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# 2D/3D Discrete Duality Finite Volume Scheme (DDFV) applied to ECG simulation.

**DDFV scheme for anisotropic- heterogeneous elliptic equations, application to a bio-mathematics problem : electrocardiogram simulation.**

**Yves COUDIÈRE\*** — **Charles PIERRE\*\*** — **Olivier ROUSSEAU\*\*\*** — **Rodolphe TURPAULT\***

*\*Laboratoire de mathématiques et applications Jean Leray, UMR CNRS 6629. Université de Nantes, France.*

*{yves.coudiere,rodolphe.turpault}@univ-nantes.fr*

*\*\*Laboratoire de Mathématiques Appliquées de Pau, UMR CNRS 5142. Université de Pau et des Pays de l'Adour, France.*

*charles.pierre@univ-pau.fr*

*\*\*\* Department of Mathematics and Statistics, University of Ottawa, Canada.*

*orous097@uottawa.ca*

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RÉSUMÉ.

*ABSTRACT. In this paper is presented a finite volume (DDFV) scheme for solving elliptic equations with heterogeneous anisotropic conductivity tensor. That method is based on the definition of a discrete divergence and a discrete gradient operator. These discrete operators have close relationships with the continuous ones, in particular they fulfil a duality property related with the Green formula. The operators are defined in dimension 2 and 3, their duality property is stated and used to establish the well posedness of the approximation scheme as well as its symmetry/positiveness. In the last part, the method is used for the resolution of a problem arising in bio-mathematics: the ECG (electrocardiogram) simulation. This is done on a 2D slice of a realistic torso defined from segmented MRI medical images.*

*MOTS-CLÉS :*

*KEYWORDS: keywords*

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## 1. Introduction

The aim of this paper is to define a finite volume discretisation (called *DDFV* discretisation) for the following elliptic equation on a bounded domain  $\Omega \subset \mathbb{R}^d$ ,  $d = 2, 3$ . For a conductivity tensor  $G = G(x)$  (symmetric positive definite and uniformly elliptic on  $\Omega$ ) that is anisotropic and also heterogeneous, and for a mixed Neumann/Dirichlet homogeneous boundary condition on  $\partial\Omega = \partial\Omega^N \cup \partial\Omega^D$ , we search  $\varphi$  such that ( $\mathbf{n}$  is a unit normal on the boundary) :

$$\operatorname{div}(G\nabla\varphi) = f, \quad G\nabla\varphi \cdot \mathbf{n} = 0 \text{ on } \partial\Omega^N, \quad \varphi|_{\partial\Omega} = 0 \text{ on } \partial\Omega^D, \quad f \in L^2(\Omega). \quad (1)$$

Precisely, one assumes that there exists one (or more) crack  $\Gamma$  in the domain that splits  $\Omega$  in  $\Omega_1, \Omega_2$  and such that  $G$  has a discontinuity across  $\Gamma$ . One thus imposes the transmission condition ( $\mathbf{n}$  is a normal to  $\Gamma$ ), in the trace sense on  $\Gamma$  :

$$\varphi|_{\Omega_1} = \varphi|_{\Omega_2}, \quad G|_{\Omega_1} \nabla\varphi|_{\Omega_1} \cdot \mathbf{n} = G|_{\Omega_2} \nabla\varphi|_{\Omega_2} \cdot \mathbf{n} \quad \text{on } \Gamma. \quad (2)$$

When  $G|_{\Omega_i}$  is smooth enough, the classical theory (see *e.g.* [LAD 68]) tells us that (1) has a unique variational solution  $\varphi \in H^1(\Omega)$  such that  $\varphi|_{\Omega_i} \in H^2(\Omega_i)$  and such that the boundary condition in (1) and the transmission conditions in (2) hold in the trace sense. Whenever  $\partial\Omega^N = \partial\Omega$ , uniqueness doesn't hold anymore and there is then a solution *iff*  $f$  has zero mean value, all solution then differ up to a constant.

