

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A DDFV mesh is a “double” mesh. It usually consists of a primal mesh, which in general can be non-orthogonal and non-conformal, and of an appropriately chosen “dual” mesh (a more general point of view is suggested in [6, §IX.B]). The case of dimension two is well studied by now (see e.g. [6, 15, 28] for description of meshes, convergence results and numerical tests). For an attempt of a unified treatment of the 2D and 3D cases, the reader can consult [3] (see also Remark 2.1 below).

In 3D, at least three types of “dual” meshes were already proposed.

(A) The construction due to Pierre (see [32, 10]) generalizes quite successfully the 2D case. Here the dual mesh is rather unusual: it recovers the domain twice.

(B) In the work [28] of Hermeline, a very wide family of finite volume schemes on 3D “double” meshes is considered; the construction includes e.g. the classical Voronoï double mesh corresponding to a well-chosen primal mesh. Numerical results of [28] show good convergence properties of such schemes, even on strongly distorted meshes. In the paper [3] of the authors and K.H. Karlsen, the very particular case of orthogonal meshes was considered. These meshes are suitable for convergence analysis in the framework of entropy solutions of nonlinear convection-diffusion problems.

(C) In the recent work [11] of Coudière and Hubert, the meshes are of the same kind as in [28], but in the finite volume approximation three meshes are involved, making it a “triple” mesh.

This note further explores the approach (B). Our goal is to provide convenient tools for the mathematical analysis of “double-mesh” discretizations on three-dimensional domains. More exactly, for a large subclass of meshes considered in [28], we exhibit a consistent discrete gradient operator which possesses the same “integration-by-parts” property as the 3D scheme of [3] or the usual 2D DDFV schemes (see e.g. [6, 15]). The discrete duality features are essential for the convergence proofs. Note that different variants of the “discrete duality property” hold for the schemes of [10, 32], of [17, 16], of [19, 20, 21, 22], of [5]. For the “complementary finite volumes” schemes as described in [23, 2, 7, 4], a discrete duality property, completely similar to the one shown in the present paper, is true in 2D (see [4] and Remark 4.2).

The practical implications of the discrete duality formula are discussed in Remark 4.3 in Section 4.

Formulae (6),(8),(7),(5) (respectively, (12),(13)) define the discrete gradient operator $\nabla^{\mathfrak{F}}$ (resp., the discrete divergence operator $\operatorname{div}^{\mathfrak{F}}$). The meaning of these formulae is explained in Remark 2.5 and Remark 2.7. Related scalar products are introduced in formulae (14),(15). The main results are those of Remark 2.6 and Proposition 3.2; the link between consistency and discrete duality is provided by the “reconstruction property” of Lemma 2.2. For simplicity, we restrict our attention to the case of convex primal volumes, and impose constraints on the choice of the “centres” of volumes and faces; these constraints can be relaxed (see Remarks 4.6, 4.7 and Example 4.8).

At the final section we also provide some comments as to the use of “double” schemes and briefly discuss the “discrete calculus” tools needed for their theoretical analysis. For the detailed techniques of the convergence analysis for DDFV discretizations of linear and nonlinear diffusion operators we refer to Domelevo and Omnès [15], Andreianov, Boyer and Hubert [6], Andreianov, Bendahmane and Karlsen [3].

2. DOUBLE MESHES AND THE ASSOCIATED GRADIENT AND DIVERGENCE OPERATORS

Let Ω be a polyhedral open bounded subset of \mathbb{R}^3 . In what follows, we introduce the notation related to “double” finite volume schemes; each piece of new notation is given in italic script. The notation is redundant in many cases, which is convenient because the role of objects we introduce is often multi-fold. Most of the notations are illustrated with the help of figures.

Throughout the paper, $\|\vec{a}\|$ denotes the euclidean norm of $\vec{a} \in \mathbb{R}^3$; $\vec{a} \cdot \vec{b}$ (respectively, $\vec{a} \times \vec{b}$) denotes the scalar product (respectively, the vector product) of $\vec{a}, \vec{b} \in \mathbb{R}^3$; $\langle \vec{a}, \vec{b}, \vec{c} \rangle$ denotes the mixed product of $\vec{a}, \vec{b}, \vec{c} \in \mathbb{R}^3$. We use extensively the geometric meaning and the properties of these products.

2.1. Construction of “double” meshes.

- A *partition* of Ω is a finite set of disjoint open polyhedral subsets of Ω such that Ω is contained in their union, up to a set of zero three-dimensional measure.

A “double” finite volume mesh of Ω is a triple $\mathfrak{T} = (\overline{\mathfrak{M}}, \overline{\mathfrak{M}^*}, \mathfrak{D})$ described below.

- We take \mathfrak{M} a partition of Ω into open polyhedra. We assume them convex.

Each $\kappa \in \mathfrak{M}$ is called *control volume* and supplied with an arbitrarily chosen *centre* x_κ ; for simplicity, we assume $x_\kappa \in \kappa$. We call $\partial\mathfrak{M}$ the set of all faces of control volumes that are included in $\partial\Omega$. These

faces are considered as *boundary control volumes*; for $K \in \partial\mathfrak{M}$, we choose a centre $x_K \in K$. We denote by $\overline{\mathfrak{M}}$ the union $\mathfrak{M} \cup \partial\mathfrak{M}$. We call *vertex* (of \mathfrak{M}) any vertex of any control volume $K \in \mathfrak{M}$.

- We call *neighbours* of K , all control volumes $L \in \overline{\mathfrak{M}}$ such that K and L have a common face. The set of all neighbours of K is denoted by $\mathcal{N}(K)$. Note that if $L \in \mathcal{N}(K)$, then $K \in \mathcal{N}(L)$; in this case we simply say that K and L are (a couple of) neighbours.

- If K and L are neighbours, we denote by $K|L$ the *interface* (face) $\partial K \cap \partial L$ between K and L .

- A generic vertex of \mathfrak{M} is denoted by x_{K^*} ; it will be associated later with a unique *dual control volume* $K^* \in \overline{\mathfrak{M}^*}$. Each face $K|L$ is supplied with a *face centre* $x_{K|L}$ which should lie in $K|L$ (the more general situation is discussed in Remarks 4.6, 4.7). For two *neighbour vertices* x_{K^*} and x_{L^*} (i.e., vertices of \mathfrak{M} joined by an edge of some polygon $K|L$), we denote by $x_{K^*|L^*}$ the midpoint of the segment $[x_{K^*}, x_{L^*}]$.

- Now if $K \in \overline{\mathfrak{M}}$ and $L \in \mathcal{N}(K)$, assume x_{K^*}, x_{L^*} are two neighbour vertices of the interface $K|L$. We denote by $T_{K^*, K^*|L^*}^K$ the tetrahedre formed by the points $x_K, x_{K^*}, x_{K|L}, x_{K^*|L^*}$. A generic tetrahedre $T_{K^*, K^*|L^*}^K$ is called an *element* of the mesh and denoted by T (see Fig. 3); the set of all elements is denoted by \mathcal{T} .

- Define the volume K^* associated with a vertice x_{K^*} of \mathfrak{M} as the union of all elements $T \in \mathcal{T}$ having x_{K^*} for one of its vertices. The collection $\overline{\mathfrak{M}^*}$ of all such K^* forms another partition of Ω .

If $x_{K^*} \in \Omega$, we say that K^* is a *dual control volume* and write $K^* \in \overline{\mathfrak{M}^*}$; and if $x_{K^*} \in \partial\Omega$, we say that K^* is a *boundary dual control volume* and write $K^* \in \partial\overline{\mathfrak{M}^*}$. Thus $\overline{\mathfrak{M}^*} = \mathfrak{M}^* \cup \partial\overline{\mathfrak{M}^*}$. We call *dual vertex* (of $\overline{\mathfrak{M}^*}$) any vertex of any dual control volume $K^* \in \overline{\mathfrak{M}^*}$. Note that by construction, the set of vertices coincides with the set of dual centres x_{K^*} ; the set of dual vertices consists of centers x_K , face centers $x_{K|L}$ and edge centers (midpoints) $x_{K^*|L^*}$.

- We denote by $\mathcal{N}^*(K^*)$ the set of (*dual*) *neighbours* of a dual control volume K^* , and by $K^*|L^*$, the (*dual*) *interface* $\partial K^* \cap \partial L^*$ between dual neighbours K^* and L^* .

- Finally, we introduce the partitions of Ω into diamonds and subdiamonds¹.

If $K, L \in \overline{\mathfrak{M}}$ are neighbours, then the convex hull of x_K, x_L and of $K|L$ is called *diamond* and denoted by $D^{K|L}$. In the sequel, to each diamond we will prescribe an orientation by fixing arbitrarily the orientation of the segment $[x_K, x_L]$.

