A posteriori error estimates in cardiac electrophysiology

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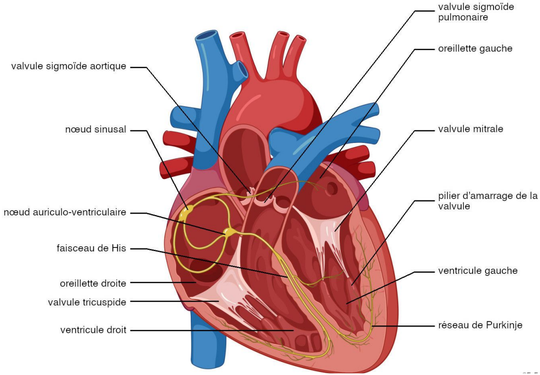
Outline

Introduction

Cardiac electrophysiology studies the electrical signals governing heart contractions and action potential propagation. These dynamics are described by the monodomain model, a fundamental system of PDEs in human-heart simulation.



Joakim Sundnes, Glenn Terje Lines, Xing Cai, Bjørn Fredrik Nielsen, Kent-Andre Mardal, and Aslak Tveito. Computing the electrical activity in the heart, volume 1 of Monographs in Computational Science and Engineering. Springer-Verlag, Berlin, 2006.

Monodomain problem

$$
\begin{aligned}
\partial_t v - \nabla \cdot (\Lambda \nabla v) + f(v,w) &= 0 \quad \text{in } \Omega \times (0,T),\\
\partial_t w + g(v,w) &= 0 \quad \text{in } \Omega \times (0,T),\\
\Lambda \nabla v \cdot \boldsymbol{n} &= 0 \quad \text{on } \partial\Omega \times (0,T),\\
v\big|_{t=0} = v^0, \quad w\big|_{t=0} = w^0 & \quad \text{in } \Omega.
\end{aligned}
$$

- unknown variables : transmembrane potential $v(t,\boldsymbol{x}) \in \mathbb{R}$, and the ionic variable $w(t,\boldsymbol{x}) \in \mathbb{R}$ (gating variable, concentration, etc) characterizing the underlying transfer of ions across the membrane in the considered medium.
- ODE : dynamic of the activation and inhibition variables for the ionic channels and $g(v,w)$ is a function representing the ionic activity.

Remark

The monodomain problem is a complex coupled nonlinear system of PDEs. Need accurate simulation and localize error within the simulation.

Phenomenological and physiological models

Two common approaches for constructing these ionic models in cardiac simulation

1. **The phenomenological model**: simplifies the underlying mechanisms and focuses on reproducing characteristic behaviors at the macroscopic scale. In terms of CPU cost, these models are competitive but do not capture the entire physical processes.

Examples (FitzHugh-Nagumo)

This model satisfies the Assumptions above

$$g(v,w) = -av + bw,$$
$$f(v,w) := f_1(v) + f_2(w)$$

with

$$f_1(v) := \lambda v(v-1)(v-\theta) \quad \text{and} \quad f_2(w) = \lambda w$$

and a, b, λ, θ are given parameters satisfying $a \geq 0$, $b \geq 0$, $\lambda > 0$ and $0 < \theta < 1$.

2. **The physiological models**: based on the cell membrane formulation developed by Hodgkin-Huxley for nerve fibers, are more realistic and capture several physical phenomena at different scales such as the mechanical response of the medium or the microscopic behavior of chemical species.
   However, the mathematical models developed in this context are **systems of nonlinear and parabolic PDEs coupled with multiple ODEs**.
   Numerical simulation would involve many unknowns and an unaffordable computational cost and memory burden.

Weak formulation

Given $f \in L^2(0,T;\left(H^1(\Omega)\right)')$, $g \in L^2(0,T;L^2(\Omega))$, $(v_0, w_0) \in (L^2(\Omega))^2$ and $\Lambda \in L^\infty(\Omega)$, a weak solution of problem is a vector $\mathbf{U} := (v, w)$ of functions s.t $v \in L^2\left(0,T;H^1(\Omega)\right)$, $\partial_t v \in L^2\left(0,T;\left(H^1(\Omega)\right)'\right)$ and $w \in C(0,T;L^2(\Omega))$ verifying

$$\frac{d}{dt}\langle v(t), \varphi\rangle_{(H^1(\Omega))', H^1(\Omega)} + (\Lambda \boldsymbol{\nabla} v(t), \boldsymbol{\nabla}\varphi)_\Omega = -\langle f(v(t), w(t)), \varphi\rangle_{(H^1(\Omega))', H^1(\Omega)} \quad \forall \varphi \in H^1(\Omega)$$
$$(\partial_t w(t), \phi)_\Omega = -(g(v(t), w(t)), \phi)_\Omega \quad \forall \phi \in L^2(\Omega).$$

Theorem (Well-posedness of Monodomain Model)

The monodomain problem admits a unique weak solution.

