Scientific Machine Learning
Final Project

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Let $\Omega = (0,1)^2$ be the spatial domain and $I = (0,T]$ a time interval. We consider the dimensionless monodomain equation, used for simulating excitable tissues, defined as:

$$\begin{aligned} \frac{\partial u}{\partial t} - \boldsymbol{\nabla} \cdot \Sigma \boldsymbol{\nabla} u + f(u) &= 0 && \text{in } \Omega \times I, \\ \mathbf{n} \cdot \boldsymbol{\nabla} u &= 0 && \text{on } \partial\Omega \times I, \\ u &= u_0 && \text{in } \Omega \times \{0\}, \end{aligned}$$

where the reaction term f is given by:

$$\begin{aligned} f(u) &= a(u - f_r)(u - f_t)(u - f_d), \\ a &= 18.515, \\ f_t &= 0.2383, \\ f_r &= 0, \\ f_d &= 1. \end{aligned}$$

We assume heterogeneous conductivity across the spatial domain:

$$\begin{aligned} \Sigma_h &= 9.5298 \times 10^{-4}, \\ \Sigma_d &\in \{10\Sigma_h, \Sigma_h, 0.1\Sigma_h\}. \end{aligned}$$

The diseased regions are defined as:

$$\begin{aligned} \Omega_{d1} &= \left\{(x,y) \in \Omega \mid (x-0.3)^2 + (y-0.7)^2 < 0.1^2\right\}, \\ \Omega_{d2} &= \left\{(x,y) \in \Omega \mid (x-0.7)^2 + (y-0.3)^2 < 0.15^2\right\}, \\ \Omega_{d3} &= \left\{(x,y) \in \Omega \mid (x-0.5)^2 + (y-0.5)^2 < 0.1^2\right\}. \end{aligned}$$

1 Finite Element Method

1.1 IMEX time integration scheme

We discretize the time interval into steps of size Δt, and denote the approximation of $u(x, t_n)$ by $U^n(x)$. The nonlinear reaction term $f(u)$ is treated explicitly, while the diffusion term is treated implicitly. The semi-discrete IMEX scheme is:

$$\frac{U^{n+1} - U^n}{\Delta t} = \boldsymbol{\nabla} \cdot \Sigma \boldsymbol{\nabla} U^{n+1} - f(U^n).$$

Rearranging terms:

$$\begin{aligned} U^{n+1} - U^n &= \Delta t\, \boldsymbol{\nabla} \cdot \Sigma \boldsymbol{\nabla} U^{n+1} - \Delta t\, f(U^n), \\ U^{n+1} - \Delta t\, \boldsymbol{\nabla} \cdot \Sigma \boldsymbol{\nabla} U^{n+1} &= U^n - \Delta t\, f(U^n). \end{aligned}$$

Assuming a spatial discretization with a mesh of size h, and denoting by A the discrete Laplace operator (stiffness matrix), we obtain the algebraic form:

$$(\mathbf{I} - \frac{\Delta t}{h^2} A) U^{n+1} = U^n - \Delta t\, f(U^n).$$

We approximate the solution at time t_n by a finite element function:

$$U^n(x) = \sum_{j=1}^{N} u_j^n \phi_j(x),$$

where $\{\phi_j\}_{j=1}^N$ is a basis for the finite element space $\mathbb{V}_h \subset \mathbb{V}$, and u_j^n are the coefficients to be computed.