If $K, L \in \overline{\mathfrak{M}}$ are neighbours, and x_{K^*}, x_{L^*} are neighbour vertices of the corresponding interface $K|L$, then the union of the four elements $T_{K^*, K^*|L^*}^K, T_{L^*, K^*|L^*}^L, T_{K^*, K^*|L^*}^L,$ and $T_{L^*, K^*|L^*}^K$ is called *subdiamond* and denoted by $S_{K^*|L^*}^{K|L}$. In this way, each diamond $D^{K|L}$ gives rise to l subdiamonds (where l is the number of vertices of $K|L$). Each subdiamond is associated with a unique interface $K|L$, and thus with a unique diamond $D^{K|L}$. We will write $S \sim D$ to signify that S is associated² with D .

We denote by $\mathfrak{D}, \mathfrak{S}$ the sets of all diamonds and the set of all subdiamonds, respectively. Generic elements of $\mathfrak{D}, \mathfrak{S}$ are denoted by D, S , respectively. Notice that \mathfrak{D} is a partition of Ω .

- (see Figure 1) Whenever the orientation of a diamond D should be cared of, the primal vertices defining it will be denoted by $x_{K_\ominus}, x_{K_\oplus}$ in such a way that the vector $\overrightarrow{x_{K_\ominus} x_{K_\oplus}}$ has the positive orientation. The oriented diamond is then denoted by $D^{K_\ominus|K_\oplus}$. We denote by $\vec{e}_{K_\ominus, K_\oplus}$ the corresponding unit vector, and by d_{K_\ominus, K_\oplus} , the length of $\overrightarrow{x_{K_\ominus} x_{K_\oplus}}$. We denote by $\vec{n}_{K_\ominus|K_\oplus}$ the unit normal vector to $K_\ominus|K_\oplus$ such that $\vec{n}_{K_\ominus|K_\oplus} \cdot \vec{e}_{K_\ominus, K_\oplus} > 0$.

The normal vector $\vec{n}_{K_\ominus|K_\oplus}$ to $K_\ominus|K_\oplus$ being fixed, this induces the orientation in the corresponding face $K_\ominus|K_\oplus$, which is a convex polygon with l vertices: we denote the vertices of $K_\ominus|K_\oplus$ by $x_{K_i^*}$, $i \in \llbracket 1, l \rrbracket$, enumerated in the direct sense. By convention, we assign $x_{K_{l+1}^*} := x_{K_1^*}$. We denote by $\vec{e}_{K_i^*, K_{i+1}^*}$ the unit normal vector pointing from $x_{K_i^*}$ towards $x_{K_{i+1}^*}$, and by $d_{K_i^*, K_{i+1}^*}$, the length of $\overrightarrow{x_{K_i^*} x_{K_{i+1}^*}}$.

In order to lighten the notation, we will drop the K 's in the subscripts and denote the objects introduced above by $x_\ominus, x_\oplus, \vec{e}_{\ominus, \oplus}, d_{\ominus, \oplus}, \vec{n}_{\ominus, \oplus}$ and by $x_i^*, \vec{e}_{i, i+1}^*, d_{i, i+1}^*$ whenever $D^{K_\ominus|K_\oplus}$ is fixed. We also denote by $x_{i, i+1}^*$ the midpoint $x_{K_i^*|K_{i+1}^*}$ of the segment $[x_i^*, x_{i+1}^*]$, and by $x_{\ominus, \oplus}^*$, the centre $x_{K_\ominus|K_\oplus}$ of $K_\ominus|K_\oplus$.

¹Their definitions should be generalized if the constraint $x_K \in K$ is dropped; see Remark 4.6.

²Because we have made the assumption that $x_{K|L} \in K|L$, the relation $S \sim D$ simply means that S is included in D . We will develop a more general point of view in Remark 4.7.

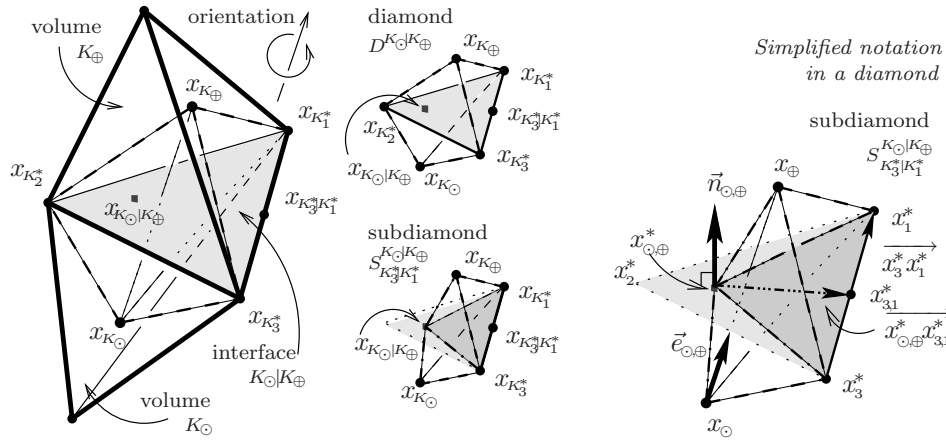


FIGURE 1. 3D neighbour volumes, diamond, subdiamond. Zoom on a subdiamond.

- For a diamond $D = D^{K_\ominus|K_\oplus}$, we denote by Proj_D the operator of orthogonal projection of \mathbb{R}^3 on the line $\langle \vec{e}_{K_\ominus|K_\oplus} \rangle$; we denote by Proj_D^* the operator of orthogonal projection of \mathbb{R}^3 on the plane containing the interface $K_\ominus|K_\oplus$.
- For $K \in \mathfrak{M}$, we denote by $\mathcal{V}(K)$ the set of all subdiamonds $s \in \mathfrak{S}$ such that x_K is a vertex of s . In the same way, for $K^* \in \mathfrak{M}^*$ we define the set $\mathcal{V}^*(K^*)$ of subdiamonds with vertex x_{K^*} .
- We denote by $\text{Vol}(A)$ the three-dimensional Lebesgue measure of A which can stand for a control volume, a dual control volume, or a diamond. For a subdiamond $s = S_{K_\ominus^*|K_\oplus^*}^{K_\ominus|K_\oplus}$, we have the formula $\text{Vol}(s) = \frac{1}{6} \langle \overrightarrow{x_\ominus x_\oplus}, \overrightarrow{x_{\ominus\oplus}^* x_{i+1}^*}, \overrightarrow{x_i^* x_{i+1}^*} \rangle$. Note the mixed product is positive, thanks to our conventions on the orientation in $D^{K_\ominus|K_\oplus}$ and because we have assumed that $x_{\ominus\oplus}^* \in K_\ominus|K_\oplus$.

Remark 2.1. *Diamonds permit to define the discrete gradient operator, while subdiamonds permit to define the discrete divergence operator (see (6), (7) and (12), (13) below, respectively).*

In the context of 2D “double” schemes, introducing diamonds is quite standard (see e.g. [6, 15]). Subdiamonds are “hidden” in the 2D construction : they actually coincide with diamonds.

The above definitions are illustrated and generalized in Remark 4.7 at the end of the paper.

2.2. Discrete functions and fields.

- A *discrete function on Ω* is a set $w^\mp = (w^\mathfrak{M}, w^{\mathfrak{M}^*})$ consisting of two sets of real values $w^\mathfrak{M} = (w_K)_{K \in \mathfrak{M}}$ and $w^{\mathfrak{M}^*} = (w_{K^*})_{K^* \in \mathfrak{M}^*}$. The set of all such functions is denoted by \mathbb{R}^\mp .

A *discrete function on $\overline{\Omega}$* is a set $w^\mp = (w^\mathfrak{M}, w^{\mathfrak{M}^*}, w^{\partial\mathfrak{M}}, w^{\partial\mathfrak{M}^*}) \equiv (w^\mp, w^{\partial\mathfrak{M}}, w^{\partial\mathfrak{M}^*})$ consisting of

$$w^\mathfrak{M} = (w_K)_{K \in \mathfrak{M}}, w^{\mathfrak{M}^*} = (w_{K^*})_{K^* \in \mathfrak{M}^*}, w^{\partial\mathfrak{M}} = (w_K)_{K \in \partial\mathfrak{M}}, w^{\partial\mathfrak{M}^*} = (w_{K^*})_{K^* \in \partial\mathfrak{M}^*}.$$

The set of all such functions is denoted by \mathbb{R}^\mp . In case all the components of $w^{\partial\mathfrak{M}}$ and of $w^{\partial\mathfrak{M}^*}$ are zero, we write $w^\mp \in \mathbb{R}_0^\mp$.

- A *discrete field on Ω* is a set $\vec{F}^\mp = (\vec{F}_D)_{D \in \mathfrak{D}}$ of vectors of \mathbb{R}^d . The set of all discrete fields is denoted by $(\mathbb{R}^d)^\mathfrak{D}$. If \vec{F}^\mp is a discrete field on Ω , we assign $\vec{F}_S = \vec{F}_D$ whenever $S \sim D$.

2.3. A reconstruction property in the plane.

Now we motivate the definition of the discrete gradient operator. Although Lemma 2.2 is a purely two-dimensional property, it is convenient to use the 3D formalism. The subsequent notation corresponds to Figure 2; within this paragraph, the reader may ignore all “asterisk” superscripts.

