A posteriori error estimates in cardiac electrophysiology

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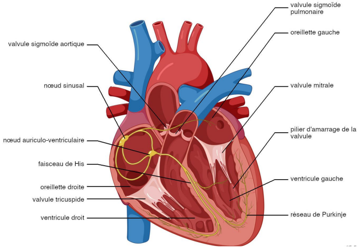
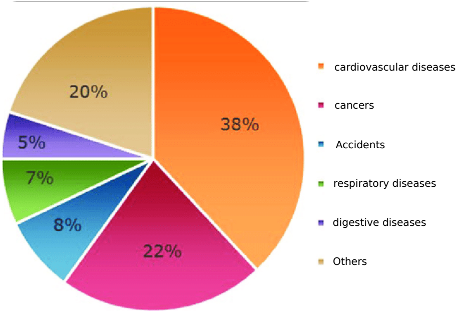
Outline

1. Introduction
2. Model problem
3. Finite element discretization
4. A posteriori error analysis
5. Conclusion

Cardiac electrophysiology studies the electrical signals governing heart contractions and action potential propagation.





We study the monodomain model, a simplified system of PDEs.

Questions : Can we estimate and localize the error within the numerical simulation ?

Monodomain problem

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

- 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) which is an auxiliary function characterizing the underlying transfer of ions across the membrane.
- 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 model

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 unfortunately 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 $0 < \theta < 1$.

Other possibility : The physiological models which are more realistic but more complicated...

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 the problem is a vector $\mathbf{U} := (v, w)$ of functions s.t $v \in L^2\left(0, T; H^1\left(\Omega\right)\right)$, $\partial_t v \in L^2\left(0, T; \left(H^1(\Omega)\right)'\right)$ and $w \in C(0, T; L^2(\Omega))$ verifying

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

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 $1 \leq n \leq N_{\mathrm{t}}$, $\mathbf{U}_h^n := (v_h^n; w_h^n) \in X_h^p \times X_h^p$ 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,

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

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

Galerkin orthogonality

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

Aposteriori Analysis

Goal

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

- 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 :

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

Remark

Violation of physical properties

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

We construct a flux $\boldsymbol{\sigma}_{h\tau} \in L^2(0,T;\mathbf{H}(\mathrm{div},\Omega))$ which "corrects" the violations.

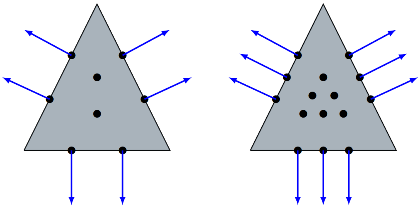
$$
\boldsymbol{\sigma}_h^{n,k} \nearrow\!\searrow \begin{cases} \boldsymbol{\sigma}_{h,\mathrm{disc}}^{n,k} & \in \mathbf{H}(\mathrm{div},\Omega) \\ \boldsymbol{\sigma}_{h,\mathrm{lin}}^{n,k} & \in \mathbf{H}(\mathrm{div},\Omega) \end{cases}
$$

Procedure of reconstruction of the flux

Raviart-Thomas subspaces of $\mathbf{H}(\mathrm{div}, \Omega)$.

$\mathbf{RT}_p(\Omega) := \{\boldsymbol{\tau}_h \in \mathbf{H}(\mathrm{div}, \Omega), \; \boldsymbol{\tau}_h|_K \in \mathbf{RT}_p(K) \, \forall K \in \mathcal{T}_h\}$ and $\mathbf{RT}_p(K) := [\mathbb{P}_p(K)]^2 + \vec{\boldsymbol{x}} \mathbb{P}_p(K)$

number of DOFs $\mathbf{RT}_0(K) = 3$.
number of DOFs $\mathbf{RT}_1(K) = 8$.
number of DOFs $\mathbf{RT}_2(K) = 15$.



