Stability and Convergence of a Finite Volume Method for a Reaction-Diffusion system of Equations in Electro-Cardiology

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RÉSUMÉ. *Pour calculer le fonctionnement électrique du myocarde, nous utilisons une méthode de volumes finis 3D sur maillages non-structurés. Pour cette méthode, nous démontrons la stabilité L^∞ et la convergence L^2 de l'approximation pour les schémas en temps d'Euler explicite et implicite, sous une condition de pas de temps. La technique de démonstration pour la stabilité est dite des « rectangles invariants ». Un résultat numérique est montré.*

ABSTRACT. *The 3D electrical activity of the heart is computed with a finite volume method on unstructured meshes. This paper gives conditions on the time-step to ensure a L^∞ stability property for an explicit and a semi-implicit time-stepping method. The proof is based on the idea of "invariant rectangles". A convergence result is proved in L^2, and a numerical example is shown.*

MOTS-CLÉS : *electro-cardiologie,volumes finis, stabilité,convergence*

KEYWORDS: *electro-cardiology,finite-volume,stability,convergence*

1. Introduction

Three dimensional computer models of the electrical activity in the myocardium are increasingly popular : the heart's activity generates an electromagnetic field in the torso, and produces a surface potential map which measure is the well-known electrocardiogram (ECG).

Despite the discrete structure of the heart muscle, recent studies in electro-cardiology assume the anisotropic cardiac tissues to be represented at a macroscopic level by a system of one or two semi-linear parabolic PDE of reaction-diffusion type and one or several ODEs. We refer to [FRA 02] for a mathematical derivation of these equations.

The different reaction terms, in the PDE and in the ODEs live at very different time scales. As a consequence, the solutions exhibit very sharp fronts propagating at high speeds, and its computation requires fine unstructured meshes. Only the recent improvement of computing capabilities allow 3D computations to be achieved. Moreover, until very recently, they were restricted to finite differences methods on structured grids and simple geometries [NAS 04]. A few researchers recently started to study computations on 3D unstructured meshes, coupled to an explicit, semi-implicit or fully-implicit time-stepping method [LIN 03, BOU 03]. The analysis of a Galerkin semi-discrete space approximation was conducted by S. Sanfelici [SAN 02]. But, to our knowledge, there has been no attempt at studying the effects of the time-stepping method on the stability of the approximation. As a matter of fact the problem of stability in time of fully discretized approximations is as difficult as the problem of global stability for the continuous solution of reaction-diffusion systems.

The main issue of this paper is to study the theoretical stability criterion for the explicit and semi-implicit Euler methods ; and to derive error estimates for the approximate solutions.

Only the results are stated here, and the detailed proofs can be found in [COU 04].

2. The Reaction-Diffusion System of Equations

2.1. *The Macroscopic Mono-domain Model in Electro-Cardiology*

At a microscopic scale, the surface membrane of the myocardiac cells delimits an intra and an extra-cellular medium, both containing ionic species. The model accounts for the dynamics of the trans-membrane ionic currents I_{ion} and difference of potential u. It writes

$$\varepsilon \frac{du}{dt} = \varepsilon^2 \nabla \cdot (\sigma \nabla u) + I_{ion}, \tag{1}$$

and can be obtained through an homogenization process [FRA 02]. The total ionic current I_{ion} is controlled both by the trans-membrane potential u and by a one or more auxiliary variable $v \in \mathbb{R}^p$:

$$I_{ion} = f(u, v), \qquad \frac{dv}{dt} = g(u, v) \tag{2}$$

and where $\varepsilon \ll 1$ measures the time and space scales differences between the variables. The variables v, called *gating variables*, have been introduced by Hodgkin and Huxley in [HOD 52], who gave a first 4 variables model for the nerve axon of the giant squid. The development of accurate models, still based on the concept of *gating variables*, is an active field of research in electro-physiology, resulting in numerous ionic models for the cardiac cell, containing up to hundreds of equations. Of course the numerical analysis is only carried out on simpler models, the most famous of which is the FitzHugh-Nagumo one [FIT 61] :

$$f(u, v) = -u(u-1)(u-a) - v, \qquad g(u, v) = ku - v, \tag{3}$$

with $0 < a < 1$ and $k > 0$. It will be referred to as the *FHN model*. A modified version proposed by Aliev and Panfilov [PAN 96] to suit the behavior of myocardiac cells writes :

$$f(u, v) = -ku(u-1)(u-a) - uv, \qquad g(u, v) = ku(1+a-u) - v, \tag{4}$$

with $k > 0$ and $0 < a < 1$.It will be referred to as the *AP model*. This model has been used recently in numerical studies [NAS 04, SER 02].