Finite element method

Time discretization : Implicite Euler scheme

Conforming space of piecewise polynomial functions

$$X_h^p := \left\{ v_h \in \mathcal{C}^0(\bar{\Omega});\ \ v_h|_K \in \mathbb{P}_p(K)\ \forall K \in \mathcal{T}_h \right\} \subset H^1(\Omega)$$

Discrete problem Given $\left(v_h^0, w_h^0\right) \in X_h^p \times X_h^p$, a discrete weak formulation consists in searching for all $1 \le n \le N_{\mathrm{t}}$, $\mathbf{U}_h^n := (v_h^n; w_h^n) \in X_h^p \times X_h^p$ such that for all φ_h and ϕ_h in X_h^p

$$\frac{1}{\Delta t_n}\left(v_h^n - v_h^{n-1}, \varphi_h\right)_\Omega + (\Lambda \boldsymbol{\nabla} v_h^n, \boldsymbol{\nabla}\varphi_h)_\Omega = -\left(f(v_h^n, w_h^n), \varphi_h\right)_\Omega$$

$$\frac{1}{\Delta t_n}\left(w_h^n - w_h^{n-1}, \phi_h\right)_\Omega = -\left(g(v_h^n, w_h^n), \phi_h\right)_\Omega,$$

Algebraic representation

$$\frac{1}{\Delta t_n}\mathbb{M}\boldsymbol{X}_{1h}^n + \mathbb{S}\boldsymbol{X}_{1h}^n = \frac{1}{\Delta t_n}\mathbb{M}\boldsymbol{X}_{1h}^{n-1} - \boldsymbol{F}(\boldsymbol{X}_h^n)$$

$$\frac{1}{\Delta t_n}\mathbb{M}\boldsymbol{X}_{2h}^n = \frac{1}{\Delta t_n}\mathbb{M}\boldsymbol{X}_{2h}^{n-1} - \boldsymbol{G}(\boldsymbol{X}_h^n)$$

Newton method

For $1 \leq n \leq N_t$ and $\boldsymbol{X}_h^{n,0} \in \mathbb{R}^{2\mathcal{N}_d^p}$ fixed, typically, $\boldsymbol{X}_h^{n,0} := \boldsymbol{X}_h^{n-1}$ where $\boldsymbol{X}_h^{n-1}$ is the last iterate from the previous time step, one looks at step $k \geq 1$ for $\boldsymbol{X}_h^{n,k} \in \mathbb{R}^{2\mathcal{N}_d^p}$ such that

$$\mathbb{A}^{n,k-1}\boldsymbol{X}_h^{n,k} = \boldsymbol{B}^{n,k-1}.$$

Here, $\mathbb{A}^{n,k-1} := \begin{pmatrix} \frac{1}{\Delta t_n}\mathbb{M} + \mathbb{S} + \mathbb{J}_{\tilde{\boldsymbol{F}}}(\boldsymbol{X}_{1h}^{n,k-1}) & \lambda\mathbb{M} \\ -a\mathbb{M} & \left(b + \frac{1}{\Delta t_n}\right)\mathbb{M} \end{pmatrix}$

$$\boldsymbol{B}^{n,k-1} := \begin{pmatrix} \mathbb{J}_{\tilde{\boldsymbol{F}}}(\boldsymbol{X}_{1h}^{n,k-1}) & \lambda\mathbb{M} \\ 0\mathbb{I}_{\mathcal{N}_d^p,\mathcal{N}_d^p} & 0\mathbb{I}_{\mathcal{N}_d^p,\mathcal{N}_d^p} \end{pmatrix} \boldsymbol{X}_h^{n,k-1} + \begin{pmatrix} \frac{1}{\Delta t_n}\mathbb{M} & 0\mathbb{I}_{\mathcal{N}_d^p,\mathcal{N}_d^p} \\ 0\mathbb{I}_{\mathcal{N}_d^p,\mathcal{N}_d^p} & \frac{1}{\Delta t_n}\mathbb{M} \end{pmatrix} \boldsymbol{X}_h^{n-1} - \begin{pmatrix} \boldsymbol{F}(\boldsymbol{X}_h^{n,k-1}) \\ \boldsymbol{0} \end{pmatrix}$$

Variational form

$$\frac{1}{\Delta t_n}\left(v_h^{n,k} - v_h^{n-1}, \psi_{h,\boldsymbol{x}_l}\right)_\Omega + \left(\Lambda \nabla v_h^{n,k}, \nabla \psi_{h,\boldsymbol{x}_l}\right)_\Omega + \Bigg(\underbrace{\mathcal{F}^{n,k}(v_h^{n,k}, w_h^{n,k})}_{\text{linearized ionic terms}}, \psi_{h,\boldsymbol{x}_l}\Bigg)_\Omega = 0$$

Goal

$$\left\| v - v_{h\tau}^{k} \right\|_{\sharp} + \left\| w - w_{h\tau}^{k} \right\|_{\flat} \leq \left(\sum_{n=1}^{N_{\mathrm{t}}} \sum_{K \in \mathcal{T}_h} (\eta_K^n (v_h^{n,k}, w_h^{n,k}))^2 \right)^{\frac{1}{2}}$$