## 2. DDFV discretisation of the problem

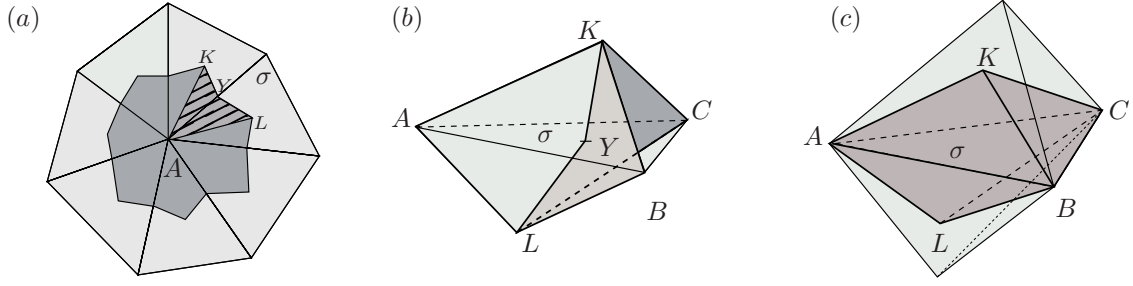
### 2.1. Mesh definition and discrete data

We consider a Delaunay triangulation/tetrahedrisation  $\mathcal{C}$  of a bounded polygonal/polyhedral subset  $\Omega \subset \mathbb{R}^d$ ,  $d = 2, 3$ . We denote by  $\mathcal{V}$  and  $\mathcal{I}$  the associated sets of vertices and interfaces (elements edges/faces). The elements  $C \in \mathcal{C}$  will be called *primal cells*. For equation (1) to be correctly discretised, we naturally assume that the internal interfaces "follow" cracks in  $G$  and that the boundary interfaces  $\sigma \subset \partial\Omega$  are dealt into two subsets  $\mathcal{I}^D, \mathcal{I}^N$  such that  $\Omega^N = \cup_{\sigma \in \mathcal{I}^N} \sigma$ ,  $\Omega^D = \cup_{\sigma \in \mathcal{I}^D} \sigma$ . The set of vertices of the interfaces  $\sigma \in \mathcal{I}^D$  is denoted by  $\mathcal{V}^D \subset \mathcal{V}$ .

To every primal cell  $C$  is associated a centre  $K \in C$  (its iso-barycentre in practice). By  $C_K$  one denotes the primal cell  $C$  of centre  $K$ . To any interface  $\sigma \in \mathcal{I}$  is associated a centre  $Y_\sigma \in \sigma$  (also its iso-barycentre in practice), also simply denoted  $Y$ . Every internal interface  $\sigma \in \mathcal{I}$  is the boundary between two primal cells  $C_1$  and  $C_2$ . This is denoted by  $\sigma = C_1|C_2$ . For more simplicity one shall denote by the same symbol any geometrical element and its measure : if  $\sigma \in \mathcal{I}$ ,  $\sigma$  also denotes its length/area ; if  $C \in \mathcal{C}$ ,  $C$  also denotes its area/volume,  $\Omega$  both denotes the domain and its measure...

To every vertex  $A \in \mathcal{V}$  is associated a **dual cell**  $P_A$ . Let us first introduce the subset  $\mathcal{I}_A \subset \mathcal{I}$  of all the interfaces having  $A$  as a vertex. To every  $\sigma \in \mathcal{I}_A$  is associated a geometrical element  $P_{A,\sigma}$ .  $P_A$  is given by  $P_A = \cup_{\sigma \in \mathcal{I}_A} P_{A,\sigma}$ .