At a macroscopic level the cells are self-organized into fibers, and the fibers into sheets, which is represented by an anisotropic tensor of conductivity $\sigma = \sigma(x)$. The fibers are tangent to the heart's boundary skin, so that the normal to $\partial\Omega$ is an eigendirection for $\sigma(x)$:

$$\forall x \in \partial\Omega, \quad \sigma(x) \cdot \mathbf{n}(x) = \lambda(x)\mathbf{n}(x), \tag{5}$$

where $\lambda(x) > 0$ and $\mathbf{n}$ is the unit vector field on $\partial\Omega$ normal to $\partial\Omega$.

The potential u shall satisfy a Neumann boundary condition :

$$\forall x \in \partial\Omega, \quad (\sigma(x)\nabla u) \cdot \mathbf{n}(x) = 0, \tag{6}$$

meaning that no current flows out of the heart.

No boundary condition is needed concerning v, since it is ruled point-wise by an ODE. Of course, an initial data is provided :

$$\forall x \in \Omega, \quad u(x, 0) = u_0(x),\ v(x, 0) = v_0(x). \tag{7}$$

2.2. *Existence, Regularity and Stability of Solutions*

Basically, local existence of solutions to (1)-(2), (6)-(7) is proved under standard assumptions on the data (f and g locally Lipschitz – fixed point theorem, th. 2.1), and stronger assumptions are needed in order to extend the solutions to all time $t > 0$ using some stability properties and resulting in strong regular solutions [HEN 81, SMO 83, BRI 86].

Specifically, stability in time is achieved by the construction of invariant regions for the solution (def. 2.2). It requires

– a good behavior of the non-linear terms outside a compact set of $\mathbb{R}^2$ (this is the case for the *FHN* and *AP* models, see fig. 1),

– a strong maximum principle for the spatial elliptic operator (lem. 2.3),

– regularity of the solution in order to apply the maximum principle (th. 2.1).

We only briefly recall below general results on existence, regularity and stability found in [HEN 81, SMO 83]. They are also needed to carry out the numerical analysis.

Theorem 2.1 *We consider the equations* (1)-(2), (6)-(7) *on Ω, a bounded open subset of $\mathbb{R}^d$, $d = 1, 2, 3$, with a C^2 regular boundary $\partial\Omega$. The conductivity tensor σ, symmetric, is assumed to have $C^{1+\nu}$ regularity on $\overline{\Omega}$ (it is $1+\nu$ Hölder continuous) and to be uniformly elliptic. The reaction terms $f,\ g : \mathbb{R}^2 \mapsto \mathbb{R}$ are assumed locally Lipschitz.*

If the initial conditions (7) satisfies $u_0 \in H^2(\Omega)$, u_0 verifying (6)*, and $v_0 \in C^\nu(\Omega)$ then* (1)-(2), (6)-(7) *have a unique weak solution $w(t,x) = (u(t,x), v(t,x))$ on $\Omega \times [0,T)$ for some $T > 0$.*

Moreover $w(t,x)$ is continuously differentiable in the variable t on $\overline{\Omega} \times (0,T)$ and $u(\cdot,t) \in C^2(\overline{\Omega})$ for $t \in (0,T)$; and then (1)-(2), (6)-(7) *hold in a strong sense.*

Definition 2.2 *The rectangular set $\Sigma = [u_-,\ u_+] \times [v_-,\ v_+] \subset \mathbb{R}^2$ is an invariant set for f and g if*

$$\forall (u,v) \in \Sigma, \quad \left| \begin{array}{l} u = u_-,\ v_- \le v \le v_+ \Rightarrow f(u,v) > 0, \\ u = u_+,\ v_- \le v \le v_+ \Rightarrow f(u,v) < 0, \\ v = v_-,\ u_- \le u \le u_+ \Rightarrow g(u,v) > 0, \\ v = v_+,\ u_- \le u \le u_+ \Rightarrow g(u,v) < 0. \end{array} \right.$$

This simply means that Σ is a strictly contracting region for the flow (f,g) in $\mathbb{R}^2$.

