First Insights into PINNs for Accelerating Immune Response Models

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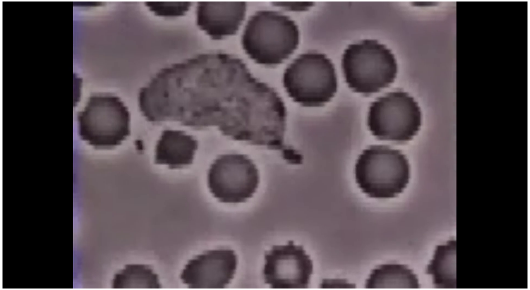
Mathematical model



The mathematical model used to describe the pathophysiology of edema formation was proposed in a previous work [1, 2]. This model includes the inflammatory part which describes the interaction between a pathogen and the human immune system.

The pathogen is modelled by:

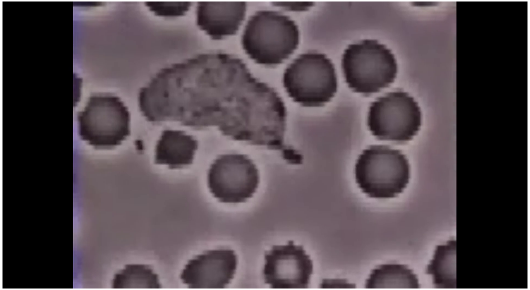
$$\begin{cases} \dfrac{d(\phi_f C_b)}{dt} = -r_b + q_b, \ t \in (0, 10] \\ C_b(0) = \delta_b, \end{cases} \tag{1}$$

where

$$q_b = c_b C_b \tag{2}$$

$$r_b = \lambda_{nb} C_n C_b \tag{3}$$

Mathematical model



The leukocyte differential model is represented by:

$$\begin{cases} \dfrac{d(\phi_f C_n)}{dt} = -r_n + q_n, \; t \in (0, 10] \\ C_b(0) = 0 \end{cases} \tag{4}$$

where

$$q_n = \gamma_n C_b (C_{n,max} - C_n) \tag{5}$$

$$r_n = \lambda_{bn} C_n C_b + \mu_n C_n \tag{6}$$

Mathematical model

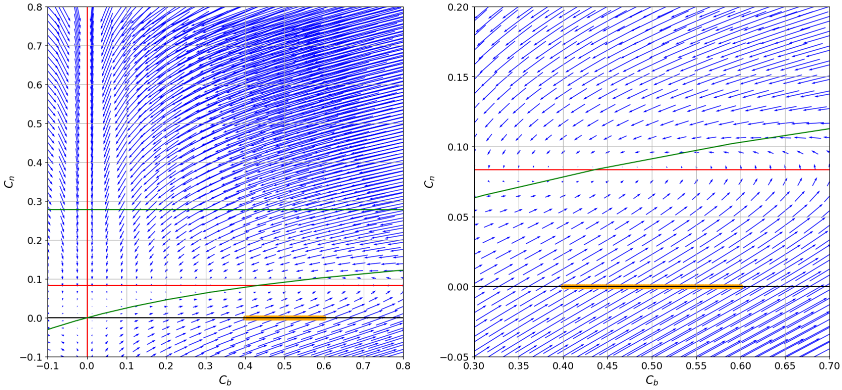


Figure 1: Phase plane for the system of equations.

Physics-Informed Neural Networks (PINN)

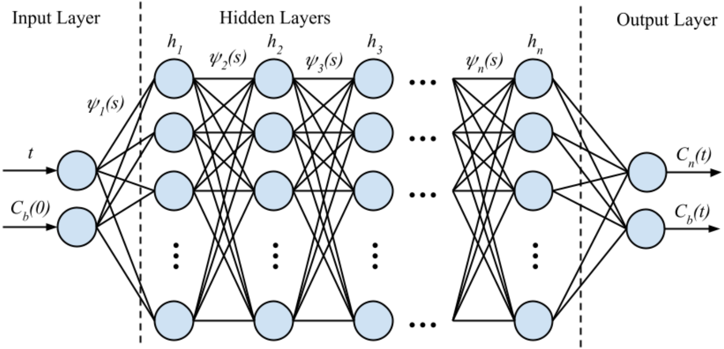


Figure 2: Neural Networks architecture.