- Fully computable upper bound on the error at each Newton step and each time step
- We employ the methodology of equilibrated flux reconstruction
- Distinguish all error components

Space-time representation of the solution (piecewise affine and continuous in time)

$$v_{h\tau}^{k}|_{I_n} := \frac{v_h^{n,k} - w_h^{n-1}}{\Delta t_n}(t - t^n) + v_h^{n,k} \quad \forall 1 \leq n \leq N_{\mathrm{t}} \quad \text{where} \quad v_{h\tau}^{n,k} := v_{h\tau}^{k}\Big|_{I_n}$$

Braess & Schoberl (2009), Ern & Vohralík (2013), Dabaghi & Martin & Vohralík (2020)

Equilibrated flux reconstruction

Recall :

$$
\begin{aligned}
&\partial_t v - \boldsymbol{\nabla}\cdot(\Lambda \boldsymbol{\nabla} v) + f(v,w) = 0 && \text{in } \Omega \times (0,T),\\
&\partial_t w + g(v,w) = 0 && \text{in } \Omega \times (0,T),\\
&\Lambda \boldsymbol{\nabla} v \cdot \boldsymbol{n} = 0 && \text{on } \partial\Omega \times (0,T),\\
&v|_{t=0} = v^0, \quad w|_{t=0} = w^0 && \text{in } \Omega.
\end{aligned}
$$

Remark

Violation of physical properties

- $\Lambda \boldsymbol{\nabla} v_{h\tau} \notin L^2(0,T;\mathbf{H}(\mathrm{div},\Omega))$
- $\boldsymbol{\nabla}\cdot(\Lambda \boldsymbol{\nabla} v_{h\tau}) \neq f(v_{h\tau}, w_{h\tau}) + \partial_t v_{h\tau}$
- $\partial_t w_{h\tau} + g(v_{h\tau}, w_{h\tau}) \neq 0$

Framework

- We construct an equilibrated flux $\boldsymbol{\sigma}_{h\tau} \in L^2(0, T; \mathbf{H}(\mathrm{div}, \Omega))$ enabling to construct local a posteriori error estimators. The laters represent and estimate the violations of physical properties of the numerical solution.
- At each Newton step we want to construct local a posteriori error estimators $\Rightarrow$ need to build two equilibrated flux reconstruction $\left(\boldsymbol{\sigma}_{h,\mathrm{disc}}^{n,k}, \boldsymbol{\sigma}_{h,\mathrm{lin}}^{n,k}\right) \in [\mathbf{H}(\mathrm{div}, \Omega)]^2$
- We can estimate each component of the error
- Adaptive procedure to save computational time.

Procedure of the flux reconstruction

The fluxes $\boldsymbol{\sigma}_{h,\mathrm{disc}}^{n,k}$ and $\boldsymbol{\sigma}_{h,\mathrm{lin}}^{n,k}$ are reconstructed in the Raviart-Thomas subspaces of $\mathbf{H}(\mathrm{div},\Omega)$. The Raviart-Thomas spaces of order $p \geq 1$ are defined by

$$\mathbf{RT}_p(\Omega) := \{\boldsymbol{\tau}_h \in \mathbf{H}(\mathrm{div},\Omega),\, \boldsymbol{\tau}_h|_K \in \mathbf{RT}_p(K) \quad \forall K \in \mathcal{T}_h\},$$

where $\mathbf{RT}_p(K) := [\mathbb{P}_p(K)]^2 + \overrightarrow{\boldsymbol{x}}\mathbb{P}_p(K)$, with $\overrightarrow{\boldsymbol{x}} = [x_1, x_2]^T$.
For $\boldsymbol{a} \in \mathcal{V}_h^{\mathrm{int}}$

$$\mathbf{V}_h^{\boldsymbol{a}} := \left\{\boldsymbol{\tau}_h \in \mathbf{RT}_p(\omega_h^{\boldsymbol{a}}), \boldsymbol{\tau}_h \cdot \mathbf{n}_{\omega_h^{\boldsymbol{a}}} = 0 \text{ on } \partial\omega_h^{\boldsymbol{a}}\right\}, \quad Q_h^{\boldsymbol{a}} := \left\{q_h \in \mathbb{P}_p\left(\mathcal{T}_h|_{\omega_h^{\boldsymbol{a}}}\right), (q_h, 1)_{\omega_h^{\boldsymbol{a}}} = 0\right\}.$$

For $\boldsymbol{a} \in \mathcal{V}_h^{\mathrm{ext}}$

$$\mathbf{V}_h^{\boldsymbol{a}} := \left\{\boldsymbol{\tau}_h \in \mathbf{RT}_p(\omega_h^{\boldsymbol{a}}), \boldsymbol{\tau}_h \cdot \mathbf{n}_{\omega_h^{\boldsymbol{a}}} = 0 \text{ on } \partial\omega_h^{\boldsymbol{a}} \backslash \partial\Omega\right\}, \quad Q_h^{\boldsymbol{a}} := \mathbb{P}_p\left(\mathcal{T}_h|_{\omega_h^{\boldsymbol{a}}}\right).$$

