

# PHYSICAL AND FINANCIAL INFORMED NEURAL NETWORKS FOR THE SOLUTION OF PARTIAL DIFERENTIAL EQUATIONS



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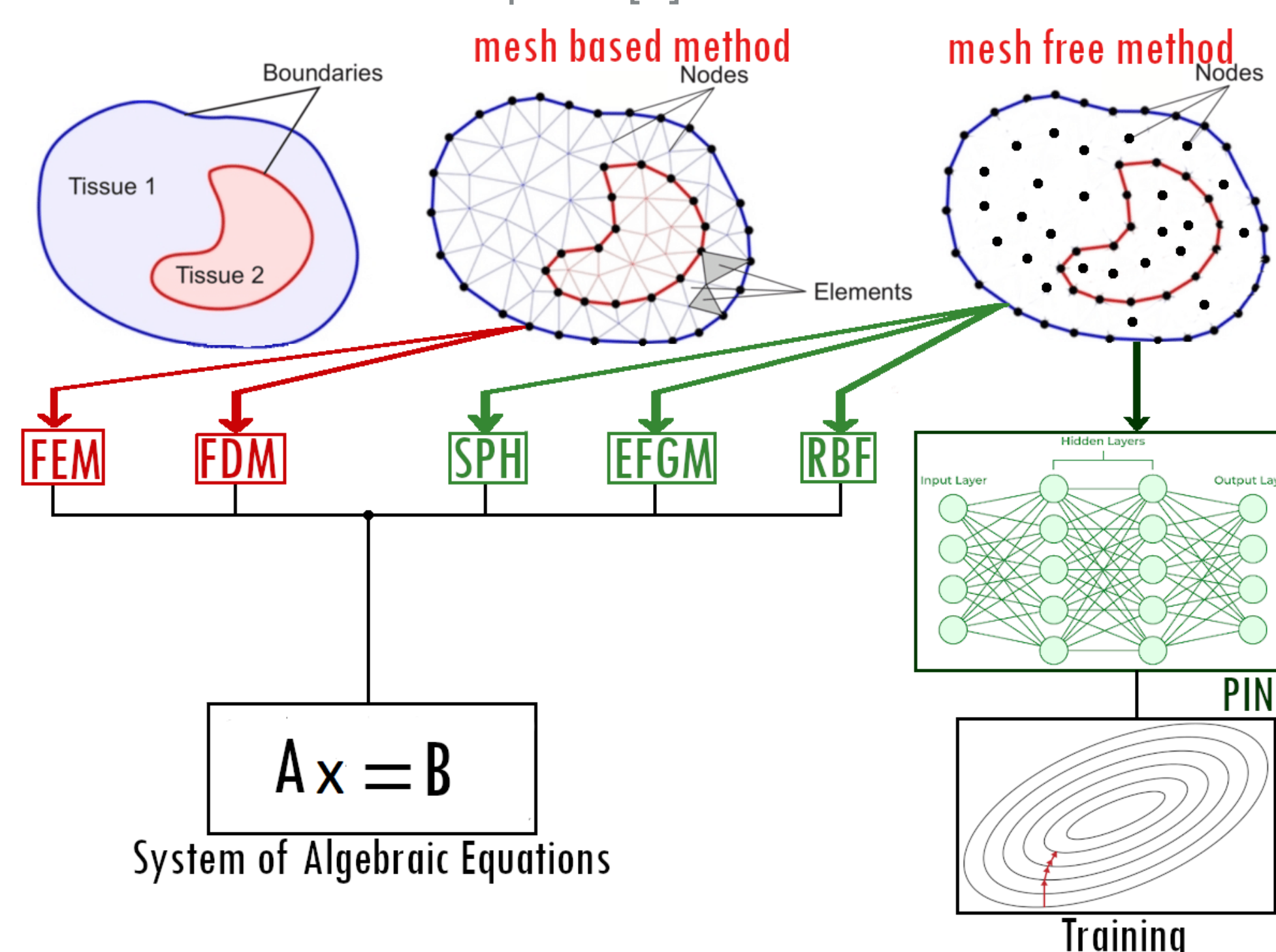
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## ABSTRACT

This work presents the application of neural networks for solving partial differential equations (PDEs) using classical approaches proposed by Raissi and Lagaris, including sub-network and sub-domain methods introduced by Jagtap that leverage parallel computing. However, these methods exhibit causality issues in high-dimensional settings. Consequently, this work proposes a temporal discretization-based Neural Networks solution and applies it to the Glioblastoma Proliferation-Invasion Model.

## INTRODUCTION

Mesh-based or mesh-free numerical methods are widely used for solving PDEs. Neural Networks are mesh-free numerical option [4].