Physics-Informed Neural Networks (PINN)

In alignment with the original formulation of Raissi et al. [3], we generally consider PDEs taking the form

$$\frac{\partial u}{\partial t} + \Phi[u] = 0,\ t \in [0,T],\ x \in \Omega \tag{7}$$

subject to the initial and boundary conditions

$$u(0,x) = g(x),\ x \in \Omega \tag{8}$$

$$\beta[u] = 0,\ t \in [0,T],\ x \in \partial\Omega \tag{9}$$

This formulation enables us to define the PDE residuals as follows:

$$\zeta_\theta(t,x) = \frac{\partial u_\theta}{\partial t}(t,x) + \Phi[u_\theta](t,x) \tag{10}$$

PINN architecture grid-search

Consequently, a physics-informed model is trained by minimising the following composite loss function:

$$L(\theta) = L_{ic}(\theta) + L_{bc}(\theta) + L_r(\theta) + L_{dt}(\theta) \tag{11}$$

$$L_{ic}(\theta) = \frac{1}{N_{ic}} \sum_{i=1}^{N_{ic}} \sqrt{(u_\theta(0, x_{ic}^i) - g(x_{ic}^i))^2} \tag{12}$$

$$L_{bc}(\theta) = \frac{1}{N_{bc}} \sum_{i=1}^{N_{bc}} \sqrt{\beta[u_\theta](t_{bc}^i, x_{bc}^i)^2} \tag{13}$$

$$L_r(\theta) = \frac{1}{N_r} \sum_{i=1}^{N_r} \sqrt{(\zeta_\theta(t_r^i, x_r^i)^2} \tag{14}$$

$$L_{dt}(\theta) = \frac{1}{N_{dt}} \sum_{i=1}^{N_{dt}} \sqrt{(u_\theta(t_{dt}^i, x_{dt}^i) - u(t_{dt}^i, x_{dt}^i))^2} \tag{15}$$

PINN architecture grid-search

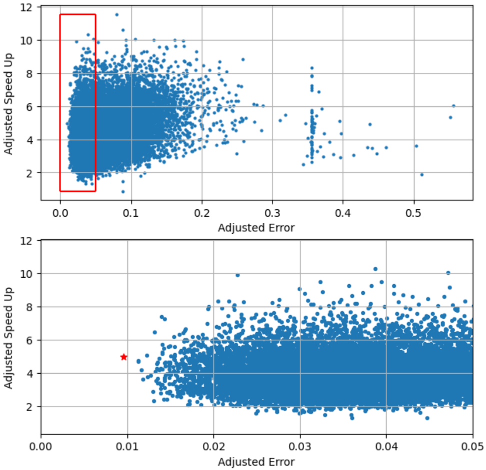


Figure 3: Adjusted error and speed up of the tested architectures.

The adjusted error and speedup are defined respectively by Equations 16 and 17.

$$E_{aj} = RMSE + RSE_{max} \tag{16}$$

$$S_{aj} = \langle S \rangle_{av} - \sigma_s \tag{17}$$

where *RMSE* stands for Root Mean Squared Error and *S* is the speed up.

PINN architecture grid-search

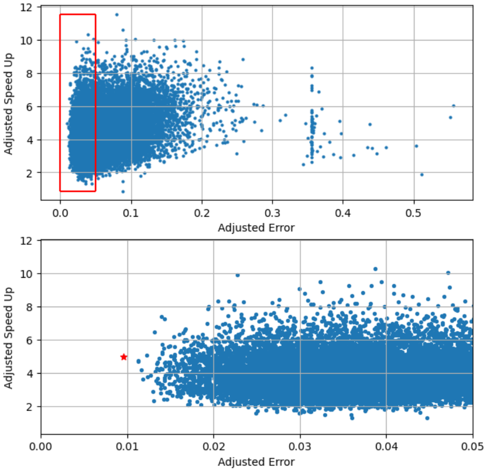


Figure 4: Adjusted error and speed up of the tested architectures.

Considering the 22465 architectures studied, the chosen one is composed by 4 hidden layers with 16, 8, 32, and 16 neurons respectively. Considering the PyTorch documentation, [4], the activation functions are defined as:

$$\psi_1 = \frac{sinh(x)}{cosh(x)} \tag{18}$$

$$\psi_2 = x \cdot \sigma(x) \tag{19}$$

$$\psi_3 = \psi_4 = max(0, x) \tag{20}$$

where x represents the values from the previous layers and $\sigma(x)$ is the logistic sigmoid function.

PINN and NN comparison

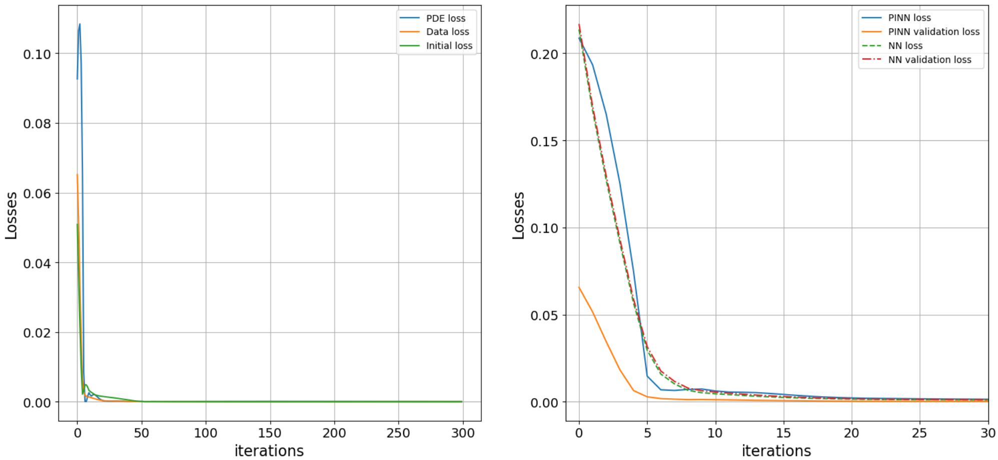


Figure 5: Learning curves for the NN and PINN training.