Total flux reconstruction

For each vertex $\boldsymbol{a} \in \mathcal{V}_h$, define $\boldsymbol{\sigma}_{h,\mathbf{tot}}^{n,k,\boldsymbol{a}} \in \mathbf{V}_h^{\boldsymbol{a}}$ and $\gamma_h^{n,\boldsymbol{a}} \in Q_h^{\boldsymbol{a}}$, by solving:

$$\begin{aligned}
\left(\boldsymbol{\sigma}_{h,\mathbf{tot}}^{n,k,\boldsymbol{a}}, \boldsymbol{\tau}_h\right)_{\omega_h^{\boldsymbol{a}}} - \left(\gamma_h^{n,k,\boldsymbol{a}}, \boldsymbol{\nabla}\cdot\boldsymbol{\tau}_h\right)_{\omega_h^{\boldsymbol{a}}} &= -\left(\psi_{h,\boldsymbol{a}}\Lambda\boldsymbol{\nabla} v_h^{n,k}, \boldsymbol{\tau}_h\right)_{\omega_h^{\boldsymbol{a}}} && \forall \boldsymbol{\tau}_h \in \mathbf{V}_h^{\boldsymbol{a}},\\
\left(\boldsymbol{\nabla}\cdot\boldsymbol{\sigma}_{h,\mathbf{tot}}^{n,k,\boldsymbol{a}}, q_h\right)_{\omega_h^{\boldsymbol{a}}} &= \left(\hat{f}_h^{n,k,\boldsymbol{a}}, q_h\right)_{\omega_h^{\boldsymbol{a}}} && \forall q_h \in Q_h^{\boldsymbol{a}},
\end{aligned}$$

At each time step $1 \leq n \leq N_{\mathbf{t}}$ the total flux reconstruction is defined by

$$\boldsymbol{\sigma}_{h,\mathbf{tot}}^{n,k} = \sum_{\boldsymbol{a}\in\mathcal{V}_h} \boldsymbol{\sigma}_{h,\mathbf{tot}}^{n,k,\boldsymbol{a}}.$$

Proposition

The total flux reconstruction $\boldsymbol{\sigma}_{h,\mathbf{tot}}^{n,k} \in \mathbf{H}(\mathbf{div},\Omega)$ and satisfies the equilibration property $\forall K \in \mathcal{T}_h$

$$\left(\boldsymbol{\nabla}\cdot\boldsymbol{\sigma}_{h,\mathbf{tot}}^{n,k} - \mathcal{F}^{n,k}(v_h^{n,k}, w_h^{n,k}) - \partial_t v_{h\tau}^{n,k}, 1\right)_K = 0.$$

Discretization flux reconstruction

We define for each vertex $\boldsymbol{a} \in \mathcal{V}_h^{\textbf{int}}$ the following quantity

$$R_{\boldsymbol{a}}^{k} := \frac{1}{\Delta t_n}\left(v_h^{n,k} - v_h^{n-1}, \psi_{h,\boldsymbol{a}}\right)_{\omega_h^{\boldsymbol{a}}} + \left(\Lambda \boldsymbol{\nabla} v_h^{n,k}, \boldsymbol{\nabla}\psi_{h,\boldsymbol{a}}\right)_{\omega_h^{\boldsymbol{a}}} + \left(f(v_h^{n,k-1}, w_h^{n,k-1}), \psi_{h,\boldsymbol{a}}\right)_{\omega_h^{\boldsymbol{a}}}.$$

For each vertex $\boldsymbol{a} \in \mathcal{V}_h$, define $\boldsymbol{\sigma}_{h,\textbf{disc}}^{n,k,\boldsymbol{a}} \in \mathbf{V}_h^{\boldsymbol{a}}$ and $\gamma_h^{n,\boldsymbol{a}} \in Q_h^{\boldsymbol{a}}$, by solving:

$$\begin{aligned}
\left(\boldsymbol{\sigma}_{h,\textbf{disc}}^{n,k,\boldsymbol{a}}, \boldsymbol{\tau}_h\right)_{\omega_h^{\boldsymbol{a}}} - \left(\gamma_h^{n,k,\boldsymbol{a}}, \boldsymbol{\nabla}\cdot\boldsymbol{\tau}_h\right)_{\omega_h^{\boldsymbol{a}}} &= -\left(\psi_{h,\boldsymbol{a}}\Lambda\boldsymbol{\nabla} v_h^{n,k}, \boldsymbol{\tau}_h\right)_{\omega_h^{\boldsymbol{a}}} && \forall \boldsymbol{\tau}_h \in \mathbf{V}_h^{\boldsymbol{a}},\\
\left(\boldsymbol{\nabla}\cdot\boldsymbol{\sigma}_{h,\textbf{disc}}^{n,k,\boldsymbol{a}}, q_h\right)_{\omega_h^{\boldsymbol{a}}} &= \left(\tilde{f}_h^{n,k,\boldsymbol{a}}, q_h\right)_{\omega_h^{\boldsymbol{a}}} && \forall q_h \in Q_h^{\boldsymbol{a}},
\end{aligned}$$

