

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 [49]. This model includes the inflammatory part which describes the interaction between a pathogen and the human immune system.

The pathogen is modelled by:

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

where

$$q_b = c_b C_b \quad (2)$$

$$r_b = \lambda_{nb} C_n C_b \quad (3)$$

Mathematical model

The leukocyte differential model is represented by:

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

where

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

$$r_b = \lambda_{bn} C_n C_b + \mu_n C_n \quad (6)$$

Mathematical model

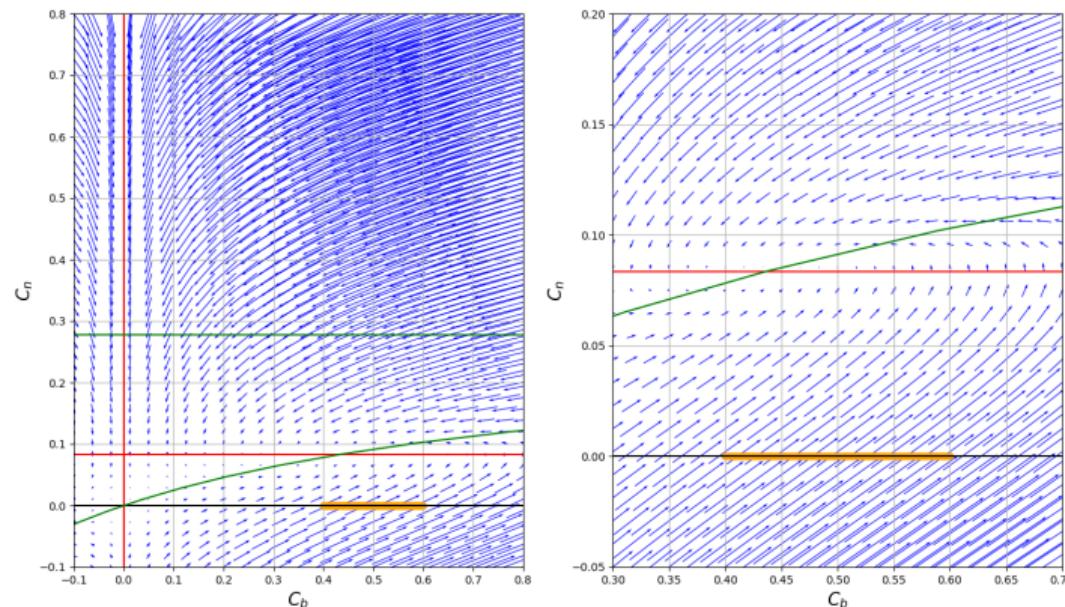


Figure 1: Phase plane for the system of equations.

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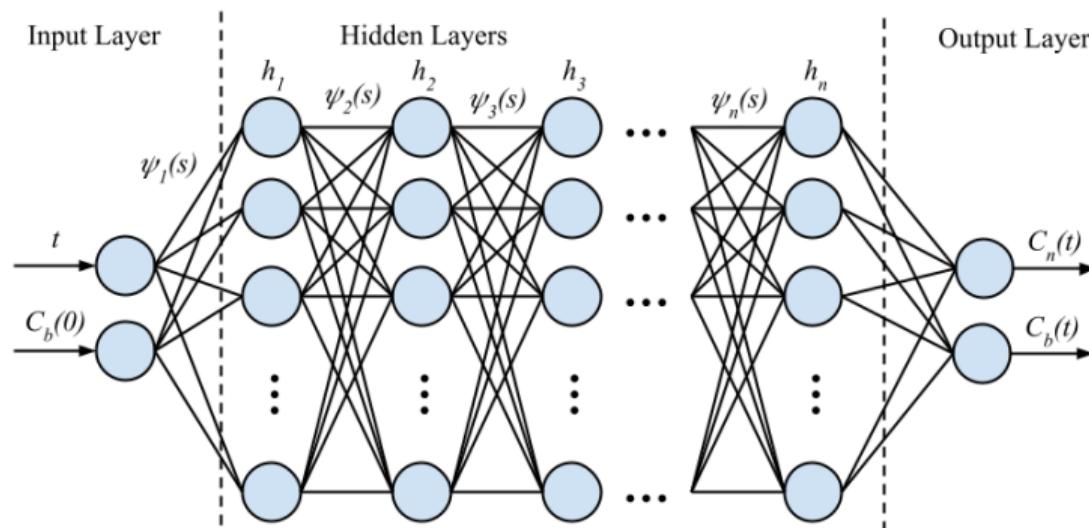


Figure 2: Neural Networks architecture.