Procedure

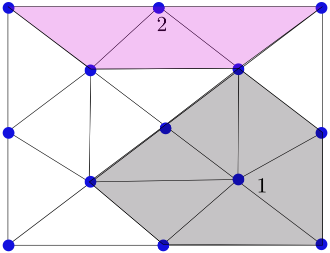
Construct for each vertices of the mesh a flux $\boldsymbol{\sigma}_h^{n,k,\boldsymbol{a}} \in \mathbf{H}(\mathrm{div}, \omega^{\boldsymbol{a}})$. The sum $\boldsymbol{\sigma}_h^{n,k} = \sum_{\boldsymbol{a} \in \mathcal{V}_h} \boldsymbol{\sigma}_h^{n,k,\boldsymbol{a}} \in \mathbf{H}(\mathrm{div}, \Omega)$

Mixed finite element system

Find $\boldsymbol{\sigma}_h^{n,k,\boldsymbol{a}} \in \mathbf{V}_h^{\boldsymbol{a}} \subset \mathbf{H}(\mathrm{div},\omega^{\boldsymbol{a}})$ and $\gamma_h^{n,k,\boldsymbol{a}} \in Q_h^{\boldsymbol{a}} \subset L^2(\omega^{\boldsymbol{a}})$ satisfying

$$\left(\boldsymbol{\sigma}_h^{n,k,\boldsymbol{a}}, \boldsymbol{\tau}_h\right)_{\omega^{\boldsymbol{a}}} - \left(\gamma_h^{n,k,\boldsymbol{a}}, \boldsymbol{\nabla}\cdot\boldsymbol{\tau}_h\right)_{\omega^{\boldsymbol{a}}} = -\left(\psi_h^{\boldsymbol{a}} \Lambda \boldsymbol{\nabla} v_h^{n,k}, \boldsymbol{\tau}_h\right)_{\omega^{\boldsymbol{a}}}$$

$$\left(\boldsymbol{\nabla}\cdot\boldsymbol{\sigma}_h^{n,k,\boldsymbol{a}}, q_h\right)_{\omega^{\boldsymbol{a}}} = -\left(\hat{f}_h^{n,k,\boldsymbol{a}}, q_h\right)_{\omega^{\boldsymbol{a}}}$$



(MFE) system $\Longleftrightarrow$ linear system of algebraic equation. Fast implementation!

$$\boldsymbol{\sigma}_h^{n,k} = \sum_{\boldsymbol{a}\in\mathcal{V}_h} \boldsymbol{\sigma}_h^{n,k,\boldsymbol{a}}$$

Lemma

The total flux reconstruction $\boldsymbol{\sigma}_h^{n,k} \in \mathbf{H}(\mathrm{div},\Omega)$ and satisfies the equilibration property

$$\left(\boldsymbol{\nabla}\cdot\boldsymbol{\sigma}_h^{n,k} - \mathcal{F}^{n,k}(v_h^{n,k}, w_h^{n,k}) - \partial_t v_h^{n,k}, 1\right)_K = 0 \quad \forall K \in \mathcal{T}_h$$

A posteriori error estimates

residual estimators

$$\eta_{\mathrm{R}_1,K}^{n,k}(t) := C_{P,K} h_K \left\| \partial_t v_{h\tau}^{n,k} + \mathcal{F}\left(v_{h\tau}^{n,k}, w_{h\tau}^{n,k}\right) + \boldsymbol{\nabla} \cdot \boldsymbol{\sigma}_{h\tau}^{n,k} \right\|_K (t)$$

$$\eta_{\mathrm{R}_2,K}^{n,k}(t) := \left\| \partial_t w_{h\tau}^{n,k} + g\left(v_{h\tau}^{n,k}, w_{h\tau}^{n,k}\right) \right\|_K (t)$$

flux estimator

$$\eta_{\mathrm{F},K}^{n,k}(t) := \left\| \Lambda \boldsymbol{\nabla} v_{h\tau}^{n,k} + \boldsymbol{\sigma}_{h\tau}^{n,k} \right\|_K (t)$$

linearization estimator

$$\eta_{\mathrm{lin},1,K}^{n,k}(t) := \left\| \mathcal{F}(v_{h\tau}^{n,k}, w_{h\tau}^{n,k}) - f(v_{h\tau}^{n,k}, w_{h\tau}^{n,k}) \right\|_K (t)$$