Let Π be a plane in \mathbb{R}^3 with a fixed unit normal vector \vec{n} , and $\sigma \subset \Pi$ be a polygon with l vertices ($l \geq 3$) denoted x_1^*, \dots, x_l^* , numbered in the direct sense with respect to the orientation of Π induced by \vec{n} . This means that for $i \in \llbracket 1, l \rrbracket$, x_i^* and x_{i+1}^* are neighbour vertices of the polygon σ , and $\langle \vec{\nu}_{i,i+1}^*, \vec{e}_{i,i+1}^*, \vec{n} \rangle = 1$; here $\vec{e}_{i,i+1}^* = \frac{\overrightarrow{x_i^* x_{i+1}^*}}{\|x_i^* x_{i+1}^*\|}$ and $\vec{\nu}_{i,i+1}^*$ is the unit normal vector to $[x_i^*, x_{i+1}^*]$ lying in Π and pointing outside σ . Here and in the sequel, x_{l+1}^* stands for x_1^* .

Further, introduce the barycenter (i.e., the midpoint) $x_{i,i+1}^*$ of $[x_i^*, x_{i+1}^*]$. For a point $x_\sigma^* \in \Pi$ and $i \in \llbracket 1, l \rrbracket$ such that $x_{i,i+1}^* \neq x_\sigma^*$, denote $\vec{\tau}_{i,i+1}^* = \frac{\overrightarrow{x_\sigma^* x_{i,i+1}^*}}{\|x_\sigma^* x_{i,i+1}^*\|}$ and $\vec{a}_{i,i+1}^* = \vec{n} \times \vec{\tau}_{i,i+1}^*$. In this way,

for each $i \in \llbracket 1, l \rrbracket$, Π is supplied with a couple of orthonormal bases $(\vec{v}_{i,i+1}^*, \vec{e}_{i,i+1}^*)$ and $(\vec{\tau}_{i,i+1}^*, \vec{a}_{i,i+1}^*)$, both oriented in the direct sense.

Finally, denote by $\theta_{i,i+1}^*$ the angle between $\vec{v}_{i,i+1}^*$ and $\vec{\tau}_{i,i+1}^*$; this is also the angle between $\vec{e}_{i,i+1}^*$ and $\vec{a}_{i,i+1}^*$. Set

$$(1) \quad m_{i,i+1} = \frac{1}{2} \langle \vec{n}, \overrightarrow{x_\sigma^* x_{i+1}^*}, \overrightarrow{x_i^* x_{i+1}^*} \rangle \quad \left(\text{we have } m_{i,i+1} = \frac{1}{2} \|\overrightarrow{x_i^* x_{i+1}^*}\| \|\overrightarrow{x_\sigma^* x_{i+1}^*}\| \cos \theta_{i,i+1}^* \right);$$

this is the (signed) area of the triangle $x_i^* x_\sigma^* x_{i+1}^*$. Denote the area of σ by m ; it is easily seen that $m = \sum_{i=1}^l m_{i,i+1}$. We also have $2 \frac{m_{i,i+1}}{\cos \theta_{i,i+1}^*} \vec{a}_{i,i+1}^* = \|\overrightarrow{x_i^* x_{i+1}^*}\| [\vec{n} \times \overrightarrow{x_\sigma^* x_{i+1}^*}]$. In the case $m_{i,i+1} = 0$ (this happens, e.g., if $x_{i+1}^* = x_\sigma^*$), the left-hand side of the above expression is meant to be zero.

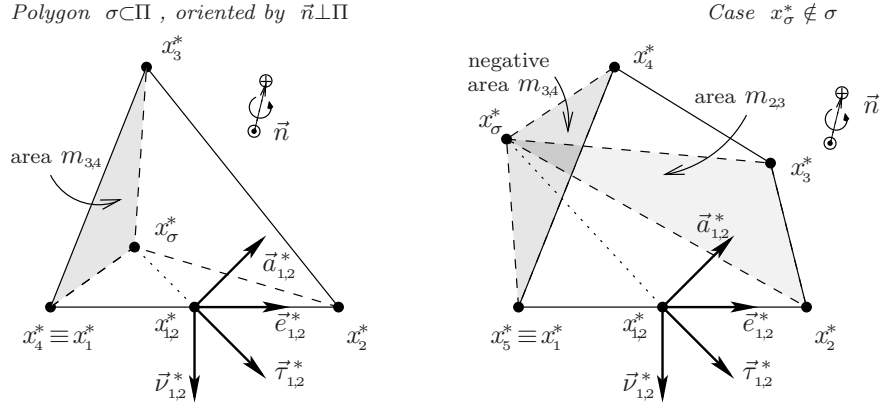


FIGURE 2. 2D Reconstruction property (zoom on a primal interface)

Lemma 2.2. *With the notation above, for all vector \vec{r} parallel to Π we have*

$$(2) \quad \vec{r} = \frac{2}{m} \sum_{i=1}^l \frac{m_{i,i+1}}{\cos \theta_{i,i+1}^*} (\vec{r} \cdot \vec{e}_{i,i+1}^*) \vec{a}_{i,i+1}^* = \frac{1}{m} \sum_{i=1}^l (\vec{r} \cdot \overrightarrow{x_i^* x_{i+1}^*}) [\vec{n} \times \overrightarrow{x_\sigma^* x_{i+1}^*}].$$

Note that, if σ admits a circumscribed circle and x_σ^* is chosen to be its center, then $\vec{\tau}_{i,i+1}^*$ is parallel to $\vec{v}_{i,i+1}^*$; in this case (2) reduces to the reconstruction property used in [3].

PROOF : Thanks to the choice of the barycenter for x_σ^* , we can apply [17, Lemma 6.1] which is a consequence of the Green-Gauss integration-by-parts formula. Note that the assumptions “ σ is convex, $x_\sigma^* \in \sigma$ ” of this lemma can be dropped. Using in addition (1), we get for all vector \vec{r} parallel to Π ,

$$(3) \quad \vec{r} = \frac{1}{m} \sum_{i=1}^l \|\overrightarrow{x_i^* x_{i+1}^*}\| (\vec{r} \cdot \overrightarrow{x_\sigma^* x_{i+1}^*}) \vec{v}_{i,i+1}^* = \frac{2}{m} \sum_{i=1}^l \frac{m_{i,i+1}}{\cos \theta_{i,i+1}^*} (\vec{r} \cdot \vec{\tau}_{i,i+1}^*) \vec{v}_{i,i+1}^*.$$

Furthermore, for all $i \in \llbracket 1, l \rrbracket$, we have $\cos \theta_{i,i+1}^* \vec{r} = (\vec{r} \cdot \vec{\tau}_{i,i+1}^*) \vec{v}_{i,i+1}^* + (\vec{r} \cdot \vec{e}_{i,i+1}^*) \vec{a}_{i,i+1}^*$. For the proof, it suffices to take the scalar product by $\vec{\tau}_{i,i+1}^*$, and then by $\vec{e}_{i,i+1}^*$, of the both sides of the relation.

Therefore

$$(4) \quad 2\vec{r} = \frac{2}{m} \sum_{i=1}^l \frac{m_{i,i+1}}{\cos \theta_{i,i+1}^*} \left((\vec{r} \cdot \vec{\tau}_{i,i+1}^*) \vec{v}_{i,i+1}^* + (\vec{r} \cdot \vec{e}_{i,i+1}^*) \vec{a}_{i,i+1}^* \right).$$

Subtracting (3) from (4) term by term, we deduce (2). \diamond

Corollary 2.3. *With the above notation, take $(w_i^*)_{i=1}^l \subset \mathbb{R}$, $w_{l+1}^* := w_1^*$. Consider the expression*

$$(5) \quad \frac{1}{\sum_{i=1}^l m_{i,i+1}} \sum_{i=1}^l (w_{i+1}^* - w_i^*) [\vec{n} \times \overrightarrow{x_\sigma^* x_{i+1}^*}].$$

In the case w_i^* are the values of an affine function w at the vertices x_i^* of the polygon σ , expression (5) gives the projection $\text{Proj}^*(\nabla w)$ of ∇w on the plane Π .

PROOF : It is sufficient to note that $\text{Proj}^*(\nabla w) \cdot \overrightarrow{x_i^* x_{i+1}^*} = \nabla w \cdot \overrightarrow{x_i^* x_{i+1}^*} = w_{i+1}^* - w_i^*$, and to substitute $m = \sum_{i=1}^l m_{i,i+1}$ into the right-hand side of (2). \diamond

Remark 2.4. Notice that Lemma 2.2 and Corollary 2.3 hold for all choice of x_σ^* in the plane Π ; the restriction $x_\sigma^* \in \sigma$ is not necessary. This restriction is equivalent to the positivity of $m_{i,i+1}$ for all i .