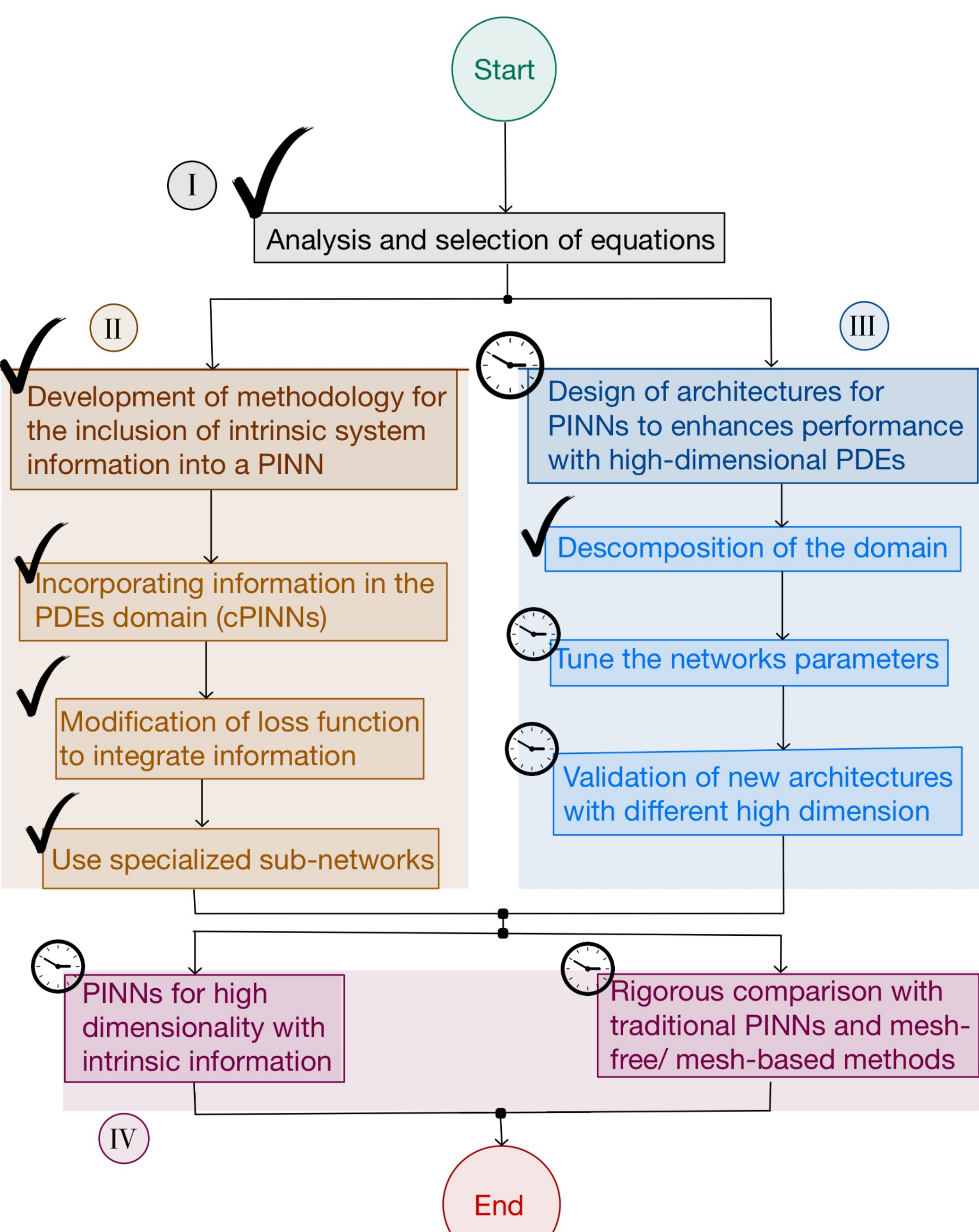
## PROBLEM STATEMENT

Given a linear, homogeneous, second-order, evolutionary physical, biological or financial differential equation of high dimension. Find a neural network  $u_\theta : \mathbb{R}^n \rightarrow \mathbb{R}^m$  and a loss function  $\mathcal{L}(\mathbf{x}, \theta, U)$ , where  $\theta$  represents the network parameters and  $U$  are the conserved quantities of the system. The pair  $(u_\theta, \mathcal{L})$  should demonstrate performance close to that of traditional methods and mesh-free methods.