initial condition estimators

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

Remark: $\eta_{\mathrm{R}_1,K}^{n,k}$ and $\eta_{\mathrm{F},K}^{n,k} \Rightarrow$ nonconformity of the flux, $\Lambda \boldsymbol{\nabla} v_{h\tau} \notin L^2(0, T; \mathbf{H}(\mathrm{div}, \Omega))$.
$\eta_{\mathrm{R}_2,K}^{n,k} \Rightarrow$ residual equation of the ODE. Indeed, $\partial_t w_{h\tau}^{n,k} + g(v_{h\tau}^{n,k}, w_{h\tau}^{n,k}) \neq 0$.

A posteriori error estimates

Theorem

$$\frac{1}{2\sqrt{C_\star}}\left(\left\|\partial_t\left(w - w_{h\tau}^{n,k}\right)\right\|_Y + \left\|w - w_{h\tau}^{n,k}\right\|_Y + \left\|\partial_t\left(v - v_{h\tau}^{n,k}\right)\right\|_Y + \left\|v - v_{h\tau}^{n,k}\right\|_X\right) \le \eta^k$$

with the global estimator η^k *defined by*

$$\eta^k := \left\{\sum_{n=1}^{N_t}\int_{I_n}\sum_{K\in\mathcal{T}_h}\left(\left(\eta_{\mathrm{R}_1,K}^{n,k} + \eta_{\mathrm{F},K}^{n,k} + \eta_{\mathrm{lin},1,K}^{n,k}\right)^2 + \left(\eta_{\mathrm{R}_2,K}^{n,k}\right)^2\right)(t)\,\mathrm{dt}\right.$$
$$\left. + \sum_{K\in\mathcal{T}_h}\left(\left(\eta_{\mathrm{IC},1,K}^{k}\right)^2 + \left(\eta_{\mathrm{IC},2,K}^{k}\right)^2\right)\right\}^{\frac{1}{2}}.$$

Space-time error

Corollary

Let $\left(v_{h\tau}^k, w_{h\tau}^k\right)$ *be the approximate solution. Let* $\boldsymbol{\sigma}_{h\tau}^k \in L^2(0, T; \mathbf{H}(\mathrm{div}, \Omega))$ *be the equilibrated flux reconstruction. Then,*

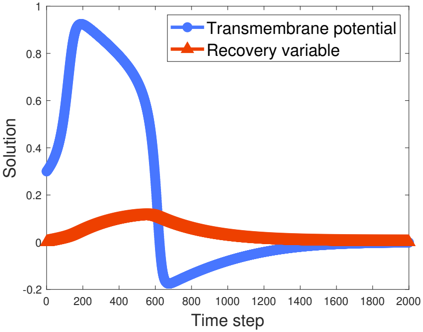
$$\eta^k \leq \eta_{\mathrm{tm}}^k + \eta_{\mathrm{FEM}}^k + \eta_{\mathrm{lin}}^k + \eta_{\mathrm{init}}^k.$$

Adaptive Newton algorithm at each time step

1. Choose an initial vector $\boldsymbol{X}_h^{n,0} \in \mathbb{R}^{2\mathcal{N}_d^p}$, typically as $\boldsymbol{X}_h^{n-1}$, and set $k = 1$.
2. From $\boldsymbol{X}_h^{n,k-1}$ define $\mathbb{A}^{n,k-1} \in \mathbb{R}^{2\mathcal{N}_d^p, 2\mathcal{N}_d^p}$ and $\boldsymbol{B}^{n,k-1} \in \mathbb{R}^{2\mathcal{N}_d^p}$.
3. Consider the linear system $\mathbb{A}^{n,k-1}\boldsymbol{X}_h^{n,k} = \boldsymbol{B}^{n,k-1}$.
4. Compute the estimators and check the stopping criterion $\eta_{\mathrm{lin}}^{n,k} \leq \gamma_{\mathrm{lin}}\eta_{\mathrm{disc}}^{n,k}$. If satisfied, return $\boldsymbol{X}_h^n = \boldsymbol{X}_h^{n,k}$. If not, set $k = k + 1$ and go back to **1**.