The elements  $P_{A,\sigma}$  are defined as follows (see figure 2.1). Let  $\sigma = C_{K_1}|C_{K_2}$  be an



**Figure 1.** (a) Two dimensional case, definition of  $P_{A,\sigma}$  (hatched dark grey) and  $P_A$  (dark grey). (b) Three dimensional case, definition of  $P_{A,\sigma}$  for an internal interface  $\sigma = C_K|C_L = ABC$ . (c) Three dimensional diamond cell  $D_\sigma$  (dark grey).  $D_\sigma = D_{\sigma,K} \cup D_{\sigma,L}$ ,  $D_{\sigma,K}$  is the part above  $\sigma$  whereas  $D_{\sigma,L}$  is the part underneath  $\sigma$ .

internal interface and let  $Y$  be  $\sigma$ 's centre. In dimension 2,  $P_{A,\sigma}$  is the quadrilateral  $AK_1YK_2$ . In dimension 3, let  $B$  and  $C$  be the two other vertices of  $\sigma$  ( $\sigma = ABC$ ). Then  $P_{A,\sigma}$  is the reunion of the two pyramids having the same quadrilateral base  $ABYC$  and  $K_1, K_2$  for apex :  $P_{A,\sigma} = ABYCK_1 \cup ABYCK_2$ . That definition has obvious extension to the case  $\sigma \subset \partial\Omega$ .

Remark that in dimension 2 the (interiors of the) dual cells are disjoint and recover the whole domain, therefore  $\sum_{A \in \mathcal{V}} P_A = \Omega$ . Whereas in dimension 3 the dual cells are no more disjoint, if  $A$  and  $B$  are two vertices of the same interface  $\sigma$ ,  $P_{A,\sigma} \cap P_{B,\sigma} \neq \emptyset$ . Actually the dual cells now recover exactly twice the whole domain, so that  $\sum_{A \in \mathcal{V}} P_A = 2\Omega$ .

To every interface  $\sigma \in \mathcal{I}$  is associated one **diamond cell**  $D_\sigma$ . For an internal interface  $\sigma = C_K|C_L$ , it is defined as  $D_\sigma = D_{\sigma,K} \cup D_{\sigma,L}$  where  $D_{\sigma,K}, D_{\sigma,L}$  are the two triangles/pyramids with base  $\sigma$  and apex  $K$  and  $L$  respectively, as depicted on figure 2.1. In the case of a boundary interface  $\sigma \subset \partial\Omega$ ,  $D_\sigma$  is a simple triangle/pyramid,  $D_\sigma = D_{\sigma,K}$ . The  $D_{\sigma,K}$  will be called sub-diamond cells.

To this different types of cells are associated the following types of data :

A **discrete vector field**  $\mathbf{X}_h$  (resp. **discrete tensor**  $G_h$ ) is a vector (resp. matrix) function, piecewise constant on each sub-diamond cell  $D_{\sigma,K}$ . To each internal interface  $\sigma = C_K|C_L$  are associated two vectors  $\mathbf{X}_{\sigma,K}$  and  $\mathbf{X}_{\sigma,L}$  (resp. matrices  $G_{\sigma,K}$  and  $G_{\sigma,L}$ ) on each side of  $\sigma$ .  $G_{\sigma,K}$  is always assumed symmetric positive definite. We shall say that  $\mathbf{X}_h$  is conservative relatively to  $G_h$  if ( $\mathbf{n}_\sigma$  being a normal to  $\sigma$ ) :

$$\forall \sigma \in \mathcal{I} \text{ such that } \sigma = C_K|C_L : G_{\sigma,K} \mathbf{X}_{\sigma,K} \cdot \mathbf{n}_\sigma = G_{\sigma,L} \mathbf{X}_{\sigma,L} \cdot \mathbf{n}_\sigma, \quad (3)$$

A **discrete scalar**  $\varphi_h$  is the data of two sets of scalars  $(\varphi_A)_{A \in \mathcal{V}}, (\varphi_K)_{C_K \in \mathcal{C}}$  associated to the vertices and primal cells centres respectively.

A **DDFV function** is a scalar function  $\tilde{\varphi}_h$ , piecewise affine on  $AY_\sigma K$  (resp.  $ABY_\sigma K$ ) whenever  $\sigma \in \mathcal{I}$ ,  $A \in \mathcal{V}$  (resp.  $A, B \in \mathcal{V}$ ) is (are) vertex(es) of  $\sigma$  in dimension 2 (resp. 3) and  $\sigma \subset C_K, C_K \in \mathcal{C}$ .