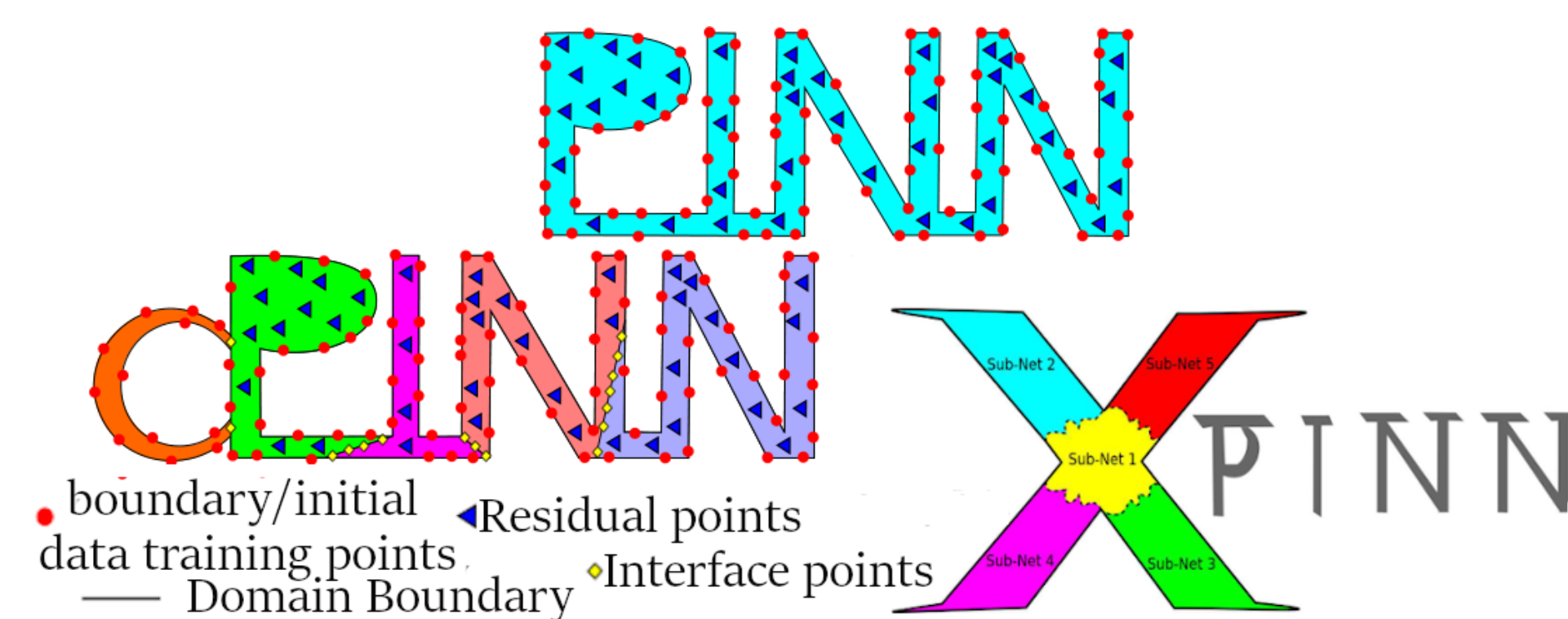
## OBJECTIVE

Design PINNs with intrinsic information for solving second-order, evolutionary, homogeneous, and high-dimensional PDEs from physical, biological and financial problems, achieving performance similar to traditional mesh-based and mesh-free methods.

