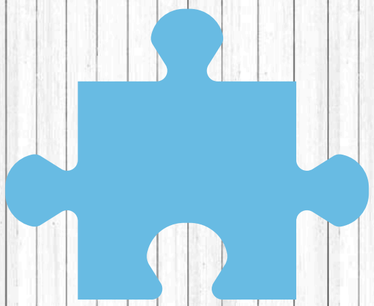
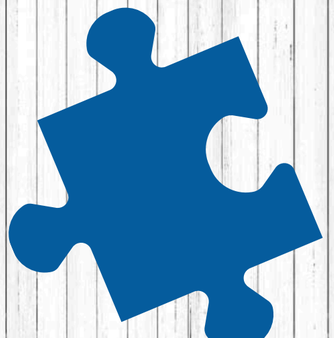
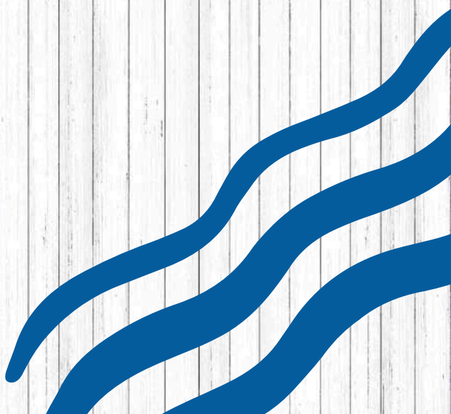
PINN for solving PDE

Quick Assessment







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