A HIGH-ORDER DISCONTINUOUS GALERKIN METHOD FOR THE BIDOMAIN PROBLEM OF CARDIAC ELECTROPHYSIOLOGY

Project N° 2

Supervisors: Christian Vergara, Paola Antonietti

Federica Botta, Matteo Calafà

Course of Numerical Analysis for Partial Differential Equations

A.Y. 2020/2021

POLITECNICO MILANO 1863

Table of Contents

POLITECNICO MILANO 1863

The physical problem

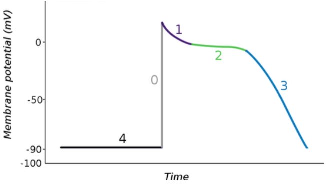
Mechanical contraction of the human heart

$\uparrow$

Electrical activation of the cardiac cells

$\downarrow$

Continuous electrical diffusion over the entire cardiac surface.



The mathematical model

Bidomain model + FitzHugh-Nagumo with Neumann B.C.

$$\begin{cases} \chi_m C_m \frac{\partial V_m}{\partial t} - \nabla \cdot (\Sigma_i \nabla \phi_i) + \chi_m I_{ion}(V_m, w) = I_i^{ext}, & \text{in } \Omega_{mus} \times (0, T], \\ -\chi_m C_m \frac{\partial V_m}{\partial t} - \nabla \cdot (\Sigma_e \nabla \phi_e) - \chi_m I_{ion}(V_m, w) = -I_e^{ext}, & \text{in } \Omega_{mus} \times (0, T], \\ I_{ion}(V_m, w) = kV_m(V_m - a)(V_m - 1) + w, & \text{in } \Omega_{mus} \times (0, T], \\ \frac{\partial w}{\partial t} = \epsilon(V_m - \gamma w), & \text{in } \Omega_{mus} \times (0, T], \\ \Sigma_i \nabla \phi_i \cdot n = b_i, & \text{on } \partial\Omega_{mus} \times (0, T], \\ \Sigma_e \nabla \phi_e \cdot n = b_e, & \text{on } \partial\Omega_{mus} \times (0, T], \\ \text{Initial conditions for } \phi_i, \phi_e, w, & \text{in } \Omega_{mus} \times \{t = 0\}. \end{cases}$$

Unknowns: $\phi_i,\ \phi_e,\ V_m = \phi_i - \phi_e,\ w$

Our objectives

What had already been done:

- Implementation of a Discontinuous Galerkin with FEM basis for the Bidomain problem.
- Implementation of a Semi-Implicit temporal scheme.

What we did:

- Implementation of a Discontinuous Galerkin with **Dubiner** basis for the Bidomain problem.
- Implementation of further temporal schemes.
- Bugs corrections and optimizations.
- Pseudo-realistic simulations.

POLITECNICO
MILANO 1863

Discretization

$$\text{Bidomain problem} \begin{array}{l} \nearrow \\ \\ \searrow \end{array}$$

space-dependent: Discontinuous Galerkin method

time-dependent: Semi-implicit, Godunov operator-splitting and quasi-implicit operator-splitting

Semi-discrete Discontinuous Galerkin formulation

For any $t \in [0, T]$ find $\Phi_h(t) = [\phi_i^h(t), \phi_e^h(t)]^T \in [V_h^p]^2$ and $w_h(t) \in V_h^p$ such that:

$$
\begin{cases}
\displaystyle\sum_{\mathcal{K}\in\tau_h}\int_{\mathcal{K}} \chi_m C_m \frac{\partial V_m^h}{\partial t} v_h d\omega + a_i(\phi_i^h, v_h) + \sum_{\mathcal{K}\in\tau_h}\int_{\mathcal{K}} \chi_m k(V_m^h - 1)(V_m^h - a)V_m^h v_h d\omega + \\
\displaystyle\qquad + \sum_{\mathcal{K}\in\tau_h}\int_{\mathcal{K}} \chi_m w_h v_h d\omega = (I_i^{ext}, v_h), \qquad \forall v_h \in V_h^p, \\
\displaystyle -\sum_{\mathcal{K}\in\tau_h}\int_{\mathcal{K}} \chi_m C_m \frac{\partial V_m^h}{\partial t} v_h d\omega + a_e(\phi_e^h, v_h) - \sum_{\mathcal{K}\in\tau_h}\int_{\mathcal{K}} \chi_m k(V_m^h - 1)(V_m^h - a)V_m^h v_h d\omega + \\
\displaystyle\qquad - \sum_{\mathcal{K}\in\tau_h}\int_{\mathcal{K}} \chi_m w_h v_h d\omega = (-I_e^{ext}, v_h), \qquad \forall v_h \in V_h^p, \\
\displaystyle\sum_{\mathcal{K}\in\tau_h}\int_{\mathcal{K}} \frac{\partial w_h}{\partial t} v_h d\omega = \sum_{\mathcal{K}\in\tau_h}\int_{\mathcal{K}} \epsilon(V_m^h - \gamma w_h) v_h d\omega, \qquad \forall v_h \in V_h^p,
\end{cases}
$$