## METHODOLOGY



## PREVIOUS PERIOD RESULTS

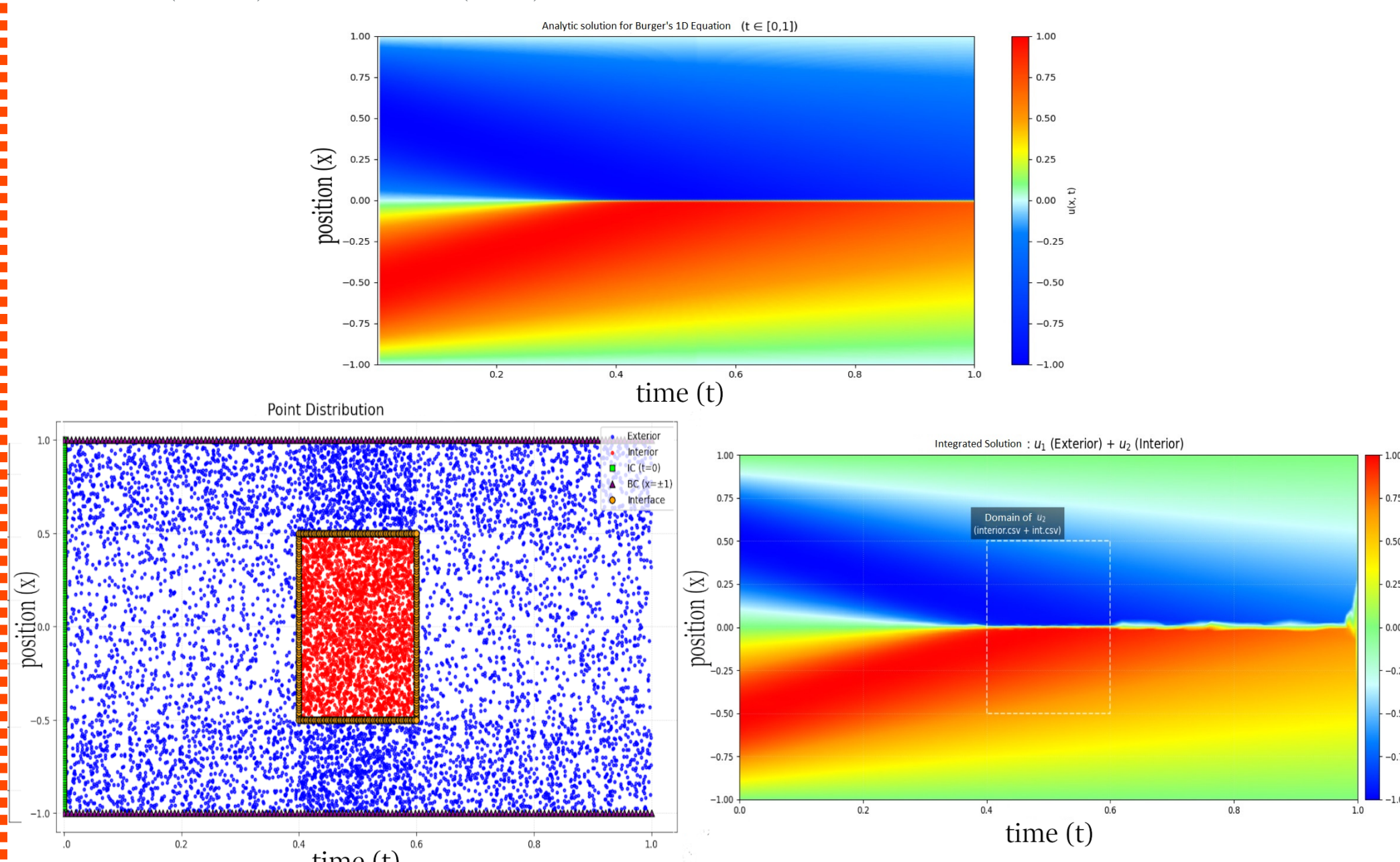


### Neural Network's approach for PDE solutions

Approach	Loss Function
Lagaris	$u_t = A(\mathbf{x}) + B(\mathbf{x})u_\theta \approx u$ $\mathcal{L} = \sum  D^n[u_t] - f(\mathbf{x}, u_t) ^2$
Raissi	$u_\theta \approx u;$ $\mathcal{L} = \sum  u_\theta(\mathbf{x}_{pde}) - F(\mathbf{x}_{pde}) ^2 + \sum  u_\theta(\mathbf{x}_{bc}) - \partial\omega ^2$
cPINN	$\mathcal{L}^p = \mathcal{L}_{pde}^p + \mathcal{L}_{bc}^p + \mathcal{L}_{av}^p + \mathcal{L}_{flux}^p$
xPINN	$\mathcal{L}^p = \mathcal{L}_{pde}^p + \mathcal{L}_{bc}^p + \mathcal{L}_{av}^p + \mathcal{L}_{int}^p$

### xPINN IMPLEMENTATION: 1D BURGER EQUATION

$\frac{\partial u(x,t)}{\partial t} + u(x,t)\frac{\partial u(x,t)}{\partial x} = \nu \frac{\partial^2 u(x,t)}{\partial x^2}$ ,  $\nu = \frac{0.01}{\pi}$   
with  $x \in [-1, 1]$ ,  $t > 0$ , boundary conditions  $u(-1, t) = u(1, t) = 0$ , and initial condition  $u(x, 0) = -\sin(\pi x)$ .



## Current Results

### CAUSALITY PROBLEM FOR PINNS

The minimization of loss function  $\mathcal{L}_{pde}$  should be based on the correct prediction of causal continuity of the network  $u$ , but usual loss function minimize  $\mathcal{L}_{pde}$  for all points simultaneously, even if prediction at  $t_i$  are incorrect:

$$\mathcal{L}_{pde} = \frac{1}{N_x} \sum_{j=1}^{N_x} \left| \frac{\partial u_\theta}{\partial t}(t, x_j) + \mathcal{N}[u_\theta](t, x_j) \right|^2$$

$$= \frac{1}{N_x N_t} \sum_{i=1}^{N_t} \sum_{j=1}^{N_x} \left| \frac{\partial u_\theta}{\partial t}(t_i, x_j) + \mathcal{N}[u_\theta](t_i, x_j) \right|^2$$