1.2 Weak formulation at time t_n

Let $v \in \mathbb{V}$. Applying the IMEX time discretization, we multiply the equation by v and integrate over Ω:

$$\int_\Omega \frac{U^{n+1} - U^n}{\Delta t} v \,\mathrm{d}x + \int_\Omega \Sigma \boldsymbol{\nabla} U^{n+1} \cdot \boldsymbol{\nabla} v \,\mathrm{d}x = \int_\Omega f(U^n) v \,\mathrm{d}x.$$

The boundary term vanishes due to the homogeneous Neumann condition:

$$\int_{\partial\Omega} (\Sigma \nabla U^{n+1} \cdot \mathbf{n}) v \,\mathrm{d}s = 0.$$

We seek $U^{n+1} \in \mathbb{V}$ such that:

$$a(U^{n+1}, v) = F(v) \quad \forall v \in \mathbb{V},$$

where

$$a(U^{n+1}, v) = \int_\Omega \frac{U^{n+1}}{\Delta t} v \, \mathrm{d}x + \int_\Omega \Sigma \boldsymbol{\nabla} U^{n+1} \cdot \boldsymbol{\nabla} v \, \mathrm{d}x,$$
$$F(v) = \int_\Omega \left(\frac{U^n}{\Delta t} + f(U^n) \right) v \, \mathrm{d}x.$$

1.3 Algebraic formulation of the FEM discretization

Using the basis functions $\{\phi_j\}$ and the expansion $U^n(x) = \sum_j u_j^n \phi_j(x)$, the weak form becomes a linear system at each time step:

$$(\mathbf{M} + \Delta t \, \mathbf{K}) \, \mathbf{u}^{n+1} = \mathbf{M} \, \mathbf{u}^n - \Delta t \, \mathbf{f}(U^n),$$

where:

$$\mathbf{M}_{ij} = \int_\Omega \phi_i(x) \phi_j(x) \, \mathrm{d}x \qquad \text{(mass matrix)},$$
$$\mathbf{K}_{ij} = \int_\Omega \Sigma(x) \boldsymbol{\nabla} \phi_i(x) \cdot \boldsymbol{\nabla} \phi_j(x) \, \mathrm{d}x \qquad \text{(stiffness matrix)},$$
$$\mathbf{f}_i(U^n) = \int_\Omega f(U^n(x)) \phi_i(x) \, \mathrm{d}x \qquad \text{(nonlinear load vector)}.$$

1.4 Simulation results

We studied the effect of different diffusivity values in the diseased region, $\Sigma_d \in \{10\Sigma_h, \Sigma_h, 0.1\Sigma_h\}$, on the dynamics of wave propagation. The results show that the activation time increases as Σ_d decreases. This is expected, as a lower diffusivity slows down the spread of excitation through the diseased region. For example, at the finest resolution ($\Delta t = 0.025$, $n_e = 256$), the activation times are approximately 26.18 for $\Sigma_d = 10\Sigma_h$, 27.78 for $\Sigma_d = \Sigma_h$, and 29.23 for $\Sigma_d = 0.1\Sigma_h$. This trend is consistent across all time steps and grid resolutions.

We also evaluated the numerical properties of the solution. In particular, we checked whether the stiffness matrix satisfies the M-matrix condition, which is associated with stability and monotonicity of the scheme. The results show that this condition is satisfied only for sufficiently small time steps and fine meshes. For instance, at $\Delta t = 0.1$, the M-matrix condition

fails in most cases, especially for smaller Σ_d. At $\Delta t = 0.025$, the condition is generally satisfied for $\Sigma_d = \Sigma_h$ and $10\Sigma_h$, but not always for $0.1\Sigma_h$.

Finally, we examined whether the numerical solution stays within the physically meaningful range $u \in [0, 1]$. Again, this requirement is met only when the mesh and time step are fine enough. Coarse discretizations tend to produce values outside the expected bounds, particularly when Σ_d is small. This suggests that smaller diffusivity increases the stiffness of the problem, requiring more careful numerical treatment to ensure accurate results.

Table 1: Results of the simulation for $\Sigma_d = 10\Sigma_h$.

Δt	n_e	Activation time	M-matrix?	$u \in [0, 1]$
0.1	64	28.60	true	false
0.1	128	29.10	true	false
0.1	256	29.20	true	false
0.05	64	26.60	false	false
0.05	128	27.15	true	true
0.05	256	27.20	true	true
0.025	64	25.60	false	false
0.025	128	26.10	true	true
0.025	256	26.175	true	true

Table 2: Results of the simulation for $\Sigma_d = \Sigma_h$.