where:

- $$a_l(\phi_l^h, v_h) = \sum_{\mathcal{K}\in\tau_h} \int_{\mathcal{K}} (\Sigma_l \nabla_h \phi_l^h) \cdot \nabla_h v_h d\omega - \sum_{F\in\mathcal{F}_h^I} \int_F \{\{\Sigma_l \nabla_h \phi_l^h\}\} \cdot [\![v_h]\!] d\sigma +$$
$$- \delta \sum_{F\in\mathcal{F}_h^I} \int_F \{\{\Sigma_l \nabla_h v_h\}\} \cdot [\![\phi_l^h]\!] d\sigma + \sum_{F\in\mathcal{F}_h^I} \int_F \Gamma [\![\phi_l^h]\!] \cdot [\![v_h]\!] d\sigma \qquad l = i, e,$$
- $$(I_i^{ext}, v_h) = \sum_{\mathcal{K}\in\tau_h} \int_{\mathcal{K}} I_i^{ext} v_h d\omega + \int_{\partial\Omega} b_i v_h d\sigma,$$
- $$(-I_e^{ext}, v_h) = - \sum_{\mathcal{K}\in\tau_h} \int_{\mathcal{K}} I_e^{ext} v_h d\omega + \int_{\partial\Omega} b_e v_h d\sigma.$$

Dubiner basis: analytical definition

Definition (Dubiner basis)

The Dubiner basis that generates the space $\mathbb{P}^p(\hat{K})$ of polynomials of degree p over the reference triangle is the set of functions:

$$\phi_{ij} : \hat{K} \to \mathbb{R},$$

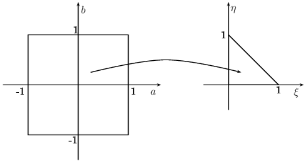
$$\phi_{ij}(\xi,\eta) = c_{ij}\, 2^j (1-\eta)^j J_i^{0,0}\left(\frac{2\xi}{1-\eta} - 1\right) J_j^{2i+1,0}(2\eta - 1),$$

for $i, j = 0, \ldots, p$ and $i + j \leq p$, where $c_{ij} := \sqrt{\frac{2(2i+1)(i+j+1)}{4^i}}$ and $J_i^{\alpha,\beta}(\cdot)$ is the i-th Jacobi polynomial.

Properties

- They consist in a pseudo tensor-product of Jacobi polynomials if the following transformation is then applied:

$$\xi = \frac{(1+a)(1-b)}{4}, \eta = \frac{(1+b)}{2}.$$



- They are $L^2(\hat{K})$ orthonormal ($\hat{K}$ is the reference triangle).

Main works

Remark

*Dubiner basis coefficients of a discretized function have **modal** meaning instead of a nodal meaning.*

Then, our main works regarded:

- Methods for the evaluation of the Dubiner functions and gradients in the reference points.
- Methods for the evaluation of the FEM coefficients of a discretized function starting from its Dubiner coefficients and viceversa.
  1. FEM $\rightarrow$ Dubiner is needed when we use the initial solution data into the Dubiner system.
  2. FEM $\leftarrow$ Dubiner is needed when we want to get the solution obtained from the Dubiner system in a comprehensible form.