Discretizing using the forward Euler scheme. For any  $1 < i < N_t - 1$ :

$$\mathcal{L}_r(t_i, \theta) \approx \frac{1}{N_x} \sum_{j=1}^{N_x} \left| \frac{u_\theta(t_i, x_j) - u_\theta(t_{i-1}, x_j)}{\Delta t} + \mathcal{N}[u_\theta](t_i, x_j) \right|^2$$

$$\approx \frac{1}{t^2 \Omega} \int_{\Omega} |u_\theta(t_i, x) - u_\theta(t_{i-1}, x) + \Delta t \mathcal{N}[u_\theta](t_i, x)|^2 dx$$

### GLIOBLASTOMA PROLIFERATION-INVASION MODEL

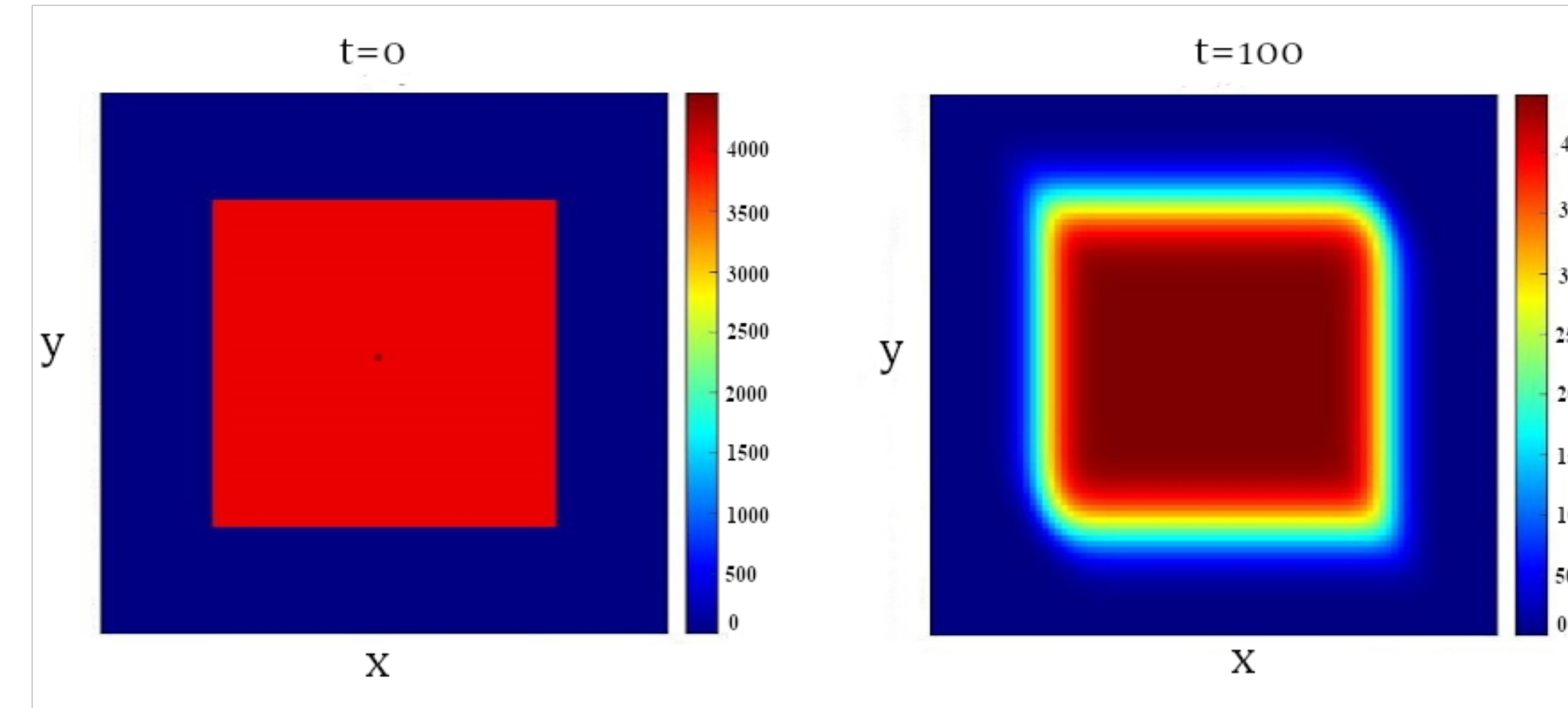
$$\frac{\partial C(x, y, t)}{\partial t} = D \left( \frac{\partial^2 C(x, y, t)}{\partial x^2} + \frac{\partial^2 C(x, y, t)}{\partial y^2} \right) + rC(x, y, t) \left( 1 - \frac{C(x, y, t)}{k} \right)$$

with  $x \in [0, 200]$ ,  $y \in [0, 200]$ ,  $t \in [0, 100]$ ,  $D = 0.3$ ,  $r = 0.002$ , and  $k = 1000$ .