Remark 2.5. Let us point out that, unless $l = 3$, formula (5) determines one among infinitely many linear forms in $(w_i^*)_{i=1}^l$ which share the property of Corollary 2.3. The choice of (5) is motivated by the calculation of Proposition 3.2: in fact, it is the discrete duality property that leads to (5). If $l = 3$, then (5) is equivalent to any of the formulas for three-point affine interpolation in the plane Π .

We guess that the affine interpolation formula (5) is well known, but to the best of our knowledge, it was not yet exploited in the context of finite volume schemes.

2.4. The discrete gradient operator.

• On the set $\mathbb{R}^{\bar{\mathfrak{X}}}$ of discrete functions $w^{\bar{\mathfrak{X}}}$ on $\bar{\Omega}$, we define the operator $\nabla^{\bar{\mathfrak{X}}}[\cdot]$ of discrete gradient

$$(6) \quad \nabla^{\bar{\mathfrak{X}}} : w^{\bar{\mathfrak{X}}} \in \mathbb{R}^{\bar{\mathfrak{X}}} \mapsto \nabla^{\bar{\mathfrak{X}}} w^{\bar{\mathfrak{X}}} = (\nabla_D w^{\bar{\mathfrak{X}}})_{D \in \mathfrak{D}} \in (\mathbb{R}^d)^{\mathfrak{D}}$$

where $\nabla^{\bar{\mathfrak{X}}} w^{\bar{\mathfrak{X}}}$ is the discrete field on Ω with the values $\nabla_D w^{\bar{\mathfrak{X}}}$ satisfying, for $D = D^{K_\circ | K_\oplus}$,

$$(7) \quad \nabla_D w^{\bar{\mathfrak{X}}} \text{ is s.t. } \begin{cases} \text{Proj}_D(\nabla_D w^{\bar{\mathfrak{X}}}) = \frac{w_\oplus - w_\circ}{d_{\circ, \oplus}} \vec{e}_{\circ, \oplus}, \text{ with } w_\circ = w_{K_\circ}, w_\oplus = w_{K_\oplus}; \\ \text{Proj}_D^*(\nabla_D w^{\bar{\mathfrak{X}}}) \text{ is the vector defined by formulae (5),(1)} \\ \text{with } w_i^* = w_{K_i^*}, \vec{n} = \vec{n}_{\circ, \oplus}, x_\sigma^* = x_{\circ, \oplus}^*. \end{cases}$$

Remark 2.6. Thus, the primal mesh $\bar{\mathfrak{M}}$ serves to reconstruct one component of the gradient, which is the one in the direction $\vec{e}_{\circ, \oplus}$. The dual mesh $\bar{\mathfrak{M}}^*$ serves to reconstruct, with the help of formula (5), the two other components which are the components in the plane Π containing $K_\circ | K_\oplus$.

For an explicit formula, note that if $\vec{p} = \text{Proj}_D(\nabla_D w^{\bar{\mathfrak{X}}})$, $\vec{p}^* = \text{Proj}_D^*(\nabla_D w^{\bar{\mathfrak{X}}})$ are given, we have

$$(8) \quad \nabla_D w^{\bar{\mathfrak{X}}} = \vec{p}^* + \frac{\vec{e}_{\circ, \oplus} \cdot (\vec{p} - \vec{p}^*)}{\vec{e}_{\circ, \oplus} \cdot \vec{n}_{\circ, \oplus}} \vec{n}_{\circ, \oplus}.$$

Notice that (7) and Corollary 2.3 imply the consistency of our gradient approximation :

Remark 2.7. Let $w_\circ, w_\oplus, (w_{i,i+1}^*)_{i=1}^l$ be the values at the points $x_\circ, x_\oplus, (x_{i,i+1}^*)_{i=1}^l$, respectively, of an affine on $D = D^{K_\circ | K_\oplus}$ function w . Then $\nabla_D w^{\bar{\mathfrak{X}}}$ coincides with the value of ∇w on D .

2.5. The discrete divergence operator.

• (see Figure 3) In a generic subdiamond, we use the following notation. Consider $s \in \mathfrak{S}$; it is associated with a unique oriented diamond which we denote $D^{K_\circ | K_\oplus}$, so that s is of the form $s = S_{K_i^* | K_{i+1}^*}^{K_\circ | K_\oplus}$. We further split s it into the two parts $S_\circ := T_{K_i^*, K_{i+1}^* | K_{i+1}^*}^{K_\circ} \cup T_{K_{i+1}^*, K_i^* | K_{i+1}^*}^{K_\circ}$, $S_\oplus := T_{K_i^*, K_{i+1}^* | K_{i+1}^*}^{K_\oplus} \cup T_{K_{i+1}^*, K_i^* | K_{i+1}^*}^{K_\oplus}$ (each one contains one flat part of the interface $K_i^* | K_{i+1}^*$). We denote $\sigma_s := s \cap K_\circ | K_\oplus$, $\sigma_{S_\circ}^* := S_\circ \cap K_i^* | K_{i+1}^*$, $\sigma_{S_\oplus}^* := S_\oplus \cap K_i^* | K_{i+1}^*$. The areas of σ_s , $\sigma_{S_\circ}^*$, $\sigma_{S_\oplus}^*$ are denoted by m_s , $m_{S_\circ}^*$, $m_{S_\oplus}^*$, respectively. We denote by \vec{n}_s , $\vec{n}_{S_\circ}^*$, $\vec{n}_{S_\oplus}^*$ the unit normal vectors to σ_s , $\sigma_{S_\circ}^*$, $\sigma_{S_\oplus}^*$, respectively. Their orientations are chosen so that to satisfy

$$(9) \quad \vec{n}_s = \vec{n}_{K_\circ | K_\oplus} \quad \text{and} \quad \langle \vec{n}_{S_\circ}^*, \vec{n}_{\circ, \oplus}, \overrightarrow{x_{\circ, \oplus}^* x_{i,i+1}^*} \rangle \geq 0, \quad \langle \vec{n}_{S_\oplus}^*, \vec{n}_{\circ, \oplus}, \overrightarrow{x_{\circ, \oplus}^* x_{i,i+1}^*} \rangle \geq 0.$$

This implies that

$$(10) \quad \begin{aligned} m_s \vec{n}_s &= \frac{1}{2} \overrightarrow{x_{\circ, \oplus}^* x_{i,i+1}^*} \times \overrightarrow{x_i^* x_{i+1}^*}, \\ m_{S_\circ}^* \vec{n}_{S_\circ}^* + m_{S_\oplus}^* \vec{n}_{S_\oplus}^* &= \frac{1}{2} \overrightarrow{x_\circ x_{\circ, \oplus}^*} \times \overrightarrow{x_{\circ, \oplus}^* x_{i,i+1}^*} + \frac{1}{2} \overrightarrow{x_{\circ, \oplus}^* x_\oplus} \times \overrightarrow{x_{\circ, \oplus}^* x_{i,i+1}^*} = \frac{1}{2} \overrightarrow{x_\circ x_\oplus} \times \overrightarrow{x_{\circ, \oplus}^* x_{i,i+1}^*}. \end{aligned}$$

Further, for $s = S_{K_i^* | K_{i+1}^*}^{K_\circ | K_\oplus}$ we define

$$(11) \quad \epsilon_s^K := \begin{cases} 0, & \text{if } K = K_\circ \\ 1, & \text{if } K = K_\oplus \end{cases}, \quad \epsilon_s^{K^*} := \begin{cases} 0, & \text{if } K^* = K_i^* \\ 1, & \text{if } K^* = K_{i+1}^* \end{cases}.$$

• For $K \in \mathfrak{M}$, we denote by $\nu(K)$ the set of all subdiamonds $s \in \mathfrak{S}$ such that $K \cap s \neq \emptyset$. In the same way, for $K^* \in \bar{\mathfrak{M}}^*$ we define the set $\nu^*(K^*)$ of the subdiamonds intersecting K^* .³

• On the set $(\mathbb{R}^d)^{\mathfrak{D}}$ of discrete fields $\vec{\mathcal{F}}^{\bar{\mathfrak{X}}}$, we define the operator $\text{div}^{\bar{\mathfrak{X}}}[\cdot]$ of discrete divergence by

$$(12) \quad \text{div}^{\bar{\mathfrak{X}}} : \vec{\mathcal{F}}^{\bar{\mathfrak{X}}} \in (\mathbb{R}^d)^{\mathfrak{D}} \mapsto v^{\bar{\mathfrak{X}}} = \text{div}^{\bar{\mathfrak{X}}}[\vec{\mathcal{F}}^{\bar{\mathfrak{X}}}] \in \mathbb{R}^{\bar{\mathfrak{X}}},$$

³These definitions should be generalized if the constraint $x_{K|L} \in K|L$ is dropped (see Remark 4.7).