First test case at convergence

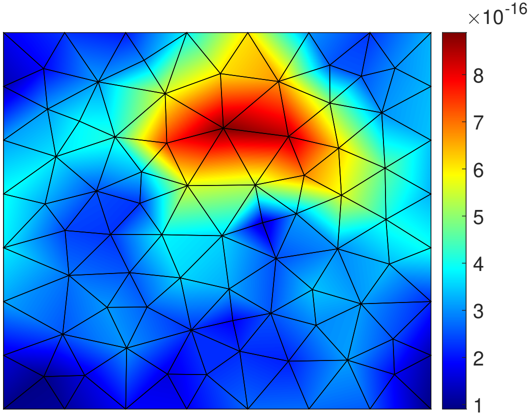
- $\Omega := [-1, 1] \times [-1, 1]$, $\mathbb{P}_1$ FEM, stopping criterion $\varepsilon = 10^{-12}$, $\Delta t_n = \Delta t = 0.1$
- For modeling ionic current flows, we employ the original FitzHugh–Nagumo model.



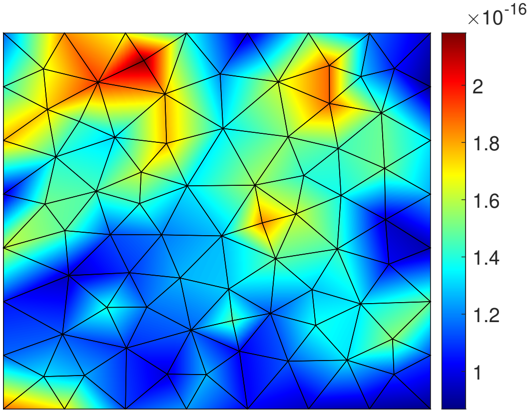
The transmembrane potential v_h (blue curve) represents the electrical activation of a cardiac cell, whereas the recovery variable w_h (red curve) accounts for the delayed response of ionic channels, such as potassium (K^+) and sodium (Na^+) channels. The overall dynamics can be divided into three main phases: rapid depolarization phase, the repolarization phase, return to the resting state phase.

Estimators

Flux estimator

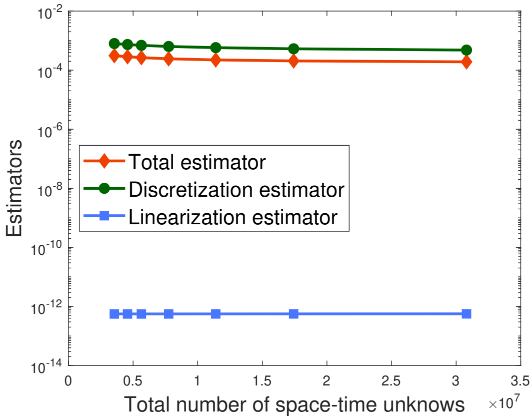


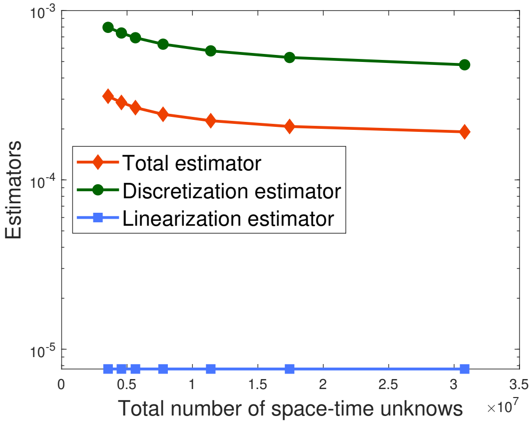
Residual estimator



These discretization estimators are very small. When the Newton solver has converged the numerical flux $\nabla v_{h\tau}^{n,k}$ is almost conforming since it is very close in the sense of the L^2 norm to the equilibrated flux $\boldsymbol{\sigma}_{h\tau}^{n,k} \in \mathbf{H}(\mathrm{div}, \Omega)$.