Δt	n_e	Activation time	M-matrix?	$u \in [0, 1]$
0.1	64	30.20	true	false
0.1	128	30.90	true	false
0.1	256	31.00	true	false
0.05	64	28.10	false	false
0.05	128	28.80	true	true
0.05	256	28.90	true	true
0.025	64	27.025	false	false
0.025	128	27.70	true	true
0.025	256	27.775	true	true

Table 3: Results of the simulation for $\Sigma_d = 0.1\Sigma_h$.

Δt	n_e	Activation time	M-matrix?	$u \in [0, 1]$
0.1	64	31.70	false	false
0.1	128	32.50	false	false
0.1	256	32.60	true	false
0.05	64	29.55	false	false
0.05	128	30.25	false	false
0.05	256	30.40	false	true
0.025	64	28.40	false	false
0.025	128	29.075	false	false
0.025	256	29.225	false	true

Overall, the results confirm that lower diffusivity in the diseased region significantly slows wave propagation and makes the numerical problem more challenging. Finer meshes and smaller time steps are necessary to maintain both accuracy and physical realism.

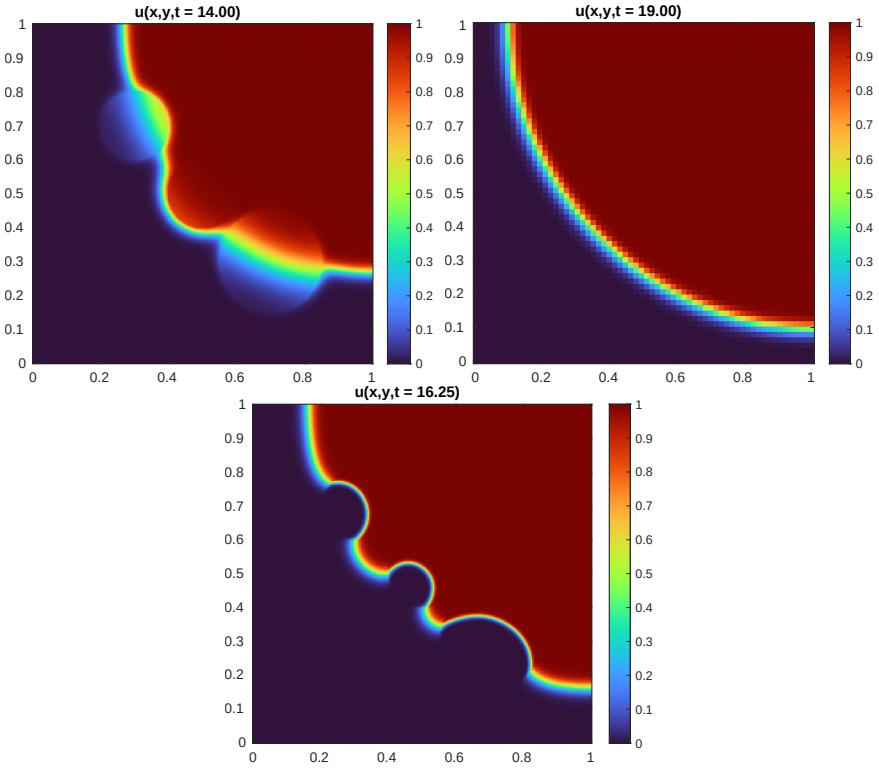

Figure 1: Snapshots of the simulation over diseased regions for $\Sigma_d \in \{10\Sigma_h, \Sigma_h, 0.1\Sigma_h\}$.

References

[1] N. McGreivy and A. Hakim. Weak baselines and reporting biases lead to overoptimism in machine learning for fluid-related partial differential equations. *Nature Machine Intelligence*, 6(10):1256–1269, Sept. 2024.