PINN and NN comparison

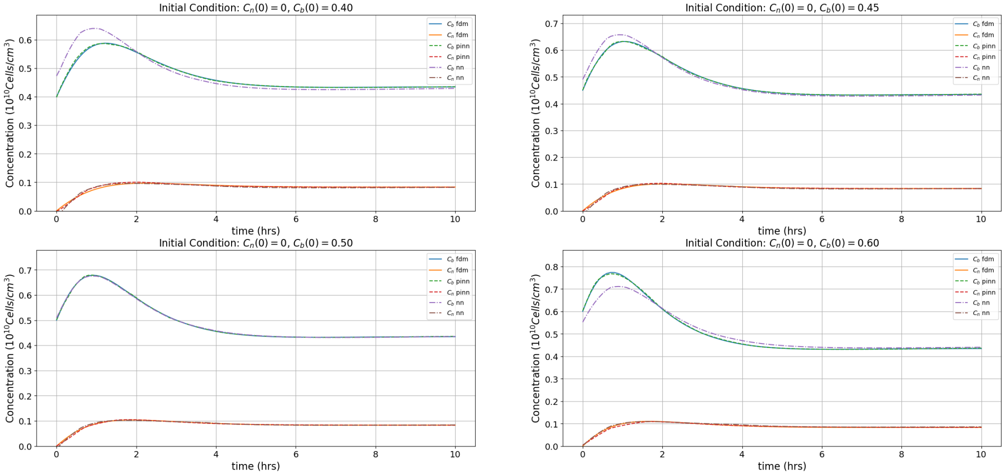


Figure 6: Concentration curves for the different computational models

PINN and NN comparison

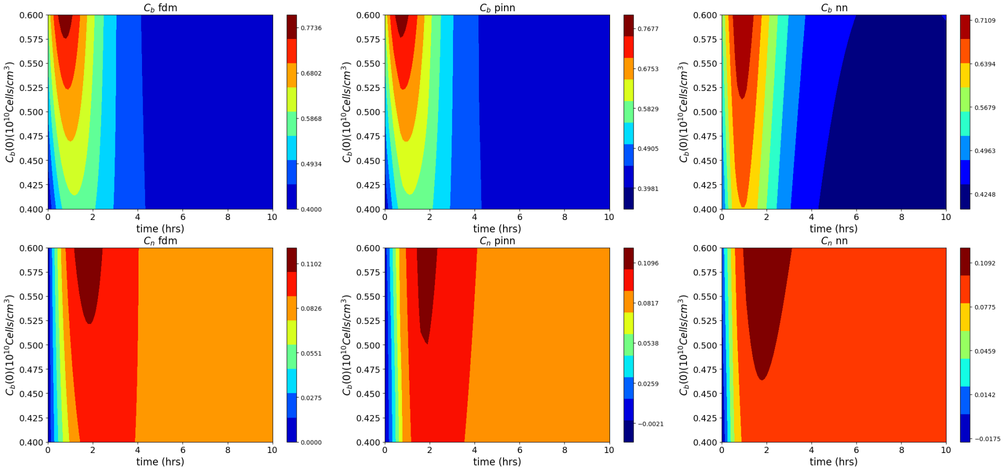


Figure 7: Concentration heat-map for the different computational models

PINN and NN comparison

Table 1 presents the results for the PINN and NN.

Table 1: Experimental results of PINN constrains implementation

Model	RMSE	RSE_{max}	Mean speed up	Speed up Standard Deviation
PINN	0.001530657	0.0080879815	5.93	0.97
NN	0.11618373	0.14936338		

[1] R. F. Reis, R. W. dos Santos, B. M. Rocha, and M. Lobosco, "On the mathematical modeling of inflammatory edema formation," *Computers & Mathematics with Applications*, vol. 78, no. 9, pp. 2994–3006, 2019.

[2] R. F. Reis, J. L. Fernandes, T. R. Schmal, B. M. Rocha, R. W. Dos Santos, and M. Lobosco, "A personalized computational model of edema formation in myocarditis based on long-axis biventricular mri images," *BMC bioinformatics*, vol. 20, pp. 1–11, 2019.

[3] M. Raissi, P. Perdikaris, and G. E. Karniadakis, "Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations," *Journal of Computational physics*, vol. 378, pp. 686–707, 2019.

[4] *PyTorch documentation*, PyTorch Foundation, 2023. [Online]. Available: https://pytorch.org/docs/stable/index.html

Thank You