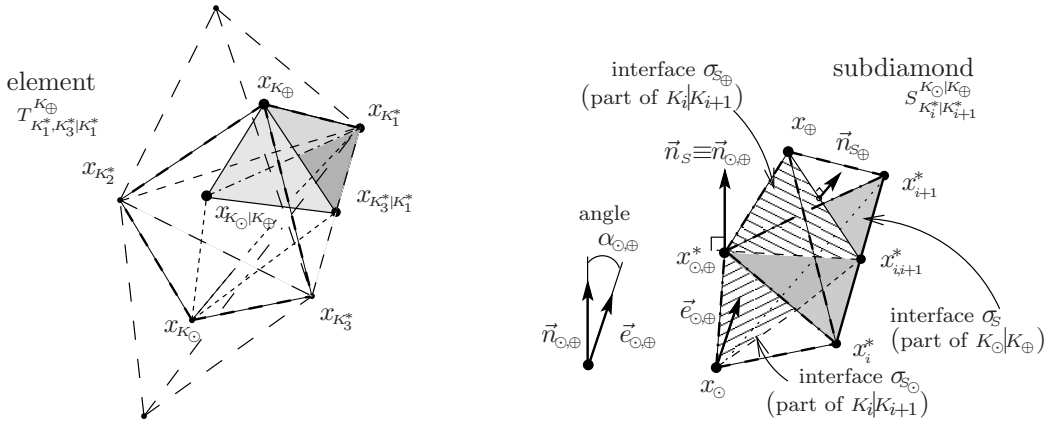


FIGURE 3. Element. Subdiamond: $\sigma_S, \sigma_{S_\oplus}, \sigma_{S_\ominus}$ and their normal vectors.

where the discrete function $v^\mp = (v^{\mathfrak{M}}, v^{\mathfrak{M}^*})$ on Ω with $v^{\mathfrak{M}} = (v_K)_{K \in \mathfrak{M}}$, $v^{\mathfrak{M}^*} = (v_{K^*})_{K^* \in \mathfrak{M}^*}$ taking the values

$$(13) \quad \begin{aligned} v_K &= \frac{1}{\text{Vol}(K)} \sum_{S \in \mathcal{V}(K)} m_S \vec{F}_S \cdot (-1)^{\epsilon_S^K} \vec{n}_S = \frac{1}{2\text{Vol}(K)} \sum_{S \in \mathcal{V}(K)} (-1)^{\epsilon_S^K} \langle \vec{F}_S, \overrightarrow{x_{\ominus\oplus}^* x_{i+1}^*}, \overrightarrow{x_i^* x_{i+1}^*} \rangle, \\ v_{K^*} &= \frac{1}{\text{Vol}(K^*)} \sum_{S \in \mathcal{V}^*(K^*)} \vec{F}_S \cdot (-1)^{\epsilon_S^{K^*}} (m_{S_\ominus}^* \vec{n}_{S_\ominus}^* + m_{S_\oplus}^* \vec{n}_{S_\oplus}^*) = \frac{1}{2\text{Vol}(K^*)} \sum_{S \in \mathcal{V}^*(K^*)} (-1)^{\epsilon_S^{K^*}} \langle \vec{F}_S, \overrightarrow{x_\ominus x_\oplus}, \overrightarrow{x_{\ominus\oplus}^* x_{i+1}^*} \rangle. \end{aligned}$$

In formulae (13), we mean that each subdiamond s in $\mathcal{V}(K)$ (or in $\mathcal{V}^*(K^*)$) has the form $s = S_{K_i^*|K_{i+1}^*}^{K_\ominus|K_\oplus}$, with some $K_\ominus, K_\oplus, K_i^*, K_{i+1}^*$; the notations $\epsilon_S^K, \epsilon_S^{K^*}, x_\ominus, x_\oplus, x_{\ominus\oplus}^*, x_{i+1}^*, x_i^*, x_{i+1}^*$, under the sign “ \sum ” refer to $s = S_{K_i^*|K_{i+1}^*}^{K_\ominus|K_\oplus}$.

Note that we have used (10) to reduce the calculation of v_K, v_{K^*} to a simple mixed product formula.

Remark 2.8. Formulae (13) correspond to the standard procedure of finite volume discretization.

The value $\text{Vol}(K) v_K$ is the flux of the vector field \vec{F}^\mp through the boundary ∂K , so that it represents $\int_K \text{div} \vec{F}^\mp$. Indeed, thanks to the constraints $x_\ominus \in K_\ominus$, $x_\oplus \in K_\oplus$ and the orientation constraints (we have $\vec{n}_S \cdot \overrightarrow{x_\ominus x_\oplus} = d_{\ominus\oplus} \vec{n}_{\ominus\oplus} \cdot \vec{e}_{\ominus\oplus} > 0$), vector \vec{n}_S points from K_\ominus to K_\oplus ; thus by definition (11) of ϵ_S^K , the vector $(-1)^{\epsilon_S^K} \vec{n}_S$ is the unit normal vector to $\sigma_S \subset \partial K$ exterior to K , for $K = K_\ominus$ and for $K = K_\oplus$.

Similarly, having chosen $x_{\ominus\oplus}^* \in K_\ominus|K_\oplus$ we ensured that $\vec{n}_{S_\ominus}^*, \vec{n}_{S_\oplus}^*$ point from K_i^* to K_{i+1}^* , thanks to (9) and to the fact that the vertices of $K_\ominus|K_\oplus$ are numbered according to the orientation of $\vec{n}_{\ominus\oplus}$. By (11), $(-1)^{\epsilon_S^{K^*}} \vec{n}_{S_\ominus}^*, (-1)^{\epsilon_S^{K^*}} \vec{n}_{S_\oplus}^*$ are the unit normal vectors to the flat portions $\sigma_{S_\ominus}^*, \sigma_{S_\oplus}^*$ of ∂K^* , exterior to K^* . Thus $\text{Vol}(K^*) v_{K^*}$ represents $\int_{K^*} \text{div} \vec{F}^\mp$ which is the flux of \vec{F}^\mp through ∂K^* .

3. THE DISCRETE DUALITY PROPERTY

Let us define the convenient multiplication of discrete functions/discrete fields and state our main result.

- Recall that \mathbb{R}^\mp is the space of all discrete functions on Ω . For $w^\mp, v^\mp \in \mathbb{R}^\mp$, set

$$(14) \quad \llbracket w^\mp, v^\mp \rrbracket = \frac{1}{3} \sum_{K \in \mathfrak{M}} \text{Vol}(K) w_K v_K + \frac{2}{3} \sum_{K^* \in \mathfrak{M}^*} \text{Vol}(K^*) w_{K^*} v_{K^*};$$

it is clear that $\llbracket \cdot, \cdot \rrbracket$ is a scalar product on \mathbb{R}^\mp .

Remark 3.1. Notice that the role of the primal and the dual meshes is not symmetric; this asymmetry is also reflected by Remark 2.5. In \mathbb{R}^d , the primal mesh would account for $\frac{1}{d}$ of the product, and the dual mesh, for $\frac{d-1}{d}$ (see [3]).

Also notice that in the 3D scheme developed by Pierre (see [10, 32]), the weights in the scalar product (14) are both equal to $\frac{1}{3}$; but, because the dual mesh in [10, 32] covers twice the domain $\Omega \subset \mathbb{R}^3$, its “weight” is doubled with respect with the “weight” of the primal mesh. This is similar to what happens in our formula (14).

As to the 3D scheme proposed by Coudière and Hubert (see [11]), a “triple” mesh is involved, and the associated scalar product takes the contributions of each of the meshes with the equal weights $\frac{1}{3}$.

• Recall that $(\mathbb{R}^3)^\mathfrak{D}$ is the space of all discrete fields on Ω . For $\vec{\mathcal{F}}^\mathfrak{x}, \vec{\mathcal{G}}^\mathfrak{x} \in (\mathbb{R}^3)^\mathfrak{D}$, set

$$(15) \quad \left\{ \vec{\mathcal{F}}^\mathfrak{x}, \vec{\mathcal{G}}^\mathfrak{x} \right\} = \sum_{D \in \mathfrak{D}} \text{Vol}(D) \vec{\mathcal{F}}_D \cdot \vec{\mathcal{G}}_D;$$

it is clear that $\left\{ \cdot, \cdot \right\}$ is a scalar product on $(\mathbb{R}^3)^\mathfrak{D}$.