Proposition

The discretization flux reconstruction $\boldsymbol{\sigma}_{h,\textbf{disc}}^{n,k} = \sum_{\boldsymbol{a}\in\mathcal{V}_h} \boldsymbol{\sigma}_{h,\textbf{disc}}^{n,k,\boldsymbol{a}} \in \mathbf{H}(\textbf{div},\Omega)$ and satisfies

$$\left(\boldsymbol{\nabla}\cdot\boldsymbol{\sigma}_{h,\textbf{disc}}^{n,k} - \partial_t v_{h\tau}^{n,k} - f(v_h^{n,k-1}, w_h^{n,k-1}) + \sum_{\boldsymbol{a}\in\mathcal{V}_K} \frac{1}{|\omega_h^{\boldsymbol{a}}|} R_a^k, 1\right)_K = 0$$

Remark

- This method works for any numerical methods
- Local implementation
- Having constructed the total flux reconstruction $\boldsymbol{\sigma}_{h,\mathbf{tot}}^{n,k}$ and the discretization flux reconstruction $\boldsymbol{\sigma}_{h,\mathbf{disc}}^{n,k}$ we deduce the linearization flux reconstruction $\boldsymbol{\sigma}_{h,\mathbf{lin}}^{n,k} = \boldsymbol{\sigma}_{h,\mathbf{tot}}^{n,k} - \boldsymbol{\sigma}_{h,\mathbf{disc}}^{n,k}$.
- When the Newton solver has converged $\mathcal{F}^{n,k}(v_h^{n,k}, w_h^{n,k}) = f(v_h^n, w_h^n)$ so that the equilibrium relation reads

$$\left(\nabla \cdot \boldsymbol{\sigma}_{h,\mathbf{tot}}^{n}, q_h\right)_K = \left(f(v_h^n, w_h^n) + \partial_t v_{h\tau}^n, q_h\right)_K \quad \forall q_h \in \mathbb{P}_p(K).$$

Residual of the equations

Sobolev spaces

$X := L^2(0,T;H^1(\Omega)),\quad Y := L^2(0,T;L^2(\Omega))\quad Z := \left\{v \in X;\ \partial_t v \in X' := L^2\left(0,T;(H^1(\Omega))'\right)\right\}$

For $v \in X$ the space-time energy norm on X is given by

$$\|v\|_X := \left\{\int_0^T \|v\|_\Omega^2(t)\,\mathbf{dt} + \int_0^T \left\|\Lambda^{\frac{1}{2}}\boldsymbol{\nabla} v\right\|_\Omega^2(t)\,\mathbf{dt}\right\}^{\frac{1}{2}}.$$

For $v \in Z$ we set

$$\|v\|_Z := \|v\|_X + \|\partial_t v\|_{X'} \quad \text{where} \quad \|\partial_t v\|_{X'} = \left\{\int_0^T \|\partial_t v\|_{(H^1(\Omega))'}^2(t)\,\mathbf{dt}\right\}^{\frac{1}{2}}$$

Definition of the residuals

$$\left\langle \mathcal{R}_1(v_{h\tau}^k),\varphi\right\rangle_{X',X} = \int_0^T \left\{-\left(\partial_t v_{h\tau}^k,\varphi\right)_\Omega - (\Lambda\boldsymbol{\nabla} v_{h\tau}^k,\boldsymbol{\nabla}\varphi)_\Omega - \langle f(v_{h\tau}^k,w_{h\tau}^k),\varphi\rangle\right\}(t)\,\mathbf{dt}$$

$$\left\langle \mathcal{R}_2(w_{h\tau}^k),\psi\right\rangle_{Y,Y} = -\int_0^T \left\{\left(\partial_t w_{h\tau}^k,\psi\right)_\Omega - \left(g(v_{h\tau}^k,w_{h\tau}^k),\psi\right)_\Omega\right\}(t)\,\mathbf{dt}$$

The dual norm of the residuals is defined by

$$\left\||\mathcal{R}_1(v_{h\tau}^k)|\right\|_{X'} = \sup_{\varphi \in X} \frac{|\left\langle \mathcal{R}_1(v_{h\tau}^k), \varphi \right\rangle_{X',X}|}{\|\varphi\|_X} \quad \text{and} \quad \||\mathcal{R}_2(w_{h\tau})|\|_Y = \sup_{\psi \in Y} \frac{|\left\langle \mathcal{R}_2(w_{h\tau}^k), \psi \right\rangle_{Y,Y}|}{\|\psi\|_Y}.$$