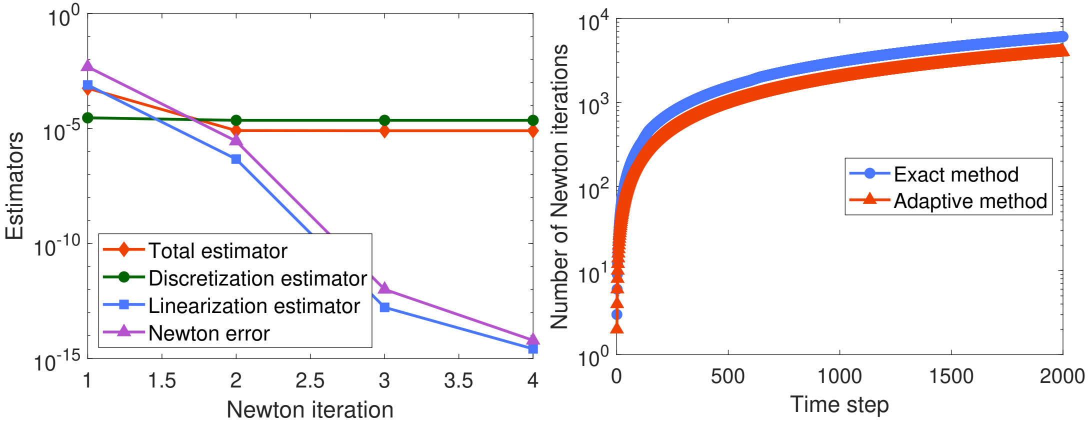
Second test case





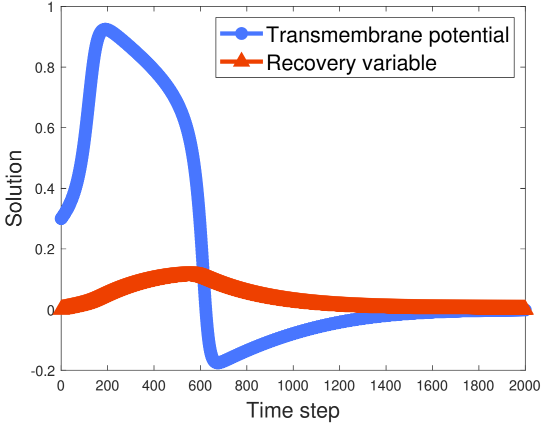
In both cases, the total estimator η^k (red curve) is nearly identical, indicating that the adaptive method achieves comparable accuracy to the exact Newton method.

Adaptivity

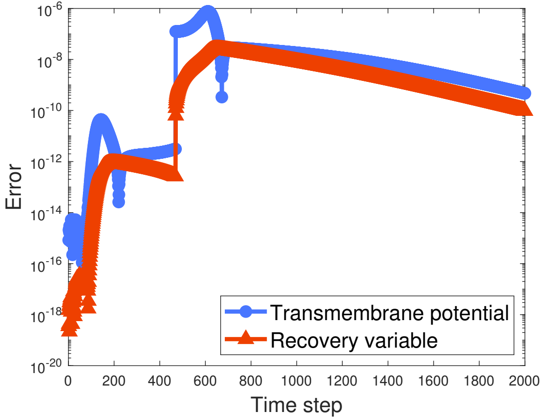


Adaptive Newton approach reduces the total number of iterations by approximately 35% by the end of the simulation.

Adaptivity



Solution
Time step
Transmembrane potential
Recovery variable
1
0.8
0.6
0.4
0.2
0
-0.2
0
200
400
600
800
1000
1200
1400
1600
1800
2000



Error
Time step
Transmembrane potential
Recovery variable
10^{-6}
10^{-8}
10^{-10}
10^{-12}
10^{-14}
10^{-16}
10^{-18}
10^{-20}
0
200
400
600
800
1000
1200
1400
1600
1800
2000

Conclusion

- In this work we devised a posteriori error estimates with adaptive stopping creteria for the monodomain problem
- Extension to more complicated formulations such as the bidomain problem is under investigation.

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