## 2.2. The discrete operators and the problem discretisation

The **discrete divergence**  $\text{div}_h$  of a discrete vector field  $\mathbf{X}_h$  is the discrete scalar :

$$(\text{div}_h \mathbf{X}_h)_A = \frac{1}{P_A} \int_{\partial P_A} \mathbf{X}_h \cdot \mathbf{n}_{\partial P_A} ds, \quad (\text{div}_h \mathbf{X}_h)_K = \frac{1}{C_K} \int_{\partial C_K} \mathbf{X}_h \cdot \mathbf{n}_{\partial C_K} ds, \quad (4)$$

where  $\mathbf{n}_{\partial E}$  is the outward unit normal on the boundary of the polygonal/polyhedral element E. That definition makes sense because there are no discontinuities of  $\mathbf{X}_h$  on the edges/faces of primal and dual cells.

The **discrete gradient** of a DDFV function  $\tilde{\varphi}_h$  is the discrete vector field :

$$(\nabla_h \tilde{\varphi}_h)_{\sigma, K} = \frac{1}{D_{\sigma, K}} \int_{D_{\sigma, K}} \nabla \varphi_h dx. \quad (5)$$

The discrete gradient for a discrete scalar is defined below, for implementation, a practical formulation is given in appendix A.

**Definition 2.1.** Let us consider a discrete scalar  $\varphi_h$  such that  $\varphi_A = 0$  for all  $A \in \mathcal{V}^D$  and a discrete tensor  $G_h$ . Then there exists a unique DDFV function  $\tilde{\varphi}_h$  such that :

$$\begin{aligned} \forall A \in \mathcal{V} : \tilde{\varphi}_h(A) &= \varphi_A, \quad \forall C_K \in \mathcal{C} : \tilde{\varphi}_h(K) = \varphi_K, \\ \forall \sigma \in \mathcal{I}^D : \tilde{\varphi}_h(Y_\sigma) &= 0, \quad \forall \sigma \in \mathcal{I}^N : G_\sigma (\nabla_h \tilde{\varphi}_h)_\sigma \cdot \mathbf{n}_\sigma = 0, \end{aligned}$$

and such that  $\nabla_h \tilde{\varphi}_h$  is conservative relatively to  $G_h$ , as defined in (3).

Relatively to  $G_h$ , the discrete gradient of  $\varphi_h$  is defined as  $\nabla_h \varphi_h = \nabla_h \tilde{\varphi}_h$ .

The previously defined discrete operators fulfil a duality property called **discrete Green formula** by analogy with the continuous case :

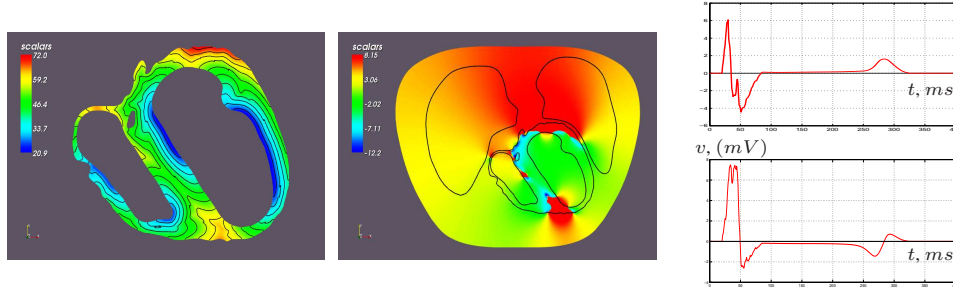
**Proposition 2.2.** Let  $G_h$  a discrete tensor,  $\varphi_h$  a discrete scalar and consider the DDFV function  $\tilde{\varphi}_h$  associated to  $\varphi_h$  relatively to  $G_h$ . If  $\mathbf{X}_h$  is a discrete vector field that satisfy  $\mathbf{X}_{\sigma, K} \cdot \mathbf{n}_\sigma = \mathbf{X}_{\sigma, L} \cdot \mathbf{n}_\sigma$  on every internal interface  $\sigma = C_K | C_L$ , then :

