Scientific Machine Learning
Final Project

Lovnesh Bhardwaj, Laurynas Varnas

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

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

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

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 $U^n(x)$. Let the nonlinear reaction term $f(u)$ be treated explicitly and the diffusion term 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 mesh 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 for 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:

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

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

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

where

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

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:

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

1.4 Simulation results

$\Sigma_d = 10$

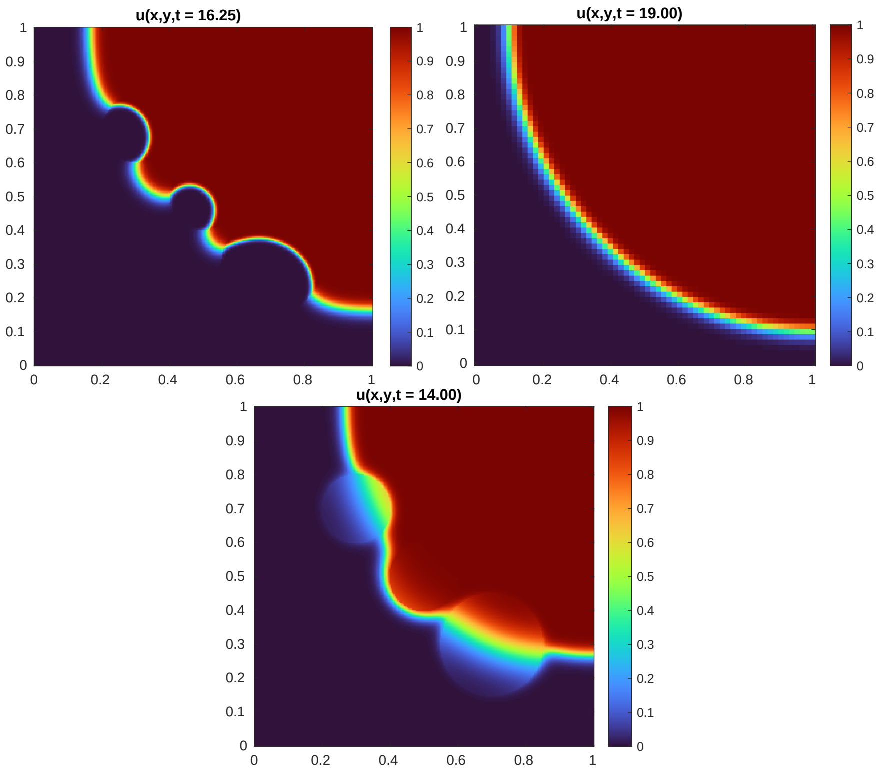
Δt	n_e	Activation time	M-matrix?	$u \in [0, 1]$
0.1	64	28.60	true	false
0.1	128	29.10	true	false
0.1	256	29.20	true	false
0.05	64	26.60	false	false
0.05	128	27.15	true	true
0.05	256	27.20	true	true
0.025	64	25.60	false	false
0.025	128	26.10	true	true
0.025	256	26.175	true	true

$\Sigma_d = 1$

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

$\Sigma_d = 0.1$

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



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.