# Scientific Machine Learning: Final Project

June 2025

## 1 Problem Definition

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:

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

where $u : \Omega \times I \to \mathbb{R}$ represents the electric potential, $\Sigma : \Omega \to \mathbb{R}$ is the electrical conductivity of the media, and $f$ is a non-linear reaction term responsible for the activation of the tissue under consideration. The monodomain equation is usually solved with homogeneous Neumann conditions (given the outer normal $\mathbf{n}$ in $\partial\Omega$) and an initial condition $u_0 : \Omega \to \mathbb{R}$. As a reference, in cardiac simulations, time is measured in milliseconds (ms) and spatial dimensions in millimeters (mm). Typically, the spatial domain extends over several tenths of millimeters, as the size of a human heart (approximately 10 cm). The temporal domain spans thousands of milliseconds, corresponding to the duration of one heartbeat (approximately 1 s).

We consider a cubic reaction term, in the form:

$$f(u) = a(u - f_r)(u - f_t)(u - f_d)$$

where $f_r \in \mathbb{R}$ is the resting potential, $f_t \in \mathbb{R}$ the threshold potential, $f_d \in \mathbb{R}$ the depolarization potential, and $a \in \mathbb{R}$ is a physical constant. We also consider a possibly heterogeneous conductivity, with $\Sigma$ varying across the spatial domain:

$$\Sigma(x) = \begin{cases} \Sigma_d, & \text{if } x \in \Omega_d, \\ \Sigma_h, & \text{if } x \in \Omega_h, \end{cases}$$

where $\Omega_h$ and $\Omega_d$ represent healthy and diseased tissues, respectively, and $\Omega = \Omega_h \cup \Omega_d$. The diseased domain $\Omega_d = \Omega_{d1} \cup \Omega_{d2} \cup \Omega_{d3}$ is defined by the following circular regions:

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

The initial condition at $t = 0$ is given by:

$$u_0 = \begin{cases} 1 & \text{if } x \geq 0.9 \text{ and } y \geq 0.9, \\ 0 & \text{otherwise.} \end{cases}$$

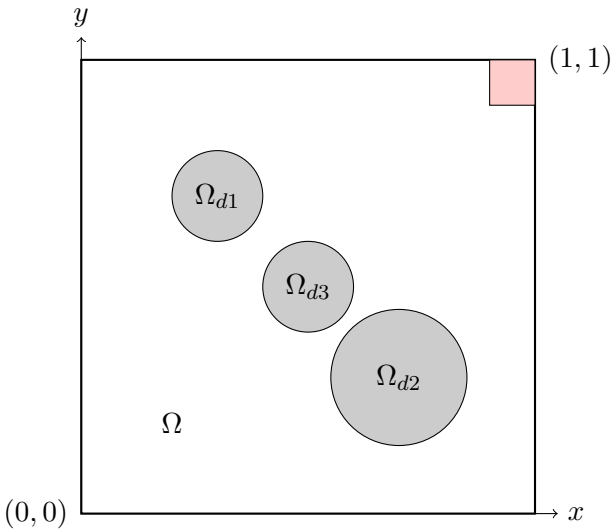


Figure 1: Sketch of the domain $\Omega$, with healthy domain $\Omega_h$ and diseased regions $\Omega_{d1}, \Omega_{d2}, \Omega_{d3}$. In red, we highlight the region where the initial stimulus is imposed.

Finally, consider the following physical parameters:

- $\Sigma_h = 9.5298 \times 10^{-4}$,
- $\Sigma_d \in \{10\Sigma_h, \Sigma_h, 0.1\Sigma_h\}$,
- $a = 18.515$,
- $f_t = 0.2383$,
- $f_r = 0$,
- $f_d = 1$,
- $T = 35$.

## 2 Finite Element Method (FEM)

1. Derive the IMEX time integration scheme for timestep $\Delta t$.
2. Write the weak formulation for time $t_n$.
3. Write the algebraic formulation of the associated FEM discretization.
4. Modify the provided `assembleDiffusion` to accept element-wise diffusivity. It should take as an additional input a vector of size number of elements
5. Write a MATLAB code that solves the problem stated at point 2. (Hint: the complete code should be around 50 lines.)
6. Adjust your code to set the diffusivity $\Sigma_d \in \{10\Sigma_h, \Sigma_h, 0.1\Sigma_h\}$ in $\Omega_d$. We consider a cell in $\Omega_d$ if its center is in falls in $\Omega_d$.
7. Run simulations with $\Sigma_d \in \{10\Sigma_h, \Sigma_h, 0.1\Sigma_h\}$, report:
   - activation time (when $u > f_t$)
   - whether the matrix is an M-matrix

- whether $u \in [0, 1]$

| $\Delta t$ | $n_e$ | Activation time | M-matrix? | $u \in [0, 1]$ |
|---|---|---|---|---|
| 0.1 | 64 | | | |
| 0.1 | 128 | | | |
| 0.1 | 256 | | | |
| 0.05 | 64 | | | |
| 0.05 | 128 | | | |
| 0.05 | 256 | | | |
| 0.025 | 64 | | | |
| 0.025 | 128 | | | |
| 0.025 | 256 | | | |

8. Generate a graphic visualization of the significant results.

## 3 Scientific Machine Learning Strategy

Solve the monodomain problem, using a SciML strategy between the ones discussed in class:

- PINNs,
- DeepRitz,
- DeepONet,
- Fourier Neural Operators,
- Hybrid methods.

It is advisable for different groups to explore different strategies, so coordination in this regard is recommended. To enhance accuracy, the use of extensions is also encouraged (such as employing pseudo-random collocation points, enforcing initial conditions via hard constraints, and incorporating adaptive strategies).

As a bonus task, in addition to the forward problem, consider also the solution of an inverse one. For example, given the computed activation at the boundary (for example with FEM), which is encoded by $u|_{\partial\Omega}$ for $t \in I$, recover the conductivity map $\Sigma$ in $\Omega$ that generated $u$.

## 4 Comparison

Design a comparative study between the two methods, following the best practices as described in [1]. In particular, discuss accuracy and the time to solution (given a target accuracy) of the two different approaches. The time used for training has to be disucssed in the analysis.

## 5 Presentation

The results of both strategies, along with their comparison, should be presented and critically discussed in an oral presentation. Each team member should speak for at least 10 minutes. A written report should also accompany the presentation. Please include clear and informative visualizations; bonus points will be awarded for sharp video output.

## References

[1] Nick McGreivy and Ammar 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, 2024.