Lemma 2.3 *Let Ω be an open bounded subset of $\mathbb{R}^d$ whose boundary $\partial\Omega$ has C^2 regularity. Let $u \in C^2(\overline{\Omega})$ satisfy the boundary condition* (6) *for a tensor $\sigma \in C^1(\overline{\Omega})$ satisfying* (5)*.*

If u has a maximum (resp. minimum) in $x \in \overline{\Omega}$ then $\nabla \cdot (\sigma \nabla u)(x) \le 0$ (resp. $\nabla \cdot (\sigma \nabla u)(x) \ge 0$).

Theorem 2.4 *We consider equations* (1)-(2), (6)-(7) *with the assumptions of theorem 2.1, so that there exists a strong solution* $w(t) = (u(t), v(t))$ *for* $t \in [0, T)$. *We moreover assume that the conductivity tensor* σ *verifies* (5).

Let Σ *be an invariant rectangle as in def. 2.2 ; then* Σ *is an invariant region for* (1)-(2), (6)-(7), *meaning that :*

$$\forall x \in \Omega,\ (u_0(x), v_0(x)) \in \Sigma \ \Rightarrow\ \forall t > 0,\ \forall x \in \Omega,\ (u(t,x), v(t,x)) \in \Sigma.$$

As a consequence, the strong solution $w(t)$ *exists for all* $t > 0$.

REMARQUE. —
Invariant regions for the *FHN* or *AP* models can be constructed as big as necessary to contain any bounded initial data, as displayed on figure 1.

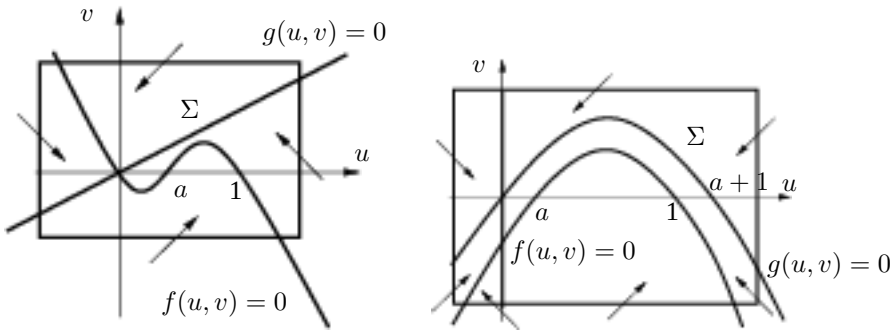

Figure 1. *Invariant regions* Σ *for FHN (left) and AP (right) models*

3. The Finite Volume Approximation

We shall approximate the solutions of system (1)-(2), (6)-(7) on Ω with a finite volume method according to the framework of [EYM 00], on admissible meshes adapted to the conductivity tensor σ defined by :

1) a partition $\mathcal{T}$ of Ω into polygonal subsets called cells. On each cells $K \in \mathcal{T}$ the conductivity tensor σ is approximated by its mean value on K

$$\forall K \in \mathcal{T}, \quad \sigma_K = \frac{1}{m(K)} \int \sigma(x) dx \tag{8}$$

where $m(K)$ stands for the measure of K ;

2) a set $\mathcal{S}$ of interfaces e that are either the frontier between two neighbor cells $K, L \in \mathcal{T}$ (we will write $e = K|L$), or on the domain boundary $e \subset \partial\Omega$;

3) two sets of points $(x_K)_{K\in\mathcal{T}}$, $(y_e)_{e\in\mathcal{S}}$ – the cells and interfaces centers – such that for each cell $K \in \mathcal{T}$ and each interface $e \subset \partial K$ the direction $y_e - x_K$ is orthogonal to e with respect to the metric defined by σ_K^{-1}.

In that framework the solution of (1)-(2), (6)-(7) is approximated by two functions $(u_K)_{K\in\mathcal{T}}$ and $(v_K)_{K\in\mathcal{T}}$ both in the subspace $L^2(\mathcal{T}) \subset L^2(\Omega)$ of the functions piecewise constant on the cells $K \in \mathcal{T}$. For a cell $K \in \mathcal{T}$ and an interface $e \in \mathcal{S}$ such that $e \subset \partial K$, either $e \subset \partial\Omega$ and the flux of $\sigma\nabla u$ is set to 0, according to the boundary condition ; or $e = K|L$, and we denote by $\mathbf{n}_{e,K}$ the unit normal vector to e pointing outward of K, and the flux of $\sigma\nabla u$ on e is approximated in a consistent manner by

$$\tau_e\,(u_L - u_K) \quad \text{for } e \in \mathcal{S},\ e = K|L, \quad \text{and } \tau_e > 0. \tag{9}$$