$$\begin{aligned} \int_{\Omega} (\nabla_h \varphi_h) \cdot \mathbf{X}_h dx &= -\frac{1}{d} \sum_{C_K \in \mathcal{C}} \varphi_K (\text{div}_h \mathbf{X}_h)_K C_K - \frac{d-1}{d} \sum_{A \in \mathcal{V}} \varphi_A (\text{div}_h \mathbf{X}_h)_A P_A \\ &+ \int_{\partial \Omega} \tilde{\varphi}_h |_{\partial \Omega} \mathbf{X}_h |_{\partial \Omega} \cdot \mathbf{n}_{\partial \Omega} ds \end{aligned} \quad (6)$$

The consequence is the following :

**Proposition 2.3.** The right hand side  $f$  in (1) being discretised in some discrete scalar  $f_h$ , we look for a discrete scalar  $\varphi_h$  such that :

$$\begin{aligned} \forall A \in \mathcal{V}^D : \varphi_A &= 0, \quad \forall \sigma \in \mathcal{I}^N : G_\sigma (\nabla_h \varphi_h)_\sigma \cdot \mathbf{n}_\sigma = 0, \quad (7) \\ \forall A \in \mathcal{V} - \mathcal{V}^D : (\text{div}_h (G_h \nabla_h \varphi_h))_A &= f_A, \quad \forall C_K \in \mathcal{C} : (\text{div}_h (G_h \nabla_h \varphi_h))_K = f_K \end{aligned}$$



**Figure 2.** (left) Simulation of  $v$  : isochrons (ms) for the excitation wave on a 2D ventricles slice mesh coming from MRI segmented images, 485000 degrees of freedom. (middle) Computation of  $\varphi$  at time  $t = 50$ ms. The four domain are separated with black lines (ventricles, ventricles cavities, lungs and torso remaining). (right) Simulated ECG for two leads (V1 and V2) located on the body surface.

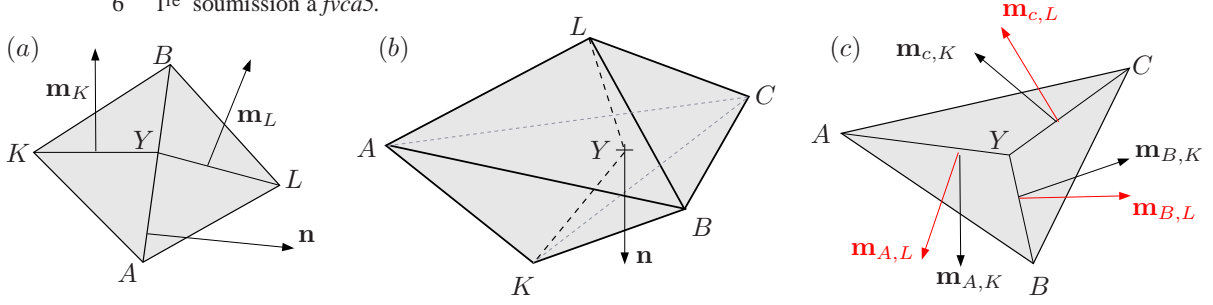
Such a  $\varphi_h$  satisfies the transmission conditions (2) in a discrete sense by construction. If  $\mathcal{I}^D \neq \emptyset$ , (7) has a unique solution. The resulting numerical linear problem to invert is moreover symmetric positive definite. The Neumann problem ( $\mathcal{I}^D = \emptyset$ ) has a solution iff  $\frac{1}{d} \sum_{C_K \in \mathcal{C}} f_K C_K + \frac{d-1}{d} \sum_{A \in \mathcal{V}} f_A P_A = 0$ . The linear problem to invert is now symmetric positive, its kernel is composed of the discrete scalar  $\psi_h$  such that  $\psi_A = C_1$ ,  $\psi_K = C_2$ .

