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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.

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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
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 ($n$ is a unit normal on the boundary):

$$\text{div}(G \nabla \varphi) = f, \quad G \nabla \varphi \cdot n = 0 \text{ on } \partial \Omega^N, \quad \varphi|_{\partial \Omega} = 0 \text{ on } \partial \Omega^D, \quad f \in L^2(\Omega).$$  (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 ($n$ is a normal to $\Gamma$), in the trace sense on $\Gamma$:

$$\varphi|_{\Omega_1} = \varphi|_{\Omega_2}, \quad G|_{\Omega_1} \nabla \varphi|_{\Omega_1} \cdot n = G|_{\Omega_2} \nabla \varphi|_{\Omega_2} \cdot n \quad \text{on } \Gamma.$$  (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 : $P_{A,\sigma} = ABYC K_1 \cup ABYC K_2$. 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 $\sum_{A \in V} P_A = \Omega$. Whereas in dimension 3 the dual cells are no more disjoints, if $A$ and $B$ are two vertices of the same interface $\sigma$, $P_{A,\sigma} \cap P_{B,\sigma} \neq \emptyset$. Actually the dual cells now recover exactly twice the whole domain, so that $\sum_{A \in V} P_A = 2\Omega$.

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 $X_h$ (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 $\sigma = C_K|C_L$, it is associated two vectors $X_{\sigma,K}$ and $X_{\sigma,L}$ (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 $X_h$ is conservative relatively to $G_h$ if ($n_\sigma$ being a normal to $\sigma$) :

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

A discrete scalar $\varphi_h$ is the data of two sets of scalars $(\varphi_A)_{A \in V}$, $(\varphi_K)_{C_K \in \mathcal{C}}$ 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 $\sigma \in \mathcal{I}$, $A \in V$ (resp. $A, B \in V$) is (are) vertex(es) of $\sigma$ in dimension 2 (resp. 3) and $\sigma \subset C_K, C_K \in \mathcal{C}$. 

$\sigma$ does not intersect $C_K$.
The discrete operators and the problem discretisation

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

$$
(\text{div}_h X_h)_A = \frac{1}{P_A} \int_{\partial P_A} X_h \cdot n_{\partial P_A} \, ds,
(\text{div}_h X_h)_K = \frac{1}{C_K} \int_{\partial C_K} X_h \cdot n_{\partial C_K} \, ds,
$$

(4)

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

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

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

(5)

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 $X_h$ is a discrete vector field that satisfy $X_{\sigma,K} \cdot n_{\sigma} = X_{\sigma,L} \cdot n_{\sigma}$ on every internal interface $\sigma = C_K|C_L$, then :

$$
\int_{\Omega} (\nabla_h \tilde{\varphi}_h) \cdot X_h \, dx = - \frac{1}{d} \sum_{C_K \in C} \varphi_K (\text{div}_h X_h)_K C_K - \frac{1}{d} \sum_{A \in V} \varphi_A (\text{div}_h X_h)_A P_A

+ \int_{\partial \Omega} \tilde{\varphi}_h|_{\partial \Omega} X_h|_{\partial \Omega} \cdot n_{\partial \Omega} \, ds
$$

(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 :

$$
\forall A \in V^D : \varphi_A = 0, \quad \forall \sigma \in I^N : G_\sigma (\nabla_h \tilde{\varphi}_h)_{\sigma} \cdot n_{\sigma} = 0,
$$

(7)

$$
\forall A \in V - V^D : (\text{div}_h (G_h \nabla_h \tilde{\varphi}_h))_A = f_A, \quad \forall C_K \in C : (\text{div}_h (G_h \nabla_h \tilde{\varphi}_h))_K = f_K
$$

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 $A \in V^D$ and a discrete tensor $G_h$. Then there exists a unique DDFV function $\tilde{\varphi}_h$ such that :

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

$$
\forall \sigma \in I^D : \tilde{\varphi}_h(Y_{\sigma}) = 0, \quad \forall \sigma \in I^N : G_\sigma (\nabla_h \tilde{\varphi}_h)_{\sigma} \cdot n_{\sigma} = 0,
$$

(7)

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

$$(\nabla_h \tilde{\varphi}_h)_{\sigma,K} = \frac{1}{D_{\sigma,K}} \int_{D_{\sigma,K}} \nabla \varphi_h \, dx.$$
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 $\frac{1}{d} \sum_{C_K \in C} f_K C_K + \frac{d-1}{d} \sum_{A \in V} f_A P_A = 0$. 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 $w(x, t) \in \mathbb{R}^N$ 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:

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

$A_m, C_m$ 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 $n, m_K, m_L$ have unit length and are respectively orthogonal to $\sigma, YK, YL$. Three dimensional case. (b) Interface $\sigma = ABC = C_K|C_L$ of centre $Y$, $n$ its unit normal from $C_K$ towards $C_L$. (c) Same interface $\sigma$ view from above, all vectors have unit length, $m_{A,K}, m_{B,K}$ and $m_{C,K}$ are orthogonal to $AY_K, BY_K$ and $CY_K$ respectively; same thing for $m_{A,L}, m_{B,L}$ and $m_{C,L}$ 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 $\tilde{G}_i = \text{Diag}(g_l^i, g_t^i)$ is a reference matrix: $g_l^i, g_t^i$ 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 $t$:

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

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:

\[ d = 2 : \quad 2D_{\sigma,K}(\nabla_h \varphi_h)_{\sigma,K} = (\tilde{\varphi}(Y) - \varphi_K) \sigma n + (\varphi_B - \varphi_A) KY m_K \]

\[ d = 3 : \quad 3D_{\sigma,K}(\nabla_h \varphi_h)_{\sigma,K} = (\tilde{\varphi}(Y) - \varphi_K) \sigma n + (\varphi_B - \varphi_C) AY K m_{A,K} + (\varphi_C - \varphi_A) BY K m_{B,K} + (\varphi_A - \varphi_B) CY K m_{C,K} \]

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

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

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

with:

\[ \alpha^{-1} = 1 + \frac{D_{\sigma,K} n_G_{\sigma,L} n}{D_{\sigma,L} n G_{\sigma,K} n} \]

\[ k = \frac{LY}{\sigma} \frac{m_L G_{\sigma,L} n}{D_{\sigma,K} n G_{\sigma,K} n + n G_{\sigma,L} n} - \frac{K Y}{\sigma} \frac{m_K G_{\sigma,K} n}{D_{\sigma,L} n G_{\sigma,L} n + n G_{\sigma,K} n} \]

\[ k_Z = \frac{ZY L}{\sigma} \frac{m_Z L G_{\sigma,L} n}{D_{\sigma,K} n G_{\sigma,K} n + n G_{\sigma,L} n} - \frac{Z Y K}{\sigma} \frac{m_Z K G_{\sigma,K} n}{D_{\sigma,L} n G_{\sigma,L} n + n G_{\sigma,K} n} \], \quad Z = A, B, C.

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

B. Bibliographie


8 1ère soumission à fyca5.