FEM-Dubiner conversion strategies

Consider:

- An element $\mathcal{K} \in \tau_h$
- $\{\psi_i\}_{i=1}^{p}, \{\varphi_j\}_{j=1}^{q}$ as the FEM and Dubiner functions with support in $\mathcal{K}$.
- $\{\hat{u}_i\}_{i=1}^{p}, \{\tilde{u}_j\}_{j=1}^{q}$ as the FEM and Dubiner coefficients of a function u_h.

FEM $\leftarrow$ Dubiner

Exploiting the nodal meaning of FEM, we compute its value in a point:

$$\hat{u}_i = \sum_{j=1}^{q} \tilde{u}_j \varphi_j(x_i),$$

FEM $\rightarrow$ Dubiner

Exploiting the L^2-orthonormality of Dubiner, we compute its Fourier coeff.:

$$\tilde{u}_j = \int_{\mathcal{K}} u_h(x)\varphi_j(x)\,dx = \int_{\mathcal{K}} \sum_{i=1}^{p} \hat{u}_i \psi_i(x)\varphi_j(x)\,dx$$

POLITECNICO MILANO 1863

Semi-implicit scheme

Idea:

- treat most of the terms of the PDE implicitly,
- treat the non-linear term semi-implictly,
- treat the ODE implictly with the exception of the term V_m.

Semi-implicit discretized system

Find $\Phi^{n+1} = [\phi_i^{n+1} \phi_e^{n+1}]^T$ and w^{n+1} $\forall n = 0, \cdots, N-1$ such that:

$$\begin{cases} (\frac{1}{\Delta t} + \epsilon\gamma)Mw^{n+1} = \epsilon M V_m^n + \frac{M}{\Delta t} w^n, \\ (B + C_{nl}(V_m^n))\Phi^{n+1} = r^{n+1}. \end{cases}$$

Godunov operator-splitting scheme

The main feature is the sub-division of the problem into two different problems to be solved sequentially, such that $L(u) = L_1(u) + L_2(u)$. In our case:

1:

$$\begin{cases} \chi_m C_m M \frac{\hat{V}_m^{n+1} - V_m^n}{\Delta t} + C(V_m^n) V_m^n + \chi_m M w^n = 0, \\ \frac{w^{n+1} - w^n}{\Delta t} = \epsilon (V_m^n - \gamma w^n). \end{cases}$$

2:

$$\begin{cases} \chi_m C_m M \frac{V_m^{n+1} - \hat{V}_m^{n+1}}{\Delta t} + A_i \phi_i^{n+1} = F_i^{n+1}, \\ -\chi_m C_m M \frac{V_m^{n+1} - \hat{V}_m^{n+1}}{\Delta t} + A_e \phi_e^{n+1} = F_e^{n+1}. \end{cases}$$

Godunov operator-splitting discretized system

$$\begin{cases} \left(\frac{\chi_m C_m}{\Delta t} \begin{bmatrix} M & -M \\ M & -M \end{bmatrix} + \begin{bmatrix} A_i & 0 \\ 0 & -A_e \end{bmatrix} \right) \begin{bmatrix} \phi_i^{n+1} \\ \phi_e^{n+1} \end{bmatrix} = \begin{bmatrix} F_i^{n+1} \\ -F_e^{n+1} \end{bmatrix} + \\ -\chi_m \begin{bmatrix} M & 0 \\ 0 & M \end{bmatrix} \begin{bmatrix} w^n \\ w^n \end{bmatrix} + \left(\frac{\chi_m C_m}{\Delta t} \begin{bmatrix} M & 0 \\ 0 & M \end{bmatrix} - \begin{bmatrix} C(V_m^n) & 0 \\ 0 & C(V_m^n) \end{bmatrix} \right) \begin{bmatrix} V_m^n \\ V_m^n \end{bmatrix}, \\ w^{n+1} = (1 - \epsilon\gamma\Delta t) w^n + \epsilon \Delta t V_m^n. \end{cases}$$

Quasi-implicit operator-splitting scheme

Idea:

- sub-division of the operator as Godunov operator-splitting
- treat implicitly all the terms except the cubic one

1:

$$\begin{cases} \chi_m C_m M \frac{\tilde{V}_m^{n+1} - V_m^n}{\Delta t} + C(V_m^n) V_m^{n+1} + \chi_m M w^{n+1} = 0, \\ \frac{w^{n+1} - w^n}{\Delta t} = \epsilon (V_m^{n+1} - \gamma w^{n+1}). \end{cases}$$