Boundary conditions:  $C(0, y, t) = C(200, y, t) = C(x, 0, t) = C(x, 200, t) = 0$

Initial condition:  $C(x, y, 0) = 4000$  for  $(x, y) \in [40, 160] \times [40, 160]$ .

### CRANK-NICOLSON NUMERICAL SOLUTION

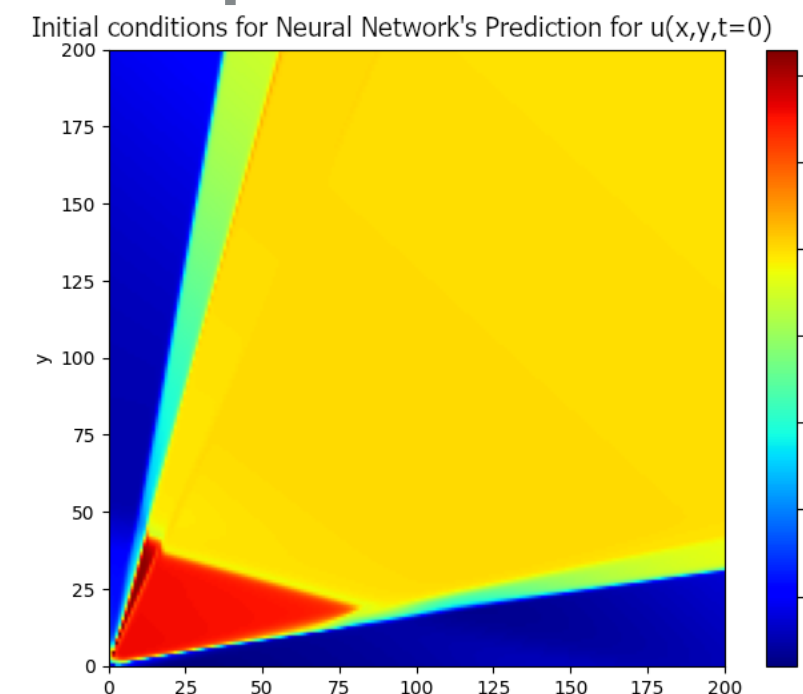


### PINN AND xPINN CAUSAL PROBLEMS FOR INITIAL CONDITIONS

#### Raissi Approach

- pde points  $(x, y, t)$  with  $x \in (0, 200)$ ,  $y \in (0, 200)$  and  $t \in (0, 100)$
- bc points  $(0, y, t)$ ,  $(200, y, t)$ ,  $(x, 0, t)$ ,  $(x, 200, t)$ , with  $x \in [0, 200]$  and  $y \in [0, 200]$
- ic point  $(x, y, 0)$  with  $40 < x < 160$  and  $40 < y < 160$
- Loss function:  
 $\mathcal{L} = \sum |\mathcal{F}[u_\theta(\mathbf{x}_{pde})]|^2 + \sum |u_\theta(\mathbf{x}_{bc})|^2 + \sum |u_\theta(\mathbf{x}_{ic}) - 1|^2$

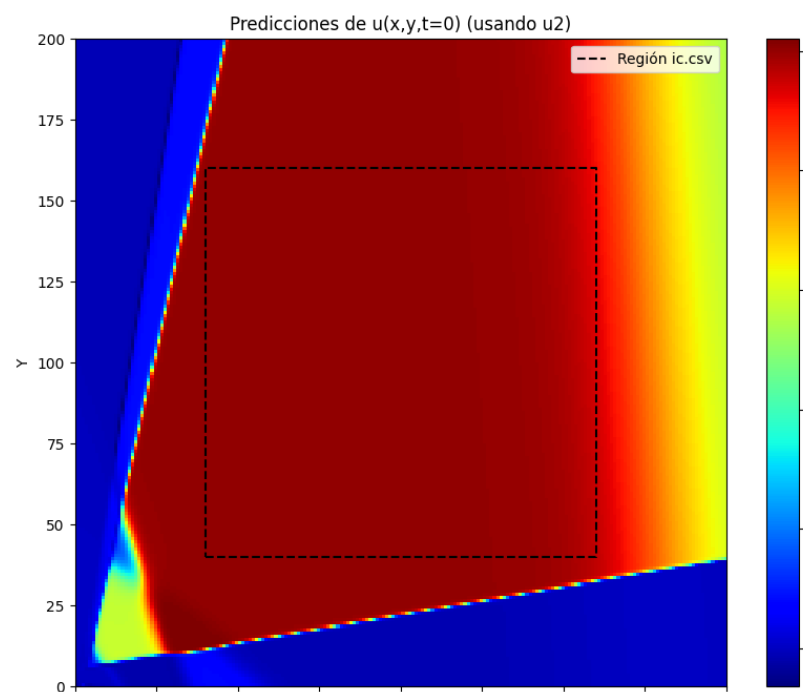
#### Implementation:



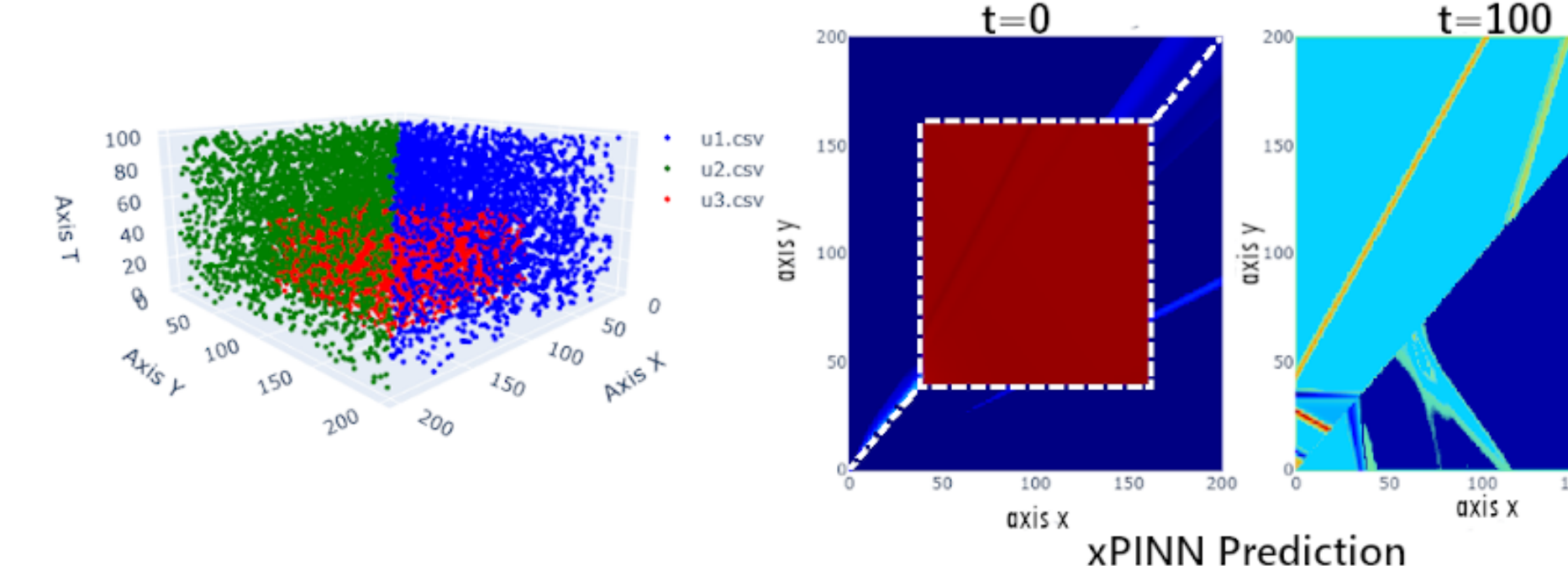
#### xPINN implementation:

##### Option 1

- Interior network's domain:  $x \in [0, 200]$ ,  $y \in [0, 200]$ ,  $t \in [0, 5]$
- Exterior networks domain:  $x \in [0, 200]$ ,  $y \in [0, 200]$ ,  $t \in (5, 100]$