The transmission coefficient τ_e associated to e (see [EYM 00] for definition) contains both geometrical informations on the mesh $\mathcal{T}$ and diffusive informations on the conductivity tensor σ. The integral formulation of (1) on each cell $K \in \mathcal{T}$ writes

$$\varepsilon u'_{\mathcal{T}}(t) = \varepsilon^2 A_{\mathcal{T}} u_{\mathcal{T}} + f(u_{\mathcal{T}}, v_{\mathcal{T}}), \tag{10}$$

$$v'_{\mathcal{T}}(t) = g(u_{\mathcal{T}}, v_{\mathcal{T}}). \tag{11}$$

The discrete operator $A_{\mathcal{T}}$ is the approximation of the diffusive operator $\nabla\cdot(\sigma\nabla\cdot)$ for the homogeneous Neumann boundary condition (6) :

$$A_{\mathcal{T}} : u_{\mathcal{T}} \in L^2(\mathcal{T}) \mapsto z_{\mathcal{T}} \in L^2(\mathcal{T}), \quad z_K = \frac{1}{\mathrm{m}(K)} \sum_{e\in\mathcal{S}, e=K|L} \tau_e(u_L - u_K). \tag{12}$$

The operator $A_{\mathcal{T}}$ is symmetric and non-positive :

$$(A_{\mathcal{T}} u_{\mathcal{T}}, u_{\mathcal{T}})_{L^2(\Omega)} = -\sum_{e\in\mathcal{S},\, e=K|L} \tau_e \left|u_L - u_K\right|^2. \tag{13}$$

Its kernel is the subspace of the functions constant on Ω.

4. Stability Analysis

We will prove that the semi-discrete and completely discretized solutions associated to an initial data bounded into an invariant rectangle Σ (def. 2.2) exists for all $t > 0$ and remains trapped in the rectangle Σ, exactly like the continuous solution.

We point out the the finite volume method provides, for very general unstructured meshes, a method consistent with the stability properties of the system of PDEs. Moreover, in the semi-discrete case, no additional assumptions on the mesh $\mathcal{T}$ is required, justifying the use of a finite volume method. Instability phenomena are only caused by the time discretization.

4.1. *The Semi-Discrete Case*

The semi-discrete formulation (10)-(11) is a system of ODEs on $L^2(\mathcal{T}) \times L^2(\mathcal{T})$. Given an initial data, it has a unique solution $w_{\mathcal{T}} \in \mathrm{C}^1([0,T); L^2(\mathcal{T}) \times L^2(\mathcal{T}))$, for some $T > 0$. Lemma 2.3 transposes easily to the semi-discrete case, as follows.

Lemma 4.1 *Let $\mathcal{T}$ be an admissible finite volume mesh of Ω adapted to the conductivity tensor σ and let $A_\mathcal{T}$ as defined in* (13) *be the discretization of the elliptic operator $\nabla \cdot (\sigma \nabla \cdot)$ on $L^2(\mathcal{T})$.*

If $u_\mathcal{T}$ has a maximum (resp. minimum) in $K \in \mathcal{T}$ then $\{A_\mathcal{T} u_\mathcal{T}\}_K \leq 0$ (resp. $\{A_\mathcal{T} u_\mathcal{T}\}_K \geq 0$).

Theorem 4.2 *We consider $\Sigma \subset \mathbb{R}^2$ as in def. 2.2. Then Σ is an invariant region for the semi-discrete solution $w_\mathcal{T}$ of* (10)-(11) *:*

$$\forall K \in \mathcal{T},\ (u_K^0, v_K^0) \in \Sigma \ \Rightarrow\ \forall t > 0,\ \forall K \in \mathcal{T},\ (u_K(t), v_K(t)) \in \Sigma.$$

Sketch of the proof. Lemma 4.1 is easily observed on (12) : $u_L - u_K \leq 0$ if u_K is a maximum of (u_K), and $\tau_e > 0$. The proof of theorem 4.2 is by contradiction : any solution $w_\mathcal{T}$ running out of Σ is such that $w'_\mathcal{T}$ points outward of Σ for some $t > 0$, despite what is deduced from lemma 4.1 and the properties of the flow (f, g).