2:

$$\begin{cases} \chi_m C_m M \frac{V_m^{n+1} - \tilde{V}_m^{n+1}}{\Delta t} + A_i \phi_i^{n+1} = F_i^{n+1}, \\ -\chi_m C_m M \frac{V_m^{n+1} - \tilde{V}_m^{n+1}}{\Delta t} + A_e \phi_e^{n+1} = F_e^{n+1}. \end{cases}$$

Quasi-implicit operator-splitting discretized system

$$\begin{cases} \left(\begin{bmatrix} Q_n & -Q_n \\ Q_n & -Q_n \end{bmatrix} + \begin{bmatrix} A_i & 0 \\ 0 & -A_e \end{bmatrix} \right) \begin{bmatrix} \phi_i^{n+1} \\ \phi_e^{n+1} \end{bmatrix} = \begin{bmatrix} R_n \\ R_n \end{bmatrix} + \begin{bmatrix} F_i^{n+1} \\ -F_e^{n+1} \end{bmatrix}, \\ w^{n+1} = \frac{w^n + \epsilon \Delta t (\phi_i^{n+1} - \phi_e^{n+1})}{1 + \epsilon \gamma \Delta t}. \end{cases}$$

Uniqueness

About uniqueness of the unkowns:

- V_m, w proved in *Existence and uniqueness of the solution for the bidomain model used in cardiac electrophysiology* by Y. Bourgault, Y. Coudière, and C. Pierre.
- ϕ_i, ϕ_e appear only through their difference V_m or their gradient. This means that there cannot be uniqueness.

POLITECNICO MILANO 1863

Uniqueness of potentials

Theorem

The classical solutions ϕ_i, ϕ_e are unique up to a constant depending only on time.

STRATEGIES

1. Imposition of the value of the function in a specific point.
   $\phi_i(\bar{x}, t) = \varphi(t) \quad \forall t \in [0, T] \quad \xrightarrow{\text{Numerical version}} \quad u_1^n = \varphi(t^n) \quad \forall n \in \{1, N\}$
2. Imposition of the function mean value.
   $\int_\Omega \phi_i \, dx = \varphi(t) \quad \forall t \in [0, T] \quad \xrightarrow{\text{Numerical version}} \quad \sum_{j=1}^{N_h} u_j^n \, w_j = \varphi(t^n) \quad \forall n \in \{1, N\}$

POLITECNICO MILANO 1863

Imposition of the value in a specific point / first coefficient

Remark

The aim is to impose the condition before or directly into the system to avoid ill-conditioning.

$$A = \begin{bmatrix} a_{11} & a_{12} & \dots & a_{1N} \\ a_{21} & a_{22} & \dots & a_{2N} \\ a_{31} & a_{32} & \dots & a_{3N} \\ \dots & \dots & \dots & \dots \\ a_{N1} & a_{N2} & \dots & a_{NN} \end{bmatrix} \quad \rightarrow \quad \tilde{A} = \begin{bmatrix} 1 & 0 & \dots & 0 \\ 0 & a_{22} & \dots & a_{2N} \\ 0 & a_{32} & \dots & a_{3N} \\ \dots & \dots & \dots & \dots \\ 0 & a_{N2} & \dots & a_{NN} \end{bmatrix}$$

$$b = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \\ \dots \\ b_N \end{bmatrix} \quad \rightarrow \quad \tilde{b} = \begin{bmatrix} c \\ b_2 - a_{21}c \\ b_3 - a_{31}c \\ \dots \\ b_N - a_{N1}c \end{bmatrix} \qquad (c \text{ is the imposed value})$$

An anaytical motivation for the mean-value imposition

Remark

The previous strategy modifies directly the system and keeps the symmetry of the matrix. This is not possible for the mean-value imposition, we should look for a different method.

Lemma

The two following problems are both well-posed and have the same solution u, moreover $\lambda = 0$.