Proposition

Let $(v, w) \in X \times Y$ be the solution of the continuous weak formulation and let $(v_{h\tau}^k, w_{h\tau}^k) \in X_h^p \times X_h^p$ be the approximate solution. Then,

$$\begin{aligned} &\left\|v - v_{h\tau}^k\right\|_X^2 + \left\|\partial_t(v - v_{h\tau}^k)\right\|_Y^2 + \left\|w - w_{h\tau}^k\right\|_Y^2 + \left\|\partial_t(w - w_{h\tau}^k)\right\|_Y^2 \\ &\quad \leq C_\star \left(\left\||\mathcal{R}_1(v_{h\tau}^k)|\right\|_Y^2 + \left\||\mathcal{R}_2(w_{h\tau}^k)|\right\|_Y^2 + \left\|(v - v_{h\tau}^k)(\cdot, 0)\right\|_\Omega^2 + \alpha_4 \left\|(w - w_{h\tau}^k)(\cdot, 0)\right\|_\Omega^2 \right) \end{aligned}$$

where $C_\star$ is a generic constant that depends on Ω, f, g and T.

A posteriori error estimates

Let $K \in \mathcal{T}_h$ and define the residual estimators by

$$\eta^{n,k}_{\mathbf{R_1},K}(t) := C_{\mathbf{P},K} h_K \left\| \partial_t v^{n,k}_{h\tau} + \mathcal{F}(v^{n,k}_{h\tau}, w^{n,k}_{h\tau}) + \boldsymbol{\nabla} \cdot \boldsymbol{\sigma}^{n,k}_{h\tau,\mathbf{tot}} \right\|_K (t)$$

$$\eta^{n,k}_{\mathbf{R_2},K}(t) := \left\| \partial_t w^{n,k}_{h\tau} + g\left(v^{n,k}_{h\tau}, w^{n,k}_{h\tau} \right) \right\|_K (t)$$

the flux estimator by

$$\eta^{n,k}_{\mathbf{F},K}(t) := \left\| \Lambda \boldsymbol{\nabla} v^{n,k}_{h\tau} + \boldsymbol{\sigma}^{n,k}_{h\tau,\mathbf{tot}} \right\|_K (t)$$

the linearization estimator by

$$\eta^{n,k}_{\mathbf{lin},\mathbf{1},K} := \left\| \mathcal{F}(v^{n,k}_{h\tau}, w^{n,k}_{h\tau}) - f(v^{n,k}_{h\tau}, w^{n,k}_{h\tau}) \right\|_K (t)$$

and the initial condition estimators by

$$\eta^{k}_{\mathbf{IC},1,K} := \left\| (v - v^{k}_{h\tau})(\cdot, 0) \right\|_K, \quad \eta^{k}_{\mathbf{IC},2,K} := \left\| (w - w^{k}_{h\tau})(\cdot, 0) \right\|_K$$

A posteriori error estimates

Theorem

$$\left\|\partial_t\left(w - w_{h\tau}^{n,k}\right)\right\|_Y^2 + \left\|w - w_{h\tau}^{n,k}\right\|_Y^2 + \left\|\partial_t\left(v - v_{h\tau}^{n,k}\right)\right\|_Y^2 + \left\|v - v_{h\tau}^{n,k}\right\|_X^2$$

$$\lesssim \left[\sum_{n=1}^{N_t}\int_{I_n}\sum_{K\in\mathcal{T}_h}\left\{\left(\eta_{\mathbf{R_1},K}^{n,k} + \eta_{\mathbf{F},K}^{n,k} + \eta_{\mathbf{lin},\mathbf{1},K}^{n,k}\right)^2 + \left(\eta_{\mathbf{R_2},K}^{n,k}\right)^2\right\}(t)\ \mathbf{dt}\right.$$

$$\left. + \sum_{K\in\mathcal{T}_h}\left\{\left(\eta_{\mathbf{IC},1,K}^{k}\right)^2 + \left(\eta_{\mathbf{IC},2,K}^{k}\right)^2\right\}\right.$$

Remark

The estimators $\eta_{\mathbf{R_1},K}^{n,k}$ and $\eta_{\mathbf{F},K}^{n,k}$ represent the nonconformity of the flux, *i.e.* $\Lambda\boldsymbol{\nabla} v_{h\tau}^{k} \notin \mathbf{H}(\mathbf{div},\Omega)$. The term $\eta_{\mathbf{R_2},K}^{n,k}$ is an estimator associated to the residual equation of the ODE. Indeed, $\partial_t w_{h\tau}^{n,k} + g(v_{h\tau}^{n,k}, w_{h\tau}^{n,k}) \neq 0$.