Proposition 3.2. *The discrete divergence and gradient operators $-\text{div}^\mathfrak{x}$, $\nabla^\mathfrak{x}$ defined in Section 2 are linked by the following duality property :*

$$(16) \quad \forall w^\mathfrak{x} \in \mathbb{R}_0^\mathfrak{x} \quad \forall \vec{\mathcal{F}}^\mathfrak{x} \in (\mathbb{R}^d)^\mathfrak{D} \quad \left[-\text{div}^\mathfrak{x}[\vec{\mathcal{F}}^\mathfrak{x}], w^\mathfrak{x} \right] = \left\{ \vec{\mathcal{F}}^\mathfrak{x}, \nabla^\mathfrak{x} w^\mathfrak{x} \right\}.$$

PROOF : The proof is by direct calculation, using the summation-by-parts procedure. Denote the product $\left[-\text{div}^\mathfrak{x}[\vec{\mathcal{F}}^\mathfrak{x}], w^\mathfrak{x} \right]$ by Z . We put together the terms in Z corresponding to adjacent couples of primal and dual volumes, which amounts to make the summation over all subdiamonds $s = S_{K_\circ^\mathfrak{x}|K_\oplus^\mathfrak{x}}^{K_\circ|K_\oplus}$ (see Figures 1,3 for the notation in s); ghost terms corresponding to the boundary volumes can be added, because $w^\mathfrak{x}$ is zero on the boundary volumes. With (14),(13),(11),(10), we find

$$\begin{aligned} Z &= \sum_{S \in \mathfrak{S}} \vec{\mathcal{F}}_s \cdot \left(\frac{1}{3}(w_\oplus - w_\circ) m_s \vec{n}_{\circ,\oplus} + \frac{2}{3}(w_{i+1}^* - w_i^*) (m_{s_\circ}^* \vec{n}_{s_\circ}^* + m_{s_\oplus}^* \vec{n}_{s_\oplus}^*) \right) \\ &= \frac{1}{3} \sum_{S \in \mathfrak{S}} \vec{\mathcal{F}}_s \cdot \left(m_s d_{\circ,\oplus} \frac{w_\oplus - w_\circ}{d_{\circ,\oplus}} \vec{n}_{\circ,\oplus} + (w_{i+1}^* - w_i^*) \overrightarrow{x_\circ x_\oplus} \times \overrightarrow{x_{\circ\oplus}^* x_{i+1}^*} \right). \end{aligned}$$

Next, we put together the terms corresponding to the subdiamonds s associated with the same diamond D ; since $\vec{\mathcal{F}}_s = \vec{\mathcal{F}}_D$ in this case, this amounts to make the summation over all diamonds $D = D^{K_\circ|K_\oplus}$ (see Figures 1,2 for the notation in D). We get

$$(17) \quad Z = \sum_{D \in \mathfrak{D}} \vec{\mathcal{F}}_D \cdot \vec{Z}_D \quad \text{with} \quad \vec{Z}_D := \sum_{S \sim D} \frac{1}{3} \left(m_s d_{\circ,\oplus} \frac{w_\oplus - w_\circ}{d_{\circ,\oplus}} \vec{n}_{\circ,\oplus} + (w_{i+1}^* - w_i^*) \overrightarrow{x_\circ x_\oplus} \times \overrightarrow{x_{\circ\oplus}^* x_{i+1}^*} \right).$$

By (15), it remains to show that the interior sum in the above formula, which we denote \vec{Z}_D , equals $\text{Vol}(D) \nabla_D^\mathfrak{x} w^\mathfrak{x}$. To this end, we calculate separately $\text{Proj}_D(\vec{Z}_D)$ and $\text{Proj}_D^*(\vec{Z}_D)$.

First, let $\alpha_{\circ\oplus}$ be the acute angle formed by the segment $[x_\circ, x_\oplus]$ and the direction normal to $K_\circ|K_\oplus$. Let m be the area of the face $K_\circ|K_\oplus$. We have $m = \sum_{S \sim D} m_s$ and since $\vec{n}_{\circ,\oplus} \cdot \vec{e}_{\circ,\oplus} > 0$,

$$(18) \quad \text{Vol}(D) = \frac{1}{3} m d_{\circ,\oplus} \cos \alpha_{\circ\oplus} = \frac{1}{3} (\vec{n}_{\circ,\oplus} \cdot \vec{e}_{\circ,\oplus}) \sum_{S \sim D} m_s d_{\circ,\oplus}.$$

Also notice that

$$(19) \quad \overrightarrow{x_\circ x_\oplus} = d_{\circ,\oplus} \cos \alpha_{\circ\oplus} \vec{n}_{\circ,\oplus} + \text{Proj}_D^*(\overrightarrow{x_\circ x_\oplus}).$$

Unless $\overrightarrow{x_{\circ\oplus}^* x_{i+1}^*}$ is zero (this case is trivial), introduce $d_{i+1/2}^* = \|\overrightarrow{x_{\circ\oplus}^* x_{i+1}^*}\|$ and $\vec{\tau}_{i,i+1}^* := \overrightarrow{x_{\circ\oplus}^* x_{i+1}^*} / d_{i+1/2}^*$, $\vec{a}_{i,i+1}^* := \vec{n}_{\circ,\oplus} \times \vec{\tau}_{i,i+1}^*$; $(\vec{\tau}_{i,i+1}^*, \vec{a}_{i,i+1}^*)$ is an orthonormal basis in the plane Π containing $K_\circ|K_\oplus$ (the so introduced notation coincides with the notation of Figure 2). We have

$$(20) \quad \begin{aligned} \text{Proj}_D^*(\overrightarrow{x_\circ x_\oplus} \times \overrightarrow{x_{\circ\oplus}^* x_{i+1}^*}) &= d_{i+1/2}^* \left(\langle \overrightarrow{x_\circ x_\oplus}, \vec{\tau}_{i,i+1}^* \rangle \vec{\tau}_{i,i+1}^* + \langle \overrightarrow{x_\circ x_\oplus}, \vec{a}_{i,i+1}^* \rangle \vec{a}_{i,i+1}^* \right) \\ &= d_{\circ,\oplus} \cos \alpha_{\circ\oplus} \langle \vec{n}_{\circ,\oplus}, \vec{\tau}_{i,i+1}^* \rangle d_{i+1/2}^* \vec{a}_{i,i+1}^* = d_{\circ,\oplus} \cos \alpha_{\circ\oplus} (\vec{n}_{\circ,\oplus} \times \overrightarrow{x_{\circ\oplus}^* x_{i+1}^*}); \end{aligned}$$

here we have used equality (19).

• Now, $\text{Proj}_D(\overrightarrow{x_\circ x_\oplus} \times \overrightarrow{x_{\circ\oplus}^* x_{i+1}^*})$ is zero. Therefore by (17) and (18),

$$\text{Proj}_D(\vec{Z}_D) = (\vec{Z}_D \cdot \vec{e}_{\circ,\oplus}) \vec{e}_{\circ,\oplus} = \frac{\text{Vol}(D)}{\vec{n}_{\circ,\oplus} \cdot \vec{e}_{\circ,\oplus}} \frac{w_\oplus - w_\circ}{d_{\circ,\oplus}} (\vec{n}_{\circ,\oplus} \cdot \vec{e}_{\circ,\oplus}) \vec{e}_{\circ,\oplus} = \text{Vol}(D) \frac{w_\oplus - w_\circ}{d_{\circ,\oplus}} \vec{e}_{\circ,\oplus}.$$

By (7), we conclude that $\text{Proj}_D(\vec{Z}_D) = \text{Vol}(D) \text{Proj}_D(\nabla_D^\mathfrak{x} w^\mathfrak{x})$.

• Similarly, $\text{Proj}_D^*(\vec{n}_{\circ,\oplus})$ is zero. By (17),(18),(20) and by the definition (7) of $\text{Proj}_D^*(\nabla_D^\mathfrak{x} w^\mathfrak{x})$,

$$\text{Proj}_D^*(\vec{Z}_D) = \frac{d_{\circ,\oplus} \cos \alpha_{\circ\oplus}}{3} m \frac{1}{m} \sum_{i=1}^l (w_{i+1}^* - w_i^*) (\vec{n}_{\circ,\oplus} \times \overrightarrow{x_{\circ\oplus}^* x_{i+1}^*}) = \text{Vol}(D) \text{Proj}_D^*(\nabla_D^\mathfrak{x} w^\mathfrak{x}).$$

◊

Remark 4.1. Note that our discrete duality property is suitable for discrete functions satisfying the homogeneous Dirichlet condition on $\partial\Omega$. For different boundary conditions see e.g. [6, 9].

Remark 4.2. In 2D, let us point out a scheme which is much simpler than the DDFV scheme and that still possesses the discrete duality property; the discrete duality follows directly from the reconstruction property of Corollary 2.3 (see [4]).

This simpler scheme is well known for the case one starts with a triangulation of $\Omega \subset \mathbb{R}^2$ (see e.g. [2, 23, 7]). Elements of the triangulation play the role of diamonds of the DDFV scheme; in particular, discrete gradient is reconstructed as being constant per triangle. The dual Voronoï mesh of the triangulation is the finite volume mesh (these are the “complementary finite volumes”, in the terminology of the paper [23]) on which one considers constant per volume discrete functions.

To the authors’ knowledge, the discrete duality property for the 3D “complementary finite volume” scheme only holds for very particular mesh geometries (e.g., uniform tetrahedral or rectangular meshes); see the discussion of [3, Appendix B].

4.1. Implications of the discrete duality property and elements of “discrete calculus”.

Remark 4.3. The discrete duality property (16) is one of the crucial tools of the “discrete calculus” for “double” schemes. It permits in particular to discretize coercive and monotone diffusion operators such as the p -laplacian with the help of coercive and monotone finite volume schemes.

