2D/3D Discrete Duality Finite Volume (DDFV) scheme for anisotropic- heterogeneous elliptic equations, application to the electrocardiogram simulation.

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

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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*

1re soumission à *fvca5*, le 22 novembre 2007.

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 Ω) 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 φ such that ($\mathbf{n}$ is a unit normal on the boundary) :

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

Precisely, one assumes that there exists one (or more) crack Γ in the domain that splits Ω in Ω_1, Ω_2 and such that G has a discontinuity across Γ. One thus imposes the transmission condition ($\mathbf{n}$ is a normal to Γ), in the trace sense on Γ :

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

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 $\sigma \in \mathcal{I}$, σ also denotes its length/area ; if $C \in \mathcal{C}$, C also denotes its area/volume, Ω 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

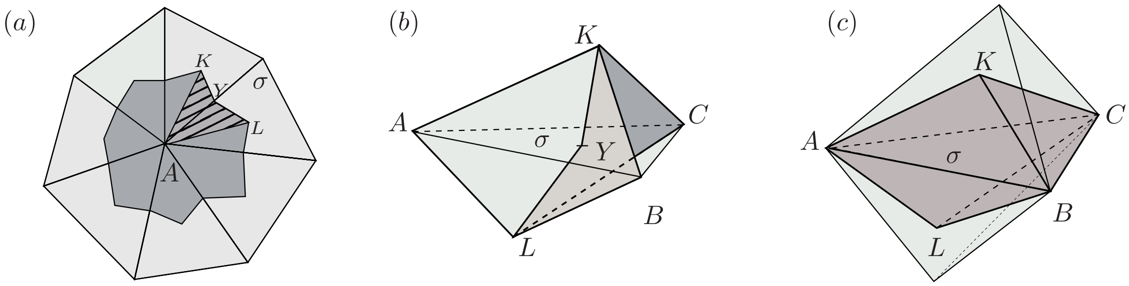

Figure 1. (a) *Two dimensional case, definition of* $P_{A,\sigma}$ *(hatched dark grey) and* P_A *(dark grey).* (b) *Three dimensional case, definition of* $P_{A,\sigma}$ *for an internal interface* $\sigma = C_K|C_L = ABC$. (c) *Three dimensional diamond cell* D_σ *(dark grey).* $D_\sigma = D_{\sigma,K}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

internal interface and let Y be σ'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 σ ($\sigma = ABC$). 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 disjoints and recover the whole domain, therefore $\sum_{A\in\mathcal{V}} P_A = \Omega$. Whereas in dimension 3 the dual cells are no more disjoints, if A and B are two vertices of the same interface σ, $P_{A,\sigma} \cap P_{B,\sigma} \neq \emptyset$. 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_σ. 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 σ and apex K and L respectively, as depicted on figure 2.1. In the case of a boundary interface $\sigma \subset \partial\Omega$, D_σ 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 σ. $G_{\sigma,K}$ 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 σ) :

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

A **discrete scalar** φ_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 σ 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 div**$_h$ of a discrete vector field $\mathbf{X}_h$ is the discrete scalar :

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

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 :

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

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 φ_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 :*

$$\forall\, A \in \mathcal{V} : \; \tilde{\varphi}_h(A) = \varphi_A \; , \;\; \forall\, C_K \in \mathcal{C} : \; \tilde{\varphi}_h(K) = \varphi_K \; ,$$

$$\forall\, \sigma \in \mathcal{I}^D : \; \tilde{\varphi}_h(Y_\sigma) = 0 \; , \;\; \forall\, \sigma \in \mathcal{I}^N : \; G_\sigma \left(\nabla_h \, \tilde{\varphi}_h\right)_\sigma \cdot \mathbf{n}_\sigma = 0 \; ,$$