Space-time adaptivity

The flux estimator $\eta^{n,k}_{\mathbf{F},K}(t)$ is split into two contributions using the triangle inequality:

$$\eta^{n,k}_{\mathbf{F},K}(t) \leq \left\| \Lambda \boldsymbol{\nabla} \left(v^{n,k}_{h\tau}(t) - v^{n,k}_{h} \right) \right\|_K + \left\| \Lambda \boldsymbol{\nabla} v^{n,k}_h + \boldsymbol{\sigma}^{n,k}_{h\tau,\mathbf{tot}} \right\|_K .$$

Using the space-time representation of the solution we have $\forall t \in I_n$

$$v^{k}_{h\tau}(t) = (1 - \rho(t))\, v^{n,k}_h + \rho(t) v^{n-1}_h \quad \text{where} \quad \rho(t) = \frac{t^n - t}{\Delta t_n}.$$

Therefore, we get

$$\eta^{n,k}_{\mathbf{F},K}(t) \leq \rho(t) \left\| \Lambda \boldsymbol{\nabla} (v^{n,k}_h - v^{n-1}_h) \right\|_K + \left\| \Lambda \boldsymbol{\nabla} v^{n,k}_h + \boldsymbol{\sigma}^{n,k}_{h\tau,\mathbf{tot}} \right\|_K .$$

Nevertheless, the function $\rho : I_n \to \mathbb{R}$ is decreasing so that

$$\eta^{n,k}_{\mathbf{F},K}(t) \leq \underbrace{\left\| \Lambda \boldsymbol{\nabla} (v^{n,k}_h - v^{n-1}_h) \right\|_K}_{\eta^{n,k}_{\mathbf{tm},K}} + \underbrace{\left\| \Lambda \boldsymbol{\nabla} v^{n,k}_h + \boldsymbol{\sigma}^{n,k}_{h\tau,\mathbf{tot}} \right\|_K}_{\eta^{n,k}_{\mathbf{DF},K}} .$$

Proposition

We have the following error estimate, distinguishing the two sources (spatial and temporal) of the error

$$\eta^k \leq \eta^k_{\mathbf{tm}} + \eta^k_{\mathbf{sp}} + \eta^k_{\mathbf{init}}$$

where

$$\eta^k_{\mathbf{sp}} = 2^{\frac{1}{2}} \left\{ \sum_{n=1}^{N_t} \int_{I_n} \sum_{K \in \mathcal{T}_h} \left(\eta^{n,k}_{\mathbf{R_1},K} + \eta^{n,k}_{\mathbf{R_2},K} + \eta^{n,k}_{\mathbf{DF},K} + \eta^{n,k}_{\mathbf{lin,1},K} \right)^2 (t) \, \mathbf{dt} \right\}^{\frac{1}{2}}$$

$$\eta^k_{\mathbf{tm}} = 2^{\frac{1}{2}} \left\{ \sum_{n=1}^{N_t} \int_{I_n} \sum_{K \in \mathcal{T}_h} \left(\eta^{n,k}_{\mathbf{tm},K} \right)^2 (t) \, \mathbf{dt} \right\}^{\frac{1}{2}}$$

$$\eta^k_{\mathbf{init}} := \left\{ \sum_{K \in \mathcal{T}_h} \left\{ \left(\eta^k_{\mathbf{IC},1,K} \right)^2 + \left(\eta^k_{\mathbf{IC},2,K} \right)^2 \right\} \right\}^{\frac{1}{2}}$$

Distinction of the spatial error components

Let $1 \leq n \leq N_\mathbf{t}$. First, we have $\boldsymbol{\sigma}_{h,\mathbf{tot}}^{n,k} = \boldsymbol{\sigma}_{h,\mathbf{disc}}^{n,k} + \boldsymbol{\sigma}_{h,\mathbf{lin}}^{n,k}$ so the triangle inequality reads

$$\eta_{\mathbf{DF},K}^{n,k}(t) \leq \underbrace{\left\| \Lambda \nabla v_h^{n,k} + \boldsymbol{\sigma}_{h\tau,\mathbf{disc}}^{n,k} \right\|_K}_{\text{discretization } \eta_{\mathbf{FEM},K}^{n,k}} + \underbrace{\left\| \boldsymbol{\sigma}_{h\tau,\mathbf{lin}}^{n,k} \right\|_K}_{\text{linearization } \eta_{\mathbf{lin2},K}^{n,k}},$$

Theorem (Distinction of the two components of the spatial error)

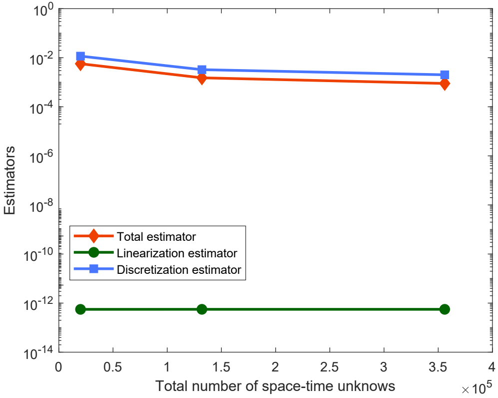
$$\eta_{\mathbf{sp}}^k \leq \eta_{\mathbf{FEM}}^k + \eta_{\mathbf{lin}}^k$$