### 3. Application

The bidomain model (see *e.g.* [KEE 98]) describes the electrical activity of the heart. It involves two compartments : the intra/extra cellular mediums, and models a trans-membrane potential  $v = \varphi_i - \varphi$ , difference between the intra/extra cellular potentials respectively. We use here the *modified monodomain* model (see [CLE 04]),  $v(x, t)$  is given through a reaction diffusion system involving a second variable  $\mathbf{w}(x, t) \in \mathbb{R}^N$  that describes the cells membrane activity ( $N$  is up to 20). It is used to simulate the normal propagation of excitation potential wave fronts ( $v$  passing from a rest value to a plateau value) and de-excitation, see figure 3. It reads :

$$A_m C_m \frac{\partial v}{\partial t} + A_m I_{ion}(v, \mathbf{w}) = \text{div}(G_1 \nabla v) + I_{app}(x, t), \quad \frac{\partial \mathbf{m}}{\partial t} = g(v, \mathbf{w}). \quad (8)$$

$A_m$ ,  $C_m$  are constants,  $G_1$  is a non constant anisotropy tensor described below,  $I_{ion}$ ,  $g$  are reaction terms and  $I_{app}$  a source term (applied current) that activates the system. The electrocardiograms (ECG) is the body surface potential resulting from that cardiac electrical activity. It is the trace on the torso  $T$  boundary  $\partial T$  of the extracellular potential  $\varphi$ . In the extra cardiac  $T - H$ ,  $\varphi(x, t)$  is given by a Poisson equation  $\text{div}(G_T \nabla \varphi) = 0$ , where  $G_T$  is isotropic heterogeneous between the different tissue layers conductivities (lungs, blood...). In the heart  $H$ , current balance between the intra and extra cellular compartments gives  $\text{div}(G_2 \nabla \varphi) = -\text{div}(G_3 \nabla v)$ . The tensors



**Figure 3.** Notations for the gradient definition. (a) Two dimensional case : interface  $\sigma = AB = C_K|C_L$  of centre  $Y$ , the three vectors  $\mathbf{n}$ ,  $\mathbf{m}_K$ ,  $\mathbf{m}_L$  have unit length and are respectively orthogonal to  $\sigma$ ,  $YK$ ,  $YL$ . Three dimensional case. (b) Interface  $\sigma = ABC = C_K|C_L$  of centre  $Y$ ,  $\mathbf{n}$  its unit normal from  $C_K$  towards  $C_L$ . (c) Same interface  $\sigma$  view from above, all vectors have unit length,  $\mathbf{m}_{A,K}$ ,  $\mathbf{m}_{B,K}$  and  $\mathbf{m}_{C,K}$  are orthogonal to  $AYK$ ,  $BYK$  and  $CYK$  respectively; same thing for  $\mathbf{m}_{A,L}$ ,  $\mathbf{m}_{B,L}$  and  $\mathbf{m}_{C,L}$  by turning  $K$  into  $L$ .

$G_i$  take into account the fibrous organisation of the heart. They read the same anisotropic/non constant form :  $G_i(x) = P^{-1}(x)\tilde{G}_iP(x)$ , where  $\tilde{G}_i = \text{Diag}(g_i^l, g_i^t)$  is a reference matrix :  $g_i^l, g_i^t$  being the longitudinal/transverse conductivities along/across the cardiac fibres.  $P(x)$  then is a change of basis matrix from the Frenet basis attached to the fibre direction at point  $x$ . On the whole domain  $T$ , this results in one global elliptic equation per time instant  $t$  :

$$\text{div}(G\nabla\varphi(t)) = f(v(t)), \quad f(v(t)) = \begin{cases} 0 & \text{in } H \\ -\text{div}(G_3\nabla v(t)) & \text{in } T - H \end{cases}, \quad (9)$$

completed with the transmission conditions (2) on the heart/torso boundary and also on the interface between different tissue layers, and also with a Neumann boundary condition on  $\partial T$  (no current flow out of the body). In that problem,  $v(x, t)$  is an entry coming from a first computation on the heart previously described.