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 φ_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, φ_h a discrete scalar and consider the DDFV function $\tilde{\varphi}_h$ associated to φ_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 :*

$$\int_\Omega (\nabla_h \varphi_h) \cdot \mathbf{X}_h dx = -\frac{1}{d} \sum_{C_K \in \mathcal{C}} \varphi_K (\mathit{div}_h \mathbf{X}_h)_K C_K - \frac{d-1}{d} \sum_{A \in \mathcal{V}} \varphi_A (\mathit{div}_h \mathbf{X}_h)_A P_A$$

$$+ \int_{\partial\Omega} \tilde{\varphi}_{h|\partial\Omega} \mathbf{X}_{h|\partial\Omega} \cdot \mathbf{n}_{\partial\Omega} ds \tag{6}$$

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 φ_h such that :*

$$\forall A \in \mathcal{V}^D \; : \; \varphi_A = 0 \;\; , \quad \forall \sigma \in \mathcal{I}^N \; : \; G_\sigma (\nabla_h \varphi_h)_\sigma \cdot \mathbf{n}_\sigma = 0 \; , \tag{7}$$

$$\forall A \in \mathcal{V} - \mathcal{V}^D : \; (\mathit{div}_h (G_h \nabla_h \varphi_h))_A = f_A \; , \;\; \forall C_K \in \mathcal{C} : \; (\mathit{div}_h (G_h \nabla_h \varphi_h))_K = f_K$$

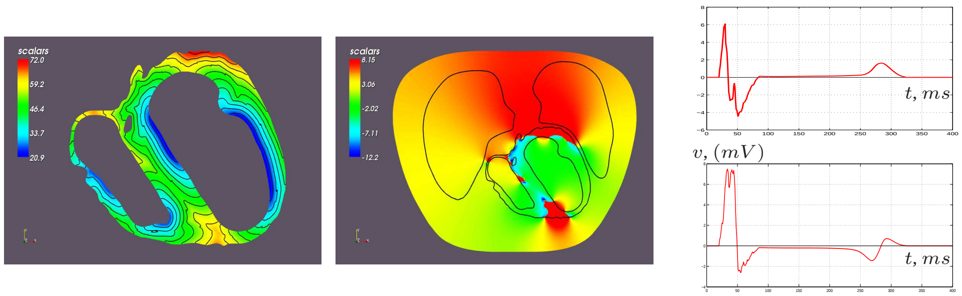

Figure 2. *(left) Simulation of v : isochrons (ms)for the excitation wave on a 2D ventricles slice mesh coming from MRI segmented images, 485000 degrees of freedom. (middle) Computation of φ at time $t = 50ms$. The four domain are separated with black lines (ventricles, ventricles cavities, lungs and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

Such a φ_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 ψ_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 :

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

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 ∂T of the extracellular potential φ. In the extra cardiac $T - H$, $\varphi(x,t)$ is given by a Poisson equation $\mathrm{div}(G_T \nabla \varphi) = 0$, 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 $\mathrm{div}(G_2 \nabla \varphi) = -\mathrm{div}(G_3 \nabla v)$. The tensors