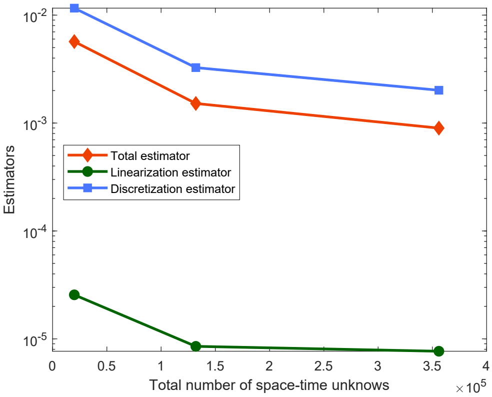
$$\eta_{\mathbf{FEM}}^k := 2^{\frac{1}{2}} \left\{ \sum_{n=1}^{N_t} \int_{I_n} \sum_{K \in \mathcal{T}_h} \left(\eta_{\mathbf{R_1},K}^{n,k} + \eta_{\mathbf{R_2},K}^{n,k} + \eta_{\mathbf{FEM},K}^{n,k} \right)^2 (t) \, \mathbf{dt} \right\}^{\frac{1}{2}},$$

$$\eta_{\mathbf{lin}}^k := 2^{\frac{1}{2}} \left\{ \sum_{n=1}^{N_t} \int_{I_n} \sum_{K \in \mathcal{T}_h} \left(\eta_{\mathbf{lin},1,K}^{n,k} + \eta_{\mathbf{lin},2,K}^{n,k} \right)^2 (t) \, \mathbf{dt} \right\}^{\frac{1}{2}}.$$

Numerical experiments

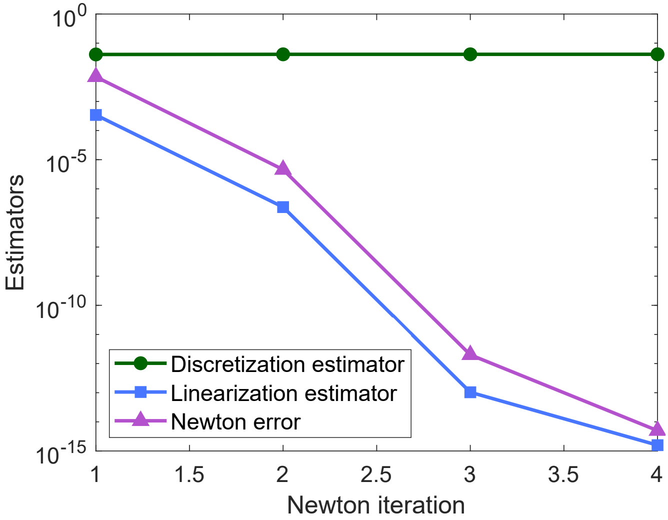
- 2D simulation
- FizHugh-Nagumo ionic model





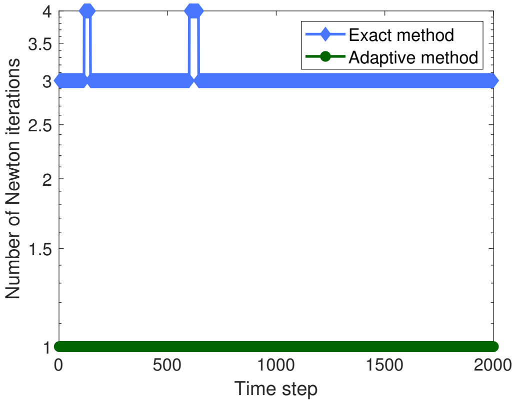
Quality and precision is preserved for adaptive Newton method

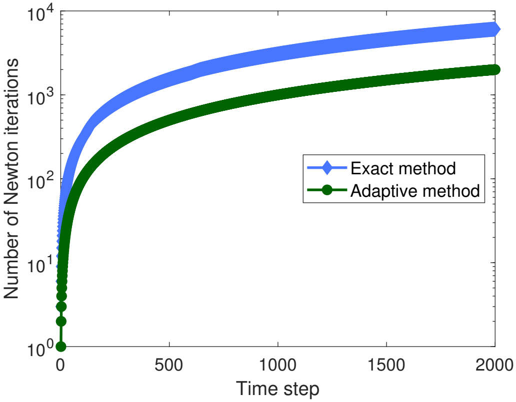
Newton adaptivity



From the first Newton iteration the linearization estimator does not influence the behavior of the discretization estimator which is constant.

Performance of the method





Conclusion

- We devised a posteriori error estimates based on equilibrated flux reconstruction for the monodomain formulation in electrophysiology
- Our approach is efficient and enable to distinguish the components of the error
- Extension to Bidomain formulation where micro-macro scale is taking into account is under investigation.

Paper in preparation F. Bader, J. Dabaghi, H. Ghazi *A posteriori error estimates and adaptive stopping criteria for cardiac monodomain model*, 2025.

Thank you for your attention !