##### Option 2:



### TIME STEPPING FOR CAUSALITY SOLUTION

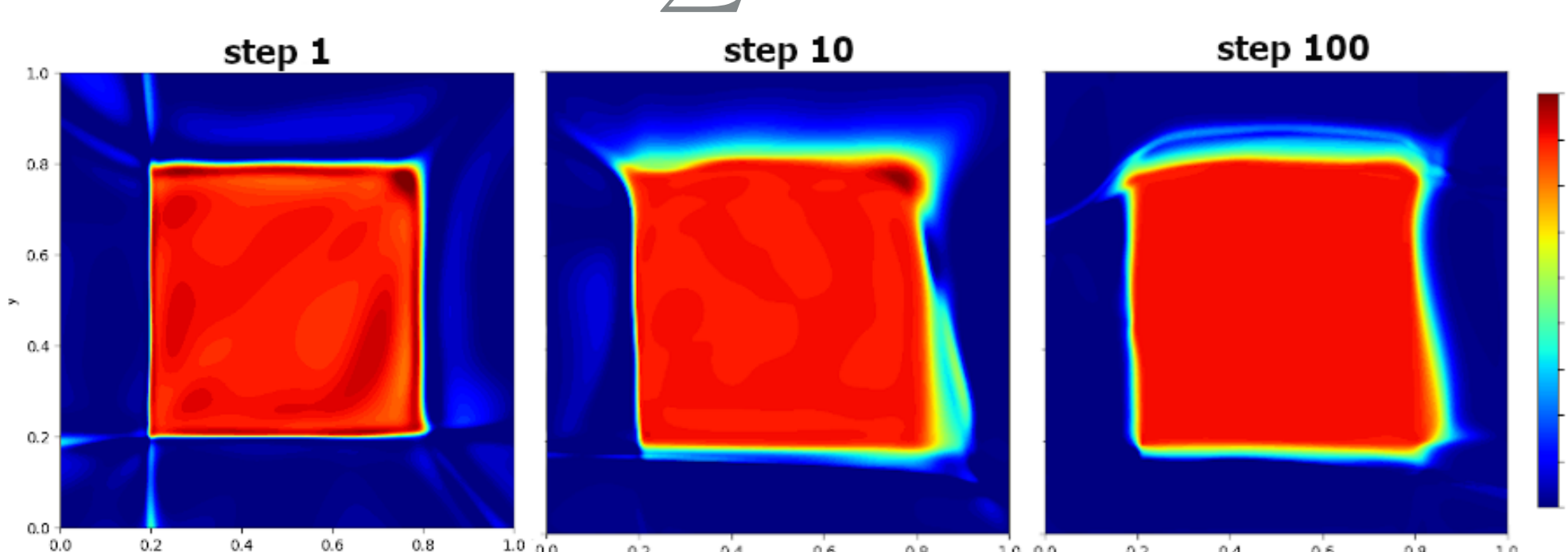
Time discretization, normalization and adimensionalization for Glioblastoma proliferation - Invasion model:

$$\mathcal{F}[u] \equiv u^i - u^{i-1} - \alpha d\hat{\tau} \left( \frac{\partial^2 u^{i-1}}{\partial \hat{x}^2} + \frac{\partial^2 u^{i-1}}{\partial \hat{y}^2} \right) - d\hat{\tau} u^{i-1} (1 - u^{i-1})$$

with  $\alpha = 0.00375$ ,  $\hat{x} \in [0, 1]$ ,  $\hat{y} \in [0, 1]$ ,  $\hat{\tau} = rt$ ,  $d\hat{\tau} = 0.0002$

For each time step, the Time Stepping loss function is:

$$\mathcal{L} = \sum |\mathcal{F}[u]|^2 + \mathcal{L}_{bc}$$



## SCHEDULE

ACTIVITIES	2023-2	2024-1	2024-2	2025-1	2025-2	2026-1	2026-2	2027-1
1- Thesis proposal writing	✓							
2- Thesis proposal defense		✓						
3- Review of the state of the art	✓							
4- Analysis and selection of equations	✓							
5- Incorporating information in the PDEs domain (cPINNs)	✓							
6- Modification of loss function to integrate information	✓							
7- Use specialized sub-networks	✓							
8- Design of new architectures to address high dimensionality of PDEs	✓							
9- Decomposition techniques of the domain	✓							
10- Tune the networks parameters	✓							
11- Validation of new architectures with different high dimensions and implementation of intrinsic information	✓							
12- Rigorous comparison of the performance of the new PINNs with mesh-based and mesh-free algorithms	✓							
13- Rigorous comparison of the performance of the new PINNs with traditional PINNs	✓							
14- Submission of article to scientist journal (ICR) and International Conference Article	✓							
15- Thesis writing	✓							
16- Administrative process for thesis defense	✓							

## REFERENCES

- [1] Silan Wang, Shyam Sankaran, and Paris Perdikaris, "Respecting Causality for Training Physics-Informed Neural Networks", arXiv preprint, 2024. Disponible en: <https://www.scienceirect.com/science/article/pii/S0045782524000696>.
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- [3] Ray Zirui Zhang, Ivan Ezhov, Michal Balcerak, Andy Zhu, Benedikt Wiestler, Björn Menze, and John S. Lowengrub, "Personalized predictions of Glioblastoma infiltration: Mathematical models, Physics-Informed Neural Networks and multimodal scans." Medical Image Analysis, vol. 101, 2025, Art. no. 103423. <https://doi.org/10.1016/j.media.2024.103423>
- [4] LuLu et al. "DeepXDE: A deep learning library for solving differential equations" In: SIAM review 63 (2021), pp. 208–228.