We then discretised (9) using the DDFV scheme. Our domain  $T$  is a torso slice mesh coming from MRI segmented data and counting 600 000 degrees of freedom. The domain is divided in four parts : the heart, the ventricles cavities (filled in with blood), the lungs and the remaining torso. each part having the different previously described conductivity properties.  $\varphi$  is computed on  $T$  at each  $ms$ , the ECG body surface potential is recorded at 6 leads located on the torso boundary, see figure 3. On a whole cardiac cycle ( $\simeq 600 ms$ ), 600 computation are thus performed. That computation necessitates the inversion of an ill-conditioned symmetric positive linear system at each  $ms$ . For this a Gm-Res solver combined with a basic SSOR preconditioning has been used.

## A. Discrete gradient implementation

With the notations of *def.* 2.1 and of figure A, the expression of  $\nabla_h \varphi_h$  is :

$$\begin{aligned} d = 2 : \quad & 2D_{\sigma,K} (\nabla_h \varphi_h)_{\sigma,K} = (\tilde{\varphi}(Y) - \varphi_K) \sigma \mathbf{n} + (\varphi_B - \varphi_A) KY \mathbf{m}_K \\ d = 3 : \quad & 3D_{\sigma,K} (\nabla_h \varphi_h)_{\sigma,K} = (\tilde{\varphi}(Y) - \varphi_K) \sigma \mathbf{n} + (\varphi_B - \varphi_C) AY K \mathbf{m}_{A,K} \\ & + (\varphi_C - \varphi_A) BY K \mathbf{m}_{B,K} + (\varphi_A - \varphi_B) CY K \mathbf{m}_{C,K} \end{aligned}$$

It involves the DDFV function  $\tilde{\varphi}_h$  in *def.* 2.1, whose definition is completed by :

$$\begin{aligned} d = 2 : \quad & \tilde{\varphi}_h(Y) = \alpha \varphi_K + (1 - \alpha) \varphi_L + k(\varphi_B - \varphi_A) \\ d = 3 : \quad & \tilde{\varphi}_h(Y) = \alpha \varphi_K + (1 - \alpha) \varphi_L + k_A(\varphi_B - \varphi_C) + k_B(\varphi_C - \varphi_A) + k_C(\varphi_A - \varphi_B) . \end{aligned}$$

with :

$$\begin{aligned} \alpha^{-1} &= 1 + \frac{D_{\sigma,K} \mathbf{n} G_{\sigma,L} \mathbf{n}}{D_{\sigma,L} \mathbf{n} G_{\sigma,K} \mathbf{n}} \\ k &= \frac{LY}{\sigma} \frac{\mathbf{m}_L G_{\sigma,L} \mathbf{n}}{\frac{D_{\sigma,L}}{D_{\sigma,K}} \mathbf{n} G_{\sigma,K} \mathbf{n} + \mathbf{n} G_{\sigma,L} \mathbf{n}} - \frac{KY}{\sigma} \frac{\mathbf{m}_K G_{\sigma,K} \mathbf{n}}{\frac{D_{\sigma,K}}{D_{\sigma,L}} \mathbf{n} G_{\sigma,L} \mathbf{n} + \mathbf{n} G_{\sigma,K} \mathbf{n}} \\ k_Z &= \frac{ZYL}{\sigma} \frac{\mathbf{m}_{Z,L} G_{\sigma,L} \mathbf{n}}{\frac{D_{\sigma,L}}{D_{\sigma,K}} \mathbf{n} G_{\sigma,K} \mathbf{n} + \mathbf{n} G_{\sigma,L} \mathbf{n}} - \frac{ZYK}{\sigma} \frac{\mathbf{m}_{Z,K} G_{\sigma,K} \mathbf{n}}{\frac{D_{\sigma,K}}{D_{\sigma,L}} \mathbf{n} G_{\sigma,L} \mathbf{n} + \mathbf{n} G_{\sigma,K} \mathbf{n}} , \quad Z = A, B, C. \end{aligned}$$

For boundary interfaces this expression is adapted as follows. For  $\sigma \in \mathcal{I}^D$ ,  $\tilde{\varphi}_h(Y) = 0$ . For  $\sigma \in \mathcal{I}^N$ , one suppresses  $D_{\sigma,L}$  by stating  $L = Y$  and  $G_{\sigma,L} = 0$ .

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