E.g. the p -laplacian $\operatorname{div} \vec{\mathbf{a}}(\nabla w)$, $\vec{\mathbf{a}}(\vec{r}) = |\vec{r}|^{p-2} \vec{r}$, would be discretized by $\operatorname{div}^{\mathfrak{T}} \vec{\mathbf{a}}(\nabla^{\mathfrak{T}} w^{\mathfrak{T}})$.

Furthermore, (16) ensures that the variational character of a diffusion operator is preserved at the discrete level. If $\vec{\mathbf{a}}(\cdot)$ is the gradient of a convex functional $\Phi(\cdot)$, so that the diffusion operator $-\operatorname{div} \vec{\mathbf{a}}(\nabla w)$ on $W_0^{1,p}(\Omega)$ derives from the functional $w \in W_0^{1,p}(\Omega) \mapsto \int_{\Omega} \Phi(\nabla w)$, then the discrete diffusion operator $-\operatorname{div}^{\mathfrak{T}} \vec{\mathbf{a}}(\nabla^{\mathfrak{T}} w^{\mathfrak{T}})$ derives from the discrete functional

$$w^{\mathfrak{T}} \in \mathbb{R}_0^{\mathfrak{T}} \mapsto \sum_{D \in \mathfrak{D}} \operatorname{Vol}(D) \Phi(\nabla^{\mathfrak{T}} w^{\mathfrak{T}})$$

(see [6]). This property allows to use the convex minimization numerical methods, such as the conjugate gradient method, in order to calculate discrete solutions in practice.

Remark 4.4. Other crucial “discrete calculus” devices involve a family of meshes \mathfrak{T}_h parametrized by the “size” h of the mesh; at this stage, uniform constraints on the mesh distortions are required. In the context of “double” finite volume schemes, we refer e.g. to [15, 6, 3] for partial results on:

- Uniform in h discrete Poincaré-Friedrichs inequalities (note that we expect that the discrete Poincaré-Friedrichs inequality for the 3D operator $\nabla^{\mathfrak{T}}$ in (13) may fail, unless the restriction $l \leq 4$ on the number l of vertices of κ_L is imposed, as in [32]);
- Uniform bounds on the Lebesgue norms of projections $\mathbb{P}^{\mathfrak{T}_h} f$ of functions f on the set $\mathbb{R}^{\mathfrak{T}_h}$ of discrete functions; asymptotic (as $h \rightarrow 0$) convergence properties for $\mathbb{P}^{\mathfrak{T}_h} f$ in the Lebesgue spaces;
- Uniform bounds on the discrete gradient $\nabla^{\mathfrak{T}_h} \mathbb{P}^{\mathfrak{T}_h} w$ in terms of the gradient ∇w for functions w in Sobolev spaces (here, the order-one consistency in the sense of Remark 2.6 is used); asymptotic convergence properties in Sobolev spaces for projections $\mathbb{P}^{\mathfrak{T}_h} w$;
- Asymptotic discrete compactness properties for sequences of discrete functions $w^{\mathfrak{T}_h}$ with uniformly bounded discrete norms of $\nabla^{\mathfrak{T}_h} w^{\mathfrak{T}_h}$.

Concerning the latter point, notice that the discrete Rellich embedding property is delicate, because bounds on $\nabla^{\mathfrak{T}_h} w^{\mathfrak{T}_h}$ do not contain enough information to control the differences $(w_K - w_{K^*})$. The results of [6, 3] state convergence of the weighted combination $\frac{1}{d} w^{\mathfrak{M}_h} + \frac{d-1}{d} w^{\mathfrak{M}_h^*}$, where $w^{\mathfrak{M}_h} := \sum_{K \in \mathfrak{M}_h} w_K^h \mathbb{1}_K$, $w^{\mathfrak{M}_h^*} := \sum_{K^* \in \mathfrak{M}_h^*} w_{K^*}^h \mathbb{1}_{K^*}$. One possibility to enforce the convergence of $w^{\mathfrak{M}_h}, w^{\mathfrak{M}_h^*}$ to the same limit is to introduce into the finite volume scheme a penalization term controlling the differences $(w_K - w_{K^*})$ for $K \cap K^* \neq \emptyset$ (see [3]). The penalization term can be chosen to derive from a discrete penalization functional such as

$$w^{\mathfrak{T}} \in \mathbb{R}_0^{\mathfrak{T}} \mapsto h^{-r} \sum_{K \in \mathfrak{M}, K^* \in \mathfrak{M}^*} \operatorname{Vol}(K \cap K^*) |w_K - w_{K^*}|^p$$

with $p \in (1, +\infty)$, $r > 0$.

Remark 4.5. The discrete duality property (16) holds without the orthogonality conditions on the meshes (which are the conditions $\vec{x}_K \vec{x}_L \perp \kappa_L$, $\vec{x}_{K^*} \vec{x}_{L^*} \perp \kappa_{L^*}$). But if one needs discrete versions of certain nonlinear analysis tools (e.g., while using the techniques of entropy or renormalized solutions), then the orthogonality condition becomes very helpful (see [4, 3]). It is also needed when one wants to ensure a

discrete maximum principle. The orthogonality is assumed in most of the classical finite volume schemes studied in [18].

4.2. On the choice of the face centers $x_{K|L}$ and other generalizations.

Remark 4.6. (i) Given a partition of Ω into convex disjoint open subsets K , one can always construct a “double” mesh \mathfrak{T} satisfying the constraints on the choice of x_K , $x_{K|L}$, $x_{K^*|L^*}$ imposed in Section 2. But if one wants to use some simpler constructions such as the classical Voronoï dual mesh in Example 4.8 below, some of the below generalizations are needed.

(ii) The barycenter (middlepoint) choice $x_{K^*|L^*} = \frac{1}{2}(x_{K^*} + x_{L^*})$ on the edges is in the heart of the consistency property of Remark 2.6 (see the proof of Lemma 2.2); we do not know whether it could be bypassed.

(iii) An important generalization concerns the choice of $x_{K|L}$. It may be convenient (as e.g. in Example 4.8 below) to let $x_{K|L}$ be the point of intersection of the plane containing the interface $K|L$ with the line passing through the centers x_K, x_L . Even if $x_K \in K$ and the volumes are convex, the intersection point can fall outside $K|L$.

In fact, the property $x_{K|L} \in K|L$ was only used in the statement that $\text{Vol}(s) = \frac{1}{6} \langle \overrightarrow{x_\ominus x_\oplus}, \overrightarrow{x_{\ominus\oplus}^* x_{i+1}^*}, \overrightarrow{x_i^* x_{i+1}^*} \rangle$ is positive, and in the second statement of Remark 2.7. In particular, no such restriction appear in Lemma 2.2, Corollary 2.3 and Remark 2.6.

Let us stress that all the formulae in terms of vector and mixed products given in this note can be used without changes, if $x_{K|L}$ belongs to the plane containing $K|L$ (see in particular remark 2.3). But it becomes necessary to generalize the notions of K^* and $\text{Vol}(K^*)$, allowing for subdiamonds and elements with negative volume. We illustrate the situation in Remark 4.7 below.

(iv) The requirement that x_K belong to K can be relaxed. The definition of diamonds and subdiamonds becomes a bit more complicated in this case, because some elements $T \in \mathfrak{T}$ may have negative volume; the situation is entirely similar to that of Remark 4.7 below. In order to have $\text{Vol}(D) > 0$, it suffices to guarantee that the normal to $K_\ominus|K_\oplus$ vector $\vec{n}_{\ominus,\oplus}$ (which, by definition, forms an acute angle with $\overrightarrow{x_\ominus x_\oplus}$) point from K_\ominus to K_\oplus . To this end, the Delaunay property is required in Example 4.8.

(v) The convexity constraint on the primal volumes K can be relaxed; e.g., if each volume K is star-shaped with respect to some point x_K , the construction goes on without any change.

Remark 4.7.

(i) Under the assumptions that $x_K \in K$ for all K , $x_{K|L} \in K|L$ for all $K|L$, the set of all elements \mathfrak{T} is a partition of Ω , and each of the partitions \mathfrak{M} , \mathfrak{M}^* , \mathfrak{D} of Ω is obtained by combining elements. More exactly, we have $K = \bigcup T_{K^*,K^*|L^*}^K$, where the sum runs over all $L \in \mathcal{N}(K)$ and all K^*, L^* which are neighbour vertices of the polygon $K|L$. Similarly, $K^* = \bigcup T_{K^*,K^*|L^*}^{K^*}$, where the union runs over all K, L^* such that $T_{K^*,K^*|L^*}^{K^*}$ makes sense. Finally,

$$D^{K|L} = \bigcup \left(T_{K^*,K^*|L^*}^K \cup T_{L^*,K^*|L^*}^K \cup T_{K^*,K^*|L^*}^{L^*} \cup T_{L^*,K^*|L^*}^{L^*} \right) = \bigcup S_{K^*|L^*}^{K|L},$$

where the sum runs over all couples $\{K^*, L^*\}$ of neighbour vertices of the interface $K|L$.