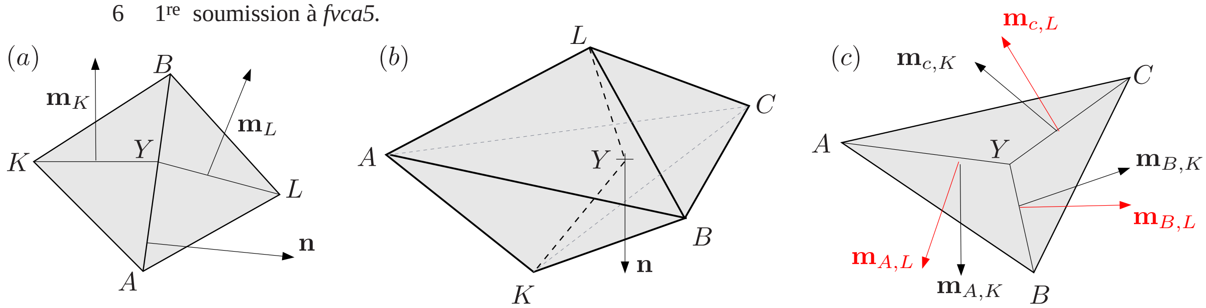

Figure 3. *Notations for the gradient definition.* (a) *Two dimensional case : interface* $\sigma = AB = C_K|C_L$ *of centre* Y*, the three vectors* $\mathbf{n}$*,* $\mathbf{m}_K$*,* $\mathbf{m}_L$ *have unit length and are respectively orthogonal to* σ*,* YK*,* YL*. Three dimensional case.* (b) *Interface* $\sigma = ABC = C_K|C_L$ *of centre* Y*,* $\mathbf{n}$ *its unit normal from* C_K *towards* C_L*.* (c) *Same interface* σ *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 : $G_i(x) = P^{-1}(x)\tilde{G}_i P(x)$, 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 :

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

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 ∂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. φ 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 :

$$d=2\ :\ \ 2D_{\sigma,K}\left(\nabla_h\varphi_h\right)_{\sigma,K}=\left(\tilde{\varphi}(Y)-\varphi_K\right)\sigma\mathbf{n}+\left(\varphi_B-\varphi_A\right)KY\mathbf{m}_K$$

$$\begin{aligned} d=3\ :\ \ 3D_{\sigma,K}\left(\nabla_h\varphi_h\right)_{\sigma,K}&=\left(\tilde{\varphi}(Y)-\varphi_K\right)\sigma\mathbf{n}+\left(\varphi_B-\varphi_C\right)AYK\mathbf{m}_{A,K}\\ &+\left(\varphi_C-\varphi_A\right)BYK\mathbf{m}_{B,K}+\left(\varphi_A-\varphi_B\right)CYK\mathbf{m}_{C,K}\end{aligned}$$

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

$$d=2\ :\ \ \tilde{\varphi}_h(Y)=\alpha\varphi_K+(1-\alpha)\varphi_L+k(\varphi_B-\varphi_A)$$

$$d=3\ :\ \ \tilde{\varphi}_h(Y)=\alpha\varphi_K+(1-\alpha)\varphi_L+k_A(\varphi_B-\varphi_C)+k_B(\varphi_C-\varphi_A)+k_C(\varphi_A-\varphi_B)\ .$$

with :

$$\alpha^{-1}=1+\frac{D_{\sigma,K}}{D_{\sigma,L}}\frac{\mathbf{n}G_{\sigma,L}\mathbf{n}}{\mathbf{n}G_{\sigma,K}\mathbf{n}}$$

$$k=\frac{LY}{\sigma}\frac{\mathbf{m}_L G_{\sigma,L}\mathbf{n}}{\dfrac{D_{\sigma,L}}{D_{\sigma,K}}\mathbf{n}G_{\sigma,K}\mathbf{n}+\mathbf{n}G_{\sigma,L}\mathbf{n}}-\frac{KY}{\sigma}\frac{\mathbf{m}_K G_{\sigma,K}\mathbf{n}}{\dfrac{D_{\sigma,K}}{D_{\sigma,L}}\mathbf{n}G_{\sigma,L}\mathbf{n}+\mathbf{n}G_{\sigma,K}\mathbf{n}}$$

$$k_Z=\frac{ZYL}{\sigma}\frac{\mathbf{m}_{Z,L} G_{\sigma,L}\mathbf{n}}{\dfrac{D_{\sigma,L}}{D_{\sigma,K}}\mathbf{n}G_{\sigma,K}\mathbf{n}+\mathbf{n}G_{\sigma,L}\mathbf{n}}-\frac{ZYK}{\sigma}\frac{\mathbf{m}_{Z,K} G_{\sigma,K}\mathbf{n}}{\dfrac{D_{\sigma,K}}{D_{\sigma,L}}\mathbf{n}G_{\sigma,L}\mathbf{n}+\mathbf{n}G_{\sigma,K}\mathbf{n}}\ ,\ \ Z=A,\ B,\ C.$$

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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