4.2. *The Semi-Implicit Euler Method*

On a finite volume mesh $\mathcal{T}$ of Ω adapted to the conductivity tensor σ and given a time-step $\Delta t > 0$, consider the semi-implicit method :

$$\varepsilon \frac{u_\mathcal{T}^{n+1} - u_\mathcal{T}^n}{\Delta t} = \varepsilon^2 A_\mathcal{T} u_\mathcal{T}^{n+1} + f(u_\mathcal{T}^n, v_\mathcal{T}^n), \tag{14}$$

$$\frac{v_\mathcal{T}^{n+1} - v_\mathcal{T}^n}{\Delta t} = g(u_\mathcal{T}^n, v_\mathcal{T}^n). \tag{15}$$

The method is implicit because a system of linear equations has to be solved in (14), which matrix is $(\mathrm{Id} - \varepsilon \Delta t A_\mathcal{T})$. With property (13), it is obviously a positive-definite matrix, so that $u_\mathcal{T}^n$ can be constructed for all $n \geq 0$.

Lemma 4.3 *Let $\Sigma \subset \mathbb{R}^2$ be an invariant rectangle (def. 2.2). If the time-step Δt verifies :*

$$\lambda_f \frac{\Delta t}{\varepsilon} \leq 1, \quad \lambda_g \Delta t \leq 1, \tag{16}$$

where

$$\lambda_f = \left| \min_\Sigma \partial_u f \right|, \quad \lambda_g = \left| \min_\Sigma \partial_v g \right|, \tag{17}$$

then Σ is an invariant region for the discrete system (14)-(15) *:*

$$\forall K \in \mathcal{T},\ (u_K^0, v_K^0) \in \Sigma \ \Rightarrow\ \forall n \geq 0,\ \forall K \in \mathcal{T},\ (u_K^n, v_K^n) \in \Sigma.$$

Sketch of the proof. Consider the C^1 mapping $\Phi : (u^n, v^n) \mapsto (u^{n+1}, v^{n+1})$. With the same argument than for theorem 4.2, Σ is proved to be invariant for Φ : $\Phi(\Sigma) \subset (\Sigma)$, under the stability assumptions (16).

4.3. *The Explicit Euler Method*

We now consider the explicit Euler method

$$\varepsilon \frac{u_{\mathcal{T}}^{n+1} - u_{\mathcal{T}}^{n}}{\Delta t} = \varepsilon^2 A_{\mathcal{T}} u_{\mathcal{T}}^{n} + f(u_{\mathcal{T}}^{n}, v_{\mathcal{T}}^{n}), \tag{18}$$

$$\frac{v_{\mathcal{T}}^{n+1} - v_{\mathcal{T}}^{n}}{\Delta t} = g(u_{\mathcal{T}}^{n}, v_{\mathcal{T}}^{n}), \tag{19}$$

on a finite volume mesh $\mathcal{T}$ of Ω adapted to the conductivity tensor σ and given a time step $\Delta t > 0$.

Lemma 4.4 *Let $\Sigma \subset \mathbb{R}^2$ be an invariant rectangle (def. 2.2). If the time-step Δt verifies :*

$$\forall K \in \mathcal{T}, \quad \eta_K \frac{\varepsilon \Delta t}{m(K)} + \lambda_f \frac{\Delta t}{\varepsilon} \leq 1, \quad \lambda_g \Delta t \leq 1, \tag{20}$$

where

$$\forall K \in \mathcal{T}, \quad \eta_K = \sum_{e \in \partial K \cap \Omega} \tau_e > 0,$$

and $\lambda_{f,g}$ are given by (17)*, then Σ is an invariant region for the discrete system* (18)-(19) *:*

$$\forall K \in \mathcal{T},\ (u_K^0, v_K^0) \in \Sigma \ \Rightarrow\ \forall n \geq 0,\ \forall K \in \mathcal{T},\ (u_K^n, v_K^n) \in \Sigma.$$

Sketch of the proof. It resemble the proof of lemma 4.3, without additional difficulties.

REMARQUE. —

Concerning the *FHN* or *AP* models, an explicit condition can be found, since

– $\lambda_f = \max(|f'(u_-)|, |f'(u_+)|)$ and $\lambda_g = 1$ in the *FHN* case,

– $\lambda_f = \max(|f'(u_-) - v - +|, |f'(u_+) - v_+|)$ and $\lambda_g = 1$ in the *AP* case.