Physics-Informed Neural Networks (PINN)

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

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

subject to the initial and boundary conditions

$$u(0, x) = g(x), \quad x \in \Omega \quad (8)$$

$$\beta[u] = 0, \quad t \in [0, T], \quad x \in \partial\Omega \quad (9)$$

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

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

PINN architecture grid-search

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

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

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

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

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

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

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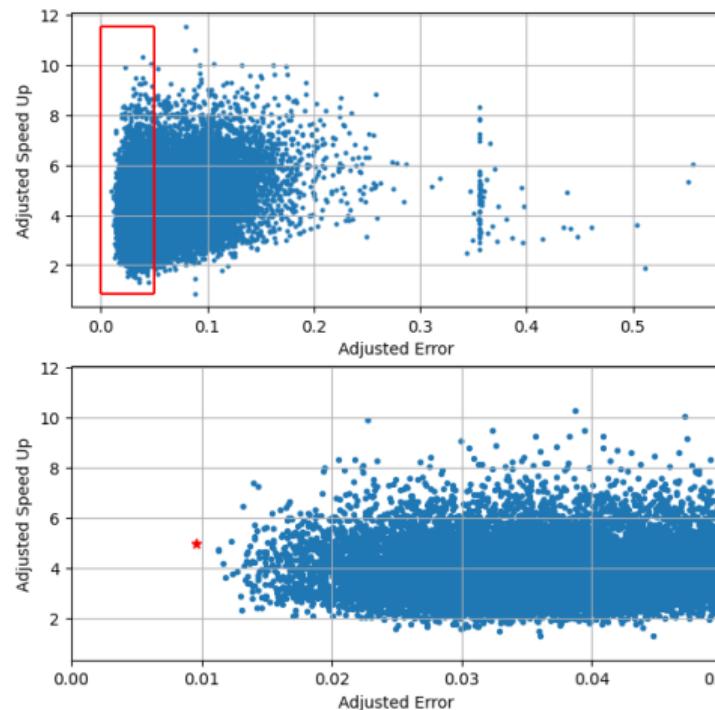


Figure 3: Adjusted error and speed up of the tested architectures.

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

$$E_{aj} = RMSE + RSE_{max} \quad (16)$$

$$S_{aj} = \langle S \rangle_{av} - \sigma_s \quad (17)$$

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

PINN architecture grid-search

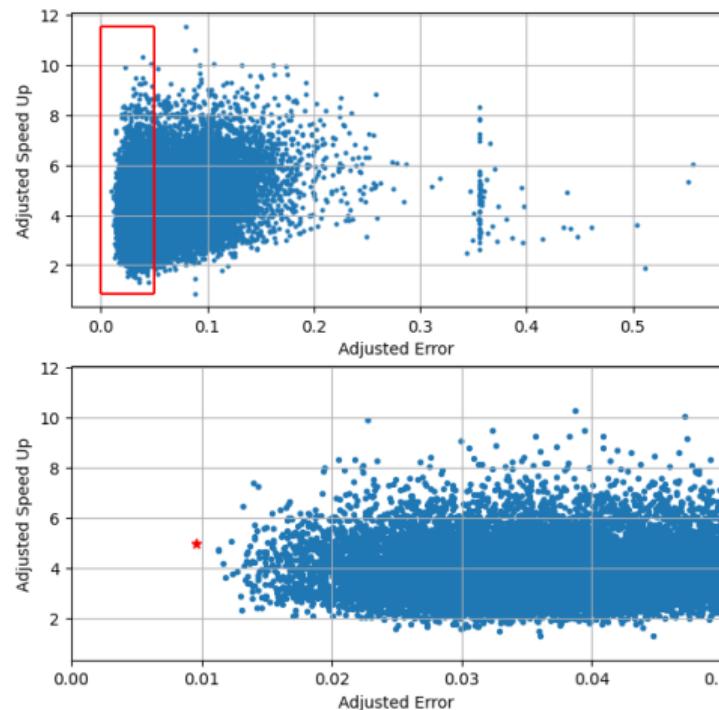


Figure 4: Adjusted error and speed up of the tested architectures.

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, [1], the activation functions are defined as:

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

$$\psi_2 = x \cdot \sigma(x) \quad (19)$$

$$\psi_3 = \psi_4 = \max(0, x) \quad (20)$$

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

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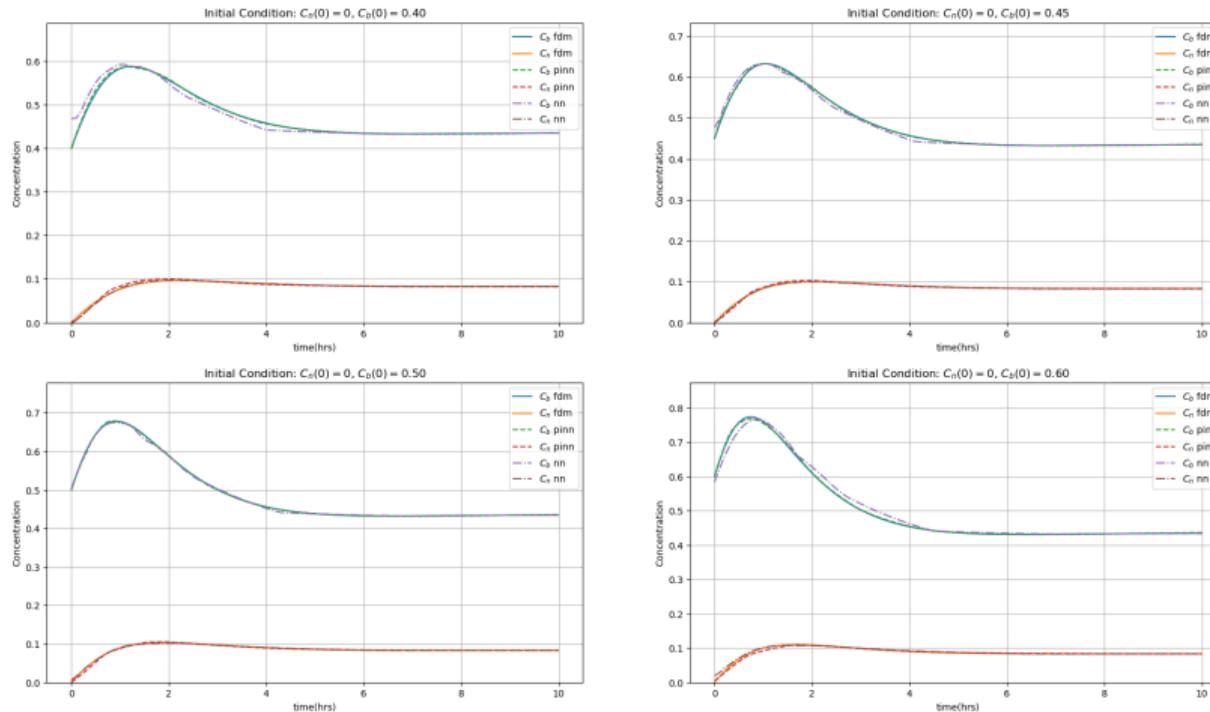


Figure 5: Concentration curves for the different computational models

PINN and NN comparison

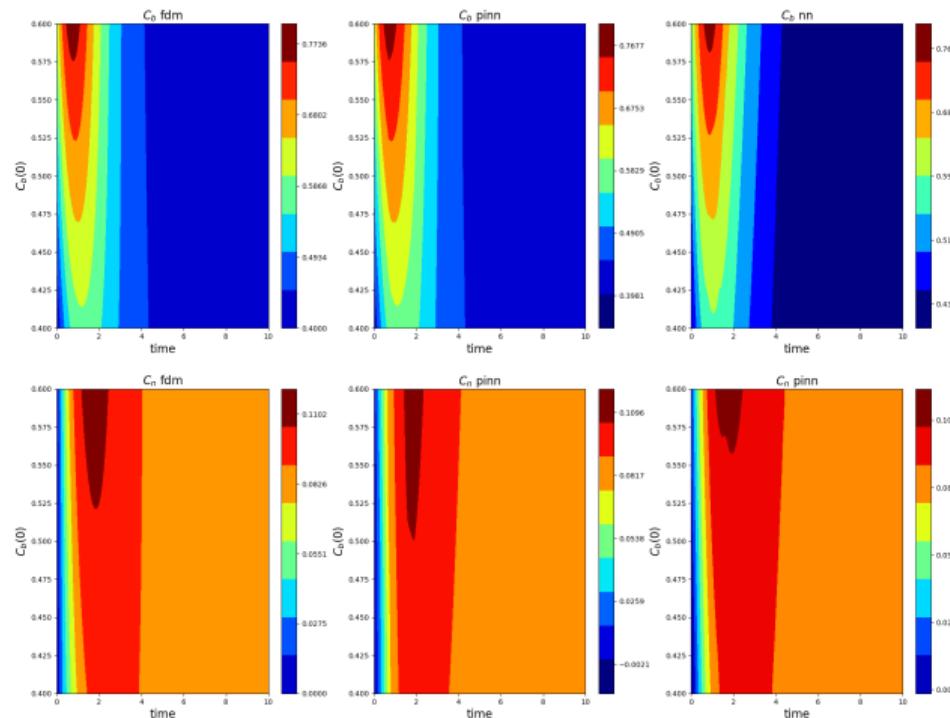


Figure 6: Concentration heat-map for the different computational models

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		
NN	0.1530657	0.80879815	5.9304240	0.96761669

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

Thank You