When an element $T \in \mathfrak{T}$ contributes to the construction of K , we say that T is associated with K , and write $T \sim K$. We therefore have $K = \bigcup_{T \sim K} T$, and $\text{Vol}(K) = \sum_{T \sim K} \text{Vol}(T)$.

Analogous meaning is given to the notation $T \sim K^*$, $T \sim D$, and $S \sim D$, $T \sim S$; e.g.,

$$(21) \quad D = \bigcup_{S \sim D} S, \quad \text{and} \quad \text{Vol}(D) = \sum_{S \sim D} \text{Vol}(S).$$

In each case, the relation “ \sim ” simply means the inclusion “ \subset ”.

(ii) Now, for one example where $x_{K|L} \notin K|L$, let $K|L$ be a triangle with vertices denoted by $x_{K^*}, x_{L^*}, x_{M^*}$, with obtuse angle at x_{L^*} ; let $x_{K|L}$ be the center of circumscribed circle of the triangle which therefore falls outside $K|L$ (this situation occurs in Example 4.8). Instead of the decomposition

$$D^{K|L} = \bigcup_{S \sim D} S = S_{K^*|L^*}^{K|L} \cup S_{L^*|M^*}^{K|L} \cup S_{M^*|K^*}^{K|L},$$

we now have

$$D^{K|L} = \left(S_{K^*|L^*}^{K|L} \cup S_{L^*|M^*}^{K|L} \right) \setminus S_{M^*|K^*}^{K|L}.$$

But if (with the notation of Figures 1,3) we keep the formula

$$(22) \quad \text{Vol}(s) = \frac{1}{6} \langle \overrightarrow{x_\ominus x_\oplus}, \overrightarrow{x_{\ominus\oplus}^* x_{i+1}^*}, \overrightarrow{x_i^* x_{i+1}^*} \rangle$$

for the volume of s , we see that $\text{Vol}(S_{M^*|K^*}^{K|L})$ becomes negative, and cancellations lead to

$$\text{Vol}(D^{K|L}) = |\text{Vol}(S_{K^*|L^*}^{K|L})| + |\text{Vol}(S_{L^*|M^*}^{K|L})| - |\text{Vol}(S_{M^*|K^*}^{K|L})| = \text{Vol}(S_{K^*|L^*}^{K|L}) + \text{Vol}(S_{L^*|M^*}^{K|L}) + \text{Vol}(S_{M^*|K^*}^{K|L}) = \sum_{S \sim D} \text{Vol}(S).$$

We see that the set-theoretic relation in (21) loses its sense, but the formula for $\text{Vol}(D)$ keeps working. Similarly, a primal volume K is a set of points of Ω that can be obtained by the operations " \cup ", " \setminus " from the elements T associated with K , and $\text{Vol}(K) = \sum_{S \sim K} \text{Vol}(T)$; the (signed) volume of T can be computed by a formula similar to (22). Let us point out that $\text{sign}(\text{Vol}(T)) = \text{sign}(\text{Vol}(S))$ when $T \subset S$, and $\text{Vol}(S) = \sum_{T \subset S} \text{Vol}(T)$.

The general situation is the same as in the above example. Notice that neither \mathcal{T} , nor \mathfrak{S} form a partition of Ω ; but each one forms a "signed partition" of Ω in the sense that

$$(23) \quad \sum_{T \in \mathcal{T}} \text{sign}(\text{Vol}(T)) \mathbb{1}_T(x) = 1 \quad \text{and} \quad \sum_{S \in \mathfrak{S}} \text{sign}(\text{Vol}(S)) \mathbb{1}_S(x) = 1 \quad \text{a.e. on } \Omega$$

(here $\mathbb{1}_A(\cdot)$ stands for the characteristic function of a set $A \subset \Omega$).

The situation with dual volumes K^* can be more intricate: K^* may in general consist of a "positive" and a "negative" part, to which no set-theoretical meaning can be given⁴; but we can give the sense of $\sum_{T \sim K^*} \text{Vol}(T)$ to $\text{Vol}(K^*)$. In this case, let us call K^* a generalized dual volume. Here a constraint appears on the choice of the family $(x_{K|L})_{K|L}$ of the face centers: one should keep $\text{Vol}(K^*) > 0$, in order that (14) be a scalar product.

Similar interpretation can be given to the statement of Remark 2.7. In formulae (13), the normal flux of $\vec{\mathcal{F}}_S$ through σ_S is automatically taken with the sign $\text{sign}(\text{Vol}(S))$, and the cancellations in $\sum_{S \in \mathcal{N}(K)} m_S \vec{\mathcal{F}}_S \cdot (-1)^{\epsilon_S^K} \vec{n}_S$ make it be equal to the normal flux of the field $\vec{\mathcal{F}}$ through ∂K . Notice that the relation " $s \in \mathcal{V}(K)$ " should be understood in the sense that $s \supset T$ for some $T \sim K$. Similarly, for a (possibly generalized) control volume K^* , the flux through its (possibly generalized) boundary ∂K^* is the sum of the signed contributions of the normal fluxes through $\sigma_{S_\odot}^*, \sigma_{S_\ominus}^* \subset s$ with $s \in \mathcal{V}^*(K^*)$. Formulae (13) take care of this convention.

(iii) Clearly, these conventions should affect the discretization of source terms on the mesh \mathfrak{T} . In the case (i) above, one naturally defines the projection of $f \in L^1(\Omega)$ on the space $\mathbb{R}^{\mathfrak{T}}$ of discrete functions by $\bar{f}^{\mathfrak{T}} = ((\bar{f}_K)_{K \in \mathfrak{M}}, (\bar{f}_{K^*})_{K^* \in \mathfrak{M}^*})$ with $\bar{f}_K = \frac{1}{\text{Vol}(K)} \int_K f$, $\bar{f}_{K^*} = \frac{1}{\text{Vol}(K^*)} \int_{K^*} f$. But in the case (ii), we should rather generalize these formulae and write

$$(24) \quad \bar{f}_{K^*} = \frac{1}{\text{Vol}(K^*)} \sum_{T \sim K^*} \text{sign}(\text{Vol}(T)) \int_T f = \left(\sum_{T \sim K^*} \text{Vol}(T) \right)^{-1} \sum_{T \sim K^*} \text{sign}(\text{Vol}(T)) \int_T f$$

when K^* is a generalized volume. The "signed partition" property (23) is a clue to the consistency of such projection operator. We guess that the "discrete calculus" properties mentioned in Remark 4.4 can be proved also in this generalized framework, under some additional restrictions such as $\text{Vol}(K^*) > 0$, $\text{Vol}(D) > 0$.

Example 4.8. Let the primal mesh \mathfrak{M} of $\Omega \subset \mathbb{R}^3$ be such that each $K \in \mathfrak{M}$ is a polyhedron admitting a circumscribed ball with center x_K (for instance, a tetrahedron), and assume that all neighbour volumes K, L satisfy the standard Delaunay condition. It follows that each face $K|L$ is an inscriptible polygon. Take for the dual mesh \mathfrak{M}^* , the standard Voronoï mesh constructed from the vertices of the primal mesh. This definition of \mathfrak{M}^* enters our framework, with the following choice:

- the center $x_{K|L}$ of a face $K|L$ is the center of its circumscribed circle;
- the center $x_{K^*|L^*}$ of an edge $K^*|L^*$ is its midpoint.

This construction does not guarantee that $x_{K|L} \in K|L$ nor that $x_K \in K$; thus we refer to the generalizations of the above Remarks 4.6, 4.7.

This "Delaunay-Voronoi" double scheme possesses the orthogonality property mentioned in Remark 4.5. See [28, 3], for two examples of the use of this scheme.

Remark 4.9. Notice that in order to get the mesh of Example 4.8, one can also reverse the construction procedure. Starting from a given set of points x_{K^*} , one constructs the Voronoï mesh which will play the role of the dual mesh \mathfrak{M}^* . A tetrahedral primal mesh \mathfrak{M} is obtained by joining appropriately the vertices of \mathfrak{M}^* ; a slightly different convention on boundary volumes is needed in this case.

5. CONCLUSIONS

This work can be viewed as a complement to the paper [28] by F. Hermeline, where a number of 3D diffusion problems were discretized with the help of "double" finite volume schemes. Many numerical examples are given in [28]. Our contribution is the purely theoretical study of the meshes and the

⁴We guess that this problem does not occur in Example 4.8, thanks to the Delaunay condition: the "negative" part of K^* is completely cancelled by its "positive" part, as in the case of the primal volumes.

associated gradient approximations leading to the “discrete duality” property, property which underlies the known convergence proofs for the 2D double schemes.

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(Boris Andreianov)
Laboratoire de Mathématiques
Université de Franche-Comté
16 route de Gray
25 030 Besançon Cedex, France
E-mail address: `boris.andreianov@univ-fcomte.fr`

(Mostafa Bendahmane)
Departamento de Ingeniería Matemática
Facultad de Ciencias Físicas y Matemáticas
Universidad de Concepción
Casilla 160-C Concepción, Chile
E-mail address: `mostafab@ing-mat.udec.cl`