REMARQUE. —

Under classical regularity assumptions on a family of meshes $(\mathcal{T}_h)_{h>0}$, we naturaly have $\eta_K / \mathrm{m}(K) = O(1/h^2)$ where $h = \mathrm{size}(\mathcal{T})$.

5. Convergence analysis

This section is devoted to the computation of some error estimates for the approximations given by methods (14)-(15) or (18)-(19), under the stability conditions given in lemmas 4.3 and 4.4.

Let $w(t,x)$ be a strong solution of (1)-(2), (6)-(7) with initial value $w_0(x) = w(0,x)$, and consider its approximation $\overline{w}_{\mathcal{T}}^n$ on finite volume mesh $\mathcal{T}$ and for $\Delta t > 0$, given by any of the two previous methods.

If w_0 lies into an invariant region Σ and if Δt satisfy the required stability condition, then both $w(t,x)$ and $\overline{w}_{\mathcal{T}}^n$ remain bounded in Σ. The functions f an g being locally Lipschitz, it is easy to compare the functions w and $\overline{w}$.

For each time step $t^n = n\Delta t$ and for each cell $K \in \mathcal{T}$, we introduce

$$w_K^n = w(t^n, x_K) = (u(t^n, x_K),\, v(t^n, x_K))\,. \tag{21}$$

As a consequence, the error is measured as being the function $e_{\mathcal{T}}^n = w_{\mathcal{T}}^n - \overline{w}_{\mathcal{T}}^n \in L^2(\mathcal{T}) \times L^2(\mathcal{T})$ for $n \geq 0$.

Theorem 5.1 *We consider system* (1)-(2), (6)-(7) *with the assumptions of theorem 2.1 and with a conductivity tensor σ satisfying* (5)*. We assume that $\Sigma \subset \mathbb{R}^2$ is an invariant region as defined by def. 2.2, and consider a solution w with initial value $w_0(x) = w(0,x)$ in Σ's interior, so that w is defined for all time and remains inside Σ.*

Let $w_{\mathcal{T}}^n$ be the approximation of w as defined in (18)-(19) *(or in* (14)-(15)*) with*

$$\forall K \in \mathcal{T}, \quad \overline{w}_K^0 = w_0(x_K) = (u_0(x_K), v_0(x_K)). \tag{22}$$

We assume furthermore that the mesh $\mathcal{T}$ and Δt satisfies the stability condition (16) *(or* (20)*) relative to Σ. Then there exists two constants C and μ, only depending on the data (Ω, w_0, f, g and Σ) such that for $n\Delta t \leq T$,*

$$\|e_{\mathcal{T}}^n\|_{L^2} \leq C \exp(\mu T)\,(\mathrm{size}(\mathcal{T}) + \Delta t)\,,$$

where $\mathrm{size}(\mathcal{T}) = \max_{K\in\mathcal{T}}$ *diam* (K).

Sketch of the proof. The solution being trapped into Σ, the non-linear terms f, g are considered as uniform Lipschitz functions on $\mathbb{R}^2$, and (1)-(2) is hardly a linear parabolic system of equations. Consequently, the proof is almost straightforward, according to the framework developped in [EYM 00].

A numerical example

As a conclusion, we show the result of a computation on a 3D mesh with 3763 vertices and 17349 tetraedra. The *AP model* is approximated with the explicit method and the time-step is computed according to lemma 4.4 : $\Delta t = 0.0031$. The method is observed to be unstable for larger time-steps (numerical blow-up within 2 or 3 iterations).

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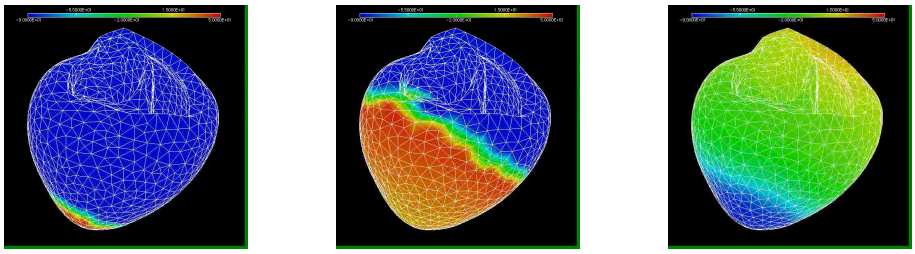

Figure 2. *Values of the unknown u at different time t. The region at rest is in black, while excited region is in light grey.*

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