Find $u \in H^1(\Omega)$ such that:

$$\begin{cases} \int_\Omega \nabla u \cdot \nabla v = \int_\Omega fv, \quad \forall v \in H^1(\Omega), \\ \int_\Omega u = 0. \end{cases}$$

Find $u \in H^1(\Omega), \lambda \in \mathbb{R}$ such that:

$$\begin{cases} \int_\Omega \nabla u \cdot \nabla v + \lambda \int_\Omega v = \int_\Omega fv, \quad \forall v \in H^1(\Omega), \\ \int_\Omega u = 0. \end{cases}$$

Imposition of the mean-value

Remark

An equivalent formulation to the Laplace problem with Neumann B.C. and null mean has been found (the very motivation passed through the Lagrange Multipliers). We can now generalize it for the Bidomain.

$$A = \begin{bmatrix} a_{11} & a_{12} & \dots & a_{1N} \\ a_{21} & a_{22} & \dots & a_{2N} \\ \dots & \dots & \dots & \dots \\ a_{N1} & a_{N2} & \dots & a_{NN} \end{bmatrix} \quad \rightarrow \quad \tilde{A} = \begin{bmatrix} a_{11} & a_{12} & \dots & a_{1N} & d_1 \\ a_{21} & a_{22} & \dots & a_{2N} & d_2 \\ \dots & \dots & \dots & \dots & \dots \\ a_{N1} & a_{N2} & \dots & a_{NN} & d_N \\ d_1 & d_2 & \dots & d_N & 0 \end{bmatrix}$$

$$b = \begin{bmatrix} b_1 \\ b_2 \\ \dots \\ b_N \end{bmatrix} \quad \rightarrow \quad \tilde{b} = \begin{bmatrix} b_1 \\ b_2 \\ \dots \\ b_N \\ c \end{bmatrix} \quad (c \text{ is the imposed value, } d_i = \textstyle\int_\Omega \varphi_i)$$

Strategies choices

Most of the times the two strategies are equivalent even if the second one is computationally more expensive. On the other hand, for very ill-posed systems, first strategy might have an overshooting effect and then a global strategy is needed.

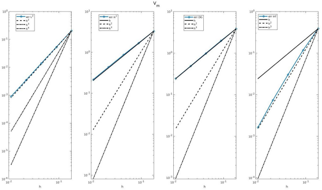
This is why we chose to adopt:

- The first coefficient imposition for error analysis studies.
- The mean value imposition for realistic simulations (where many terms are null).

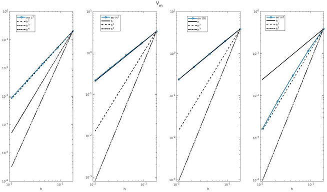
Chosen data

Domain	$\begin{bmatrix} 0 & 1 \\ 0 & 1 \end{bmatrix}$
dt	0.0001
T	0.001
χm	10^5
Σ_i	$\begin{bmatrix} 0.12 & 0 \\ 0 & 0.12 \end{bmatrix}$
Σ_e	$\begin{bmatrix} 0.12 & 0 \\ 0 & 0.12 \end{bmatrix}$
C_m	10^{-2}
k	19.5
ε	1.2
γ	0.1
a	$13 \cdot 10^{-3}$
V_m exact solution	$sin(2\pi x)sin(2\pi y)e^{-5t}$
w exact solution	$\frac{\varepsilon}{\varepsilon\gamma-5}sin(2\pi x)sin(2\pi y)e^{-5t}$

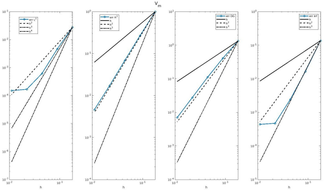
Comparison between FEM and Dubiner



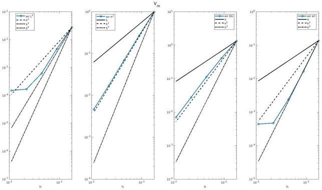
D1



P1

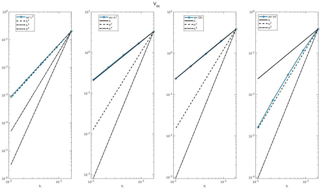


D2

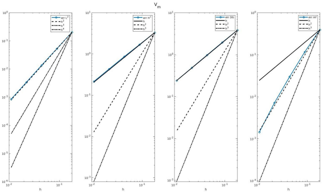


P2

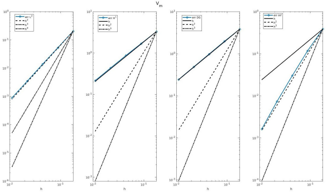
Comparison between temporal schemes



Semi-implicit

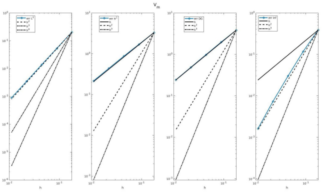


Godunov OS

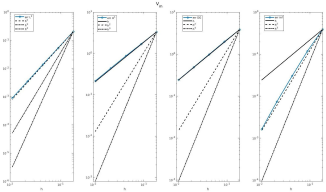


Quasi-implicit OS

Comparison between uniqueness imposition strategies



First coefficient imposition



Mean value imposition

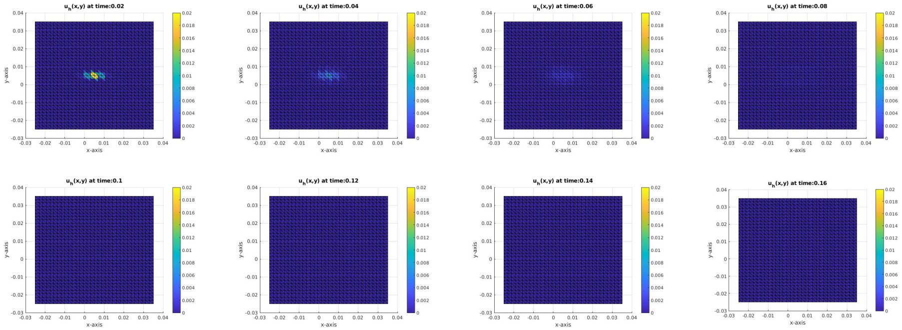
Moreover, condition number passes from $\approx 10^{17}$ to $\approx 10^{7}$.

POLITECNICO MILANO 1863

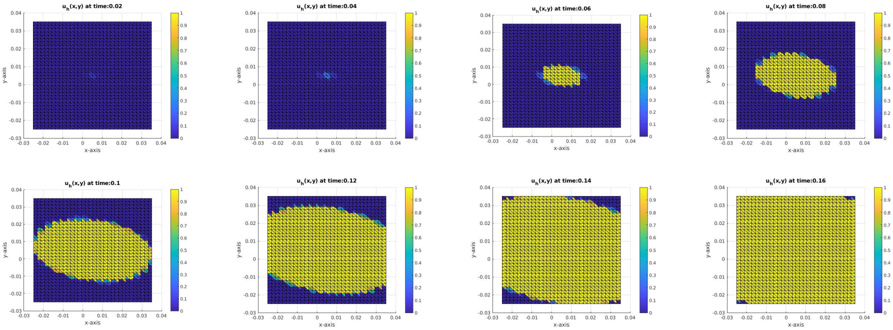
Chosen data

Domain	$\begin{bmatrix} -0.025 & 0.035 \\ -0.025 & 0.035 \end{bmatrix}$
Initial condition for V_m	0
Initial condition for w	0
I_i^{ext}	$I \cdot 10^3 \, \chi_{[0.001,0.002]}(t) \, \chi_{[0.0045,0.0055]}(x) \, \chi_{[0.0045,0.0055]}(y)$
I_e^{ext}	$I \cdot 10^3 \, \chi_{[0.001,0.002]}(t) \, \chi_{[0.0045,0.0055]}(x) \, \chi_{[0.0045,0.0055]}(y)$
b_i	0
b_e	0
Σ_i	$\begin{bmatrix} 0.34 & 0 \\ 0 & 0.06 \end{bmatrix}$
Σ_e	$\begin{bmatrix} 0.62 & 0 \\ 0 & 0.24 \end{bmatrix}$

Missed activation, $I = 500 \cdot 10^3$



Achieved activation, $I = 700 \cdot 10^3$



Conclusions

- Simulations truthfully represent the physical phenomenon: the threshold value for the activation, the propagation, the constant height etc.
- However, the rest and activation values are 0 and 1, different from the physiological values. Moreover, the repolarization phase misses. This is probably due to the ionic model that is too poor and a too wide mesh.

Further researches might:

- Do a mesh-adaptivity study.
- Adopt and compare different ionic models.