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To cite this version:
Yves Coudiere, Charles Pierre, Olivier Rousseau, Rodolphe Turpault. 2D/3D Discrete Duality Finite Volume (DDFV) scheme for anisotropic- heterogeneous elliptic equations, application to the electrocardiogram simulation. Int. symposium on Finite Volumes for Complex Applications V, 2008, Aussois, France. pp.313-320. hal-00189765

HAL Id: hal-00189765
https://hal.archives-ouvertes.fr/hal-00189765
Submitted on 22 Nov 2007
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 fulfill 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 $\Omega$) 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 $\phi$ such that ($n$ is a unit normal on the boundary):

$$\text{div}(G\nabla \phi) = f, \quad G\nabla \phi \cdot n = 0 \text{ on } \partial \Omega^N, \quad \phi|_{\partial \Omega} = 0 \text{ on } \partial \Omega^D, \quad f \in L^2(\Omega).$$  \hspace{1cm} (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 $\Gamma$:

$$\phi|_{\Gamma_1} = \phi|_{\Gamma_2}, \quad G|_{\Gamma_1} \nabla \phi|_{\Gamma_1} \cdot n = G|_{\Gamma_2} \nabla \phi|_{\Gamma_2} \cdot n \text{ on } \Gamma.$$ \hspace{1cm} (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 $\phi \in H^1(\Omega)$ such that $\phi|_{\Omega_1} \in H^2(\Omega_1)$ 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 if $f$ 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 $\Omega^N = \bigcup_{\sigma \in \mathcal{I}^N} \sigma$, $\Omega^D = \bigcup_{\sigma \in \mathcal{I}^D} \sigma$. 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
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 \textbf{diamond cell} \( D_{\sigma} \). For an internal interface \( \sigma = C_K|C_L = ABC \), it is defined as \( D_{\sigma} = D_{\sigma,K} \cup D_{\sigma,L} \) where \( D_{\sigma,K} \) and \( D_{\sigma,L} \) 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 \textbf{discrete vector field} \( \mathbf{X}_h \) (resp. \textbf{discrete tensor} \( \mathbf{G}_h \)) 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 \( \mathbf{G}_{\sigma,K} \) and \( \mathbf{G}_{\sigma,L} \)) on each side of \( \sigma \). \( \mathbf{G}_{\sigma,K} \) is always assumed symmetric positive definite. We shall say that \( \mathbf{X}_h \) is conservative relatively to \( \mathbf{G}_h \) if (\( n_\sigma \) being a normal to \( \sigma \)):

\[
\forall \sigma \in \mathcal{I} \text{ such that } \sigma = C_K|C_L : \quad \mathbf{G}_{\sigma,K} \mathbf{X}_{\sigma,K} \cdot n_\sigma = \mathbf{G}_{\sigma,L} \mathbf{X}_{\sigma,L} \cdot n_\sigma, \quad (3)
\]

A \textbf{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 \textbf{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 \( \sigma \subset C_K, C_K \in \mathcal{C} \).
2.2. The discrete operators and the problem discretisation

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

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

(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 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:

- $\forall A \in V : \tilde{\varphi}_h(A) = \varphi_A$, $\forall C_K \in C : \tilde{\varphi}_h(K) = \varphi_K$,
- $\forall \sigma \in T^D : \tilde{\varphi}_h(Y_{\sigma}) = 0$, $\forall \sigma \in \mathcal{I}^N : G_{\sigma} (\nabla_h \tilde{\varphi}_h)_{\sigma} \cdot n_{\sigma} = 0$,

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 $\varphi_h$ 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 $X_h$ 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:

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

(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:

- $\forall A \in V^D : \varphi_A = 0$, $\forall \sigma \in \mathcal{I}^N : G_{\sigma} (\nabla_h \varphi_h)_{\sigma} \cdot n_{\sigma} = 0$,
- $\forall A \in V - V^D : (\text{div}_h (G_h \nabla_h \varphi_h))_A = f_A$, $\forall C_K \in C : (\text{div}_h (G_h \nabla_h \varphi_h))_K = f_K$. 

(7)
2D/3D DDFV scheme

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 $\phi$ 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 ($V_1$ and $V_2$) located on the body surface.

Such a $\phi_h$ 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

$$
\sum_{C \in \mathcal{C}} f_K C_K + \sum_{A \in \mathcal{V}} f_A P_A = 0.
$$

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 $w(x, t) \in \mathbb{R}^N$ 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:

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

(8)

$A_m$, $C_m$ are constants, $G_1$ is a non constant anisotropy tensor described below, $I_{\text{ion}}$, $g$ are reaction terms and $I_{\text{app}}$ 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 \( AYK, BYK \) and \( CYK \) respectively; same thing for \( m_{A,L}, m_{B,L} \) and \( m_{C,L} \) by turning \( K \) into \( L \).
A. Discrete gradient implementation

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

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

$d = 3 : 3D_{\sigma,K} (\nabla_h \varphi_h)_{\sigma,K} = (\hat{\varphi}(Y) - \varphi_K) \sigma n + (\varphi_B - \varphi_C) AY K m_{A,K}$

$+ (\varphi_C - \varphi_A) BY K m_{B,K} + (\varphi_A - \varphi_B) CY K m_{C,K}$

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

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

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

with:

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

$k = \frac{LY}{D_{\sigma,K} G_{\sigma,K} n + n G_{\sigma,L} n} - \frac{KY}{D_{\sigma,K} G_{\sigma,L} n + n G_{\sigma,K} n}$

$k_Z = \frac{Z Y L}{D_{\sigma,K} G_{\sigma,K} n + n G_{\sigma,L} n} - \frac{Z Y K}{D_{\sigma,K} G_{\sigma,L} n + n G_{\sigma,K} n}$, $Z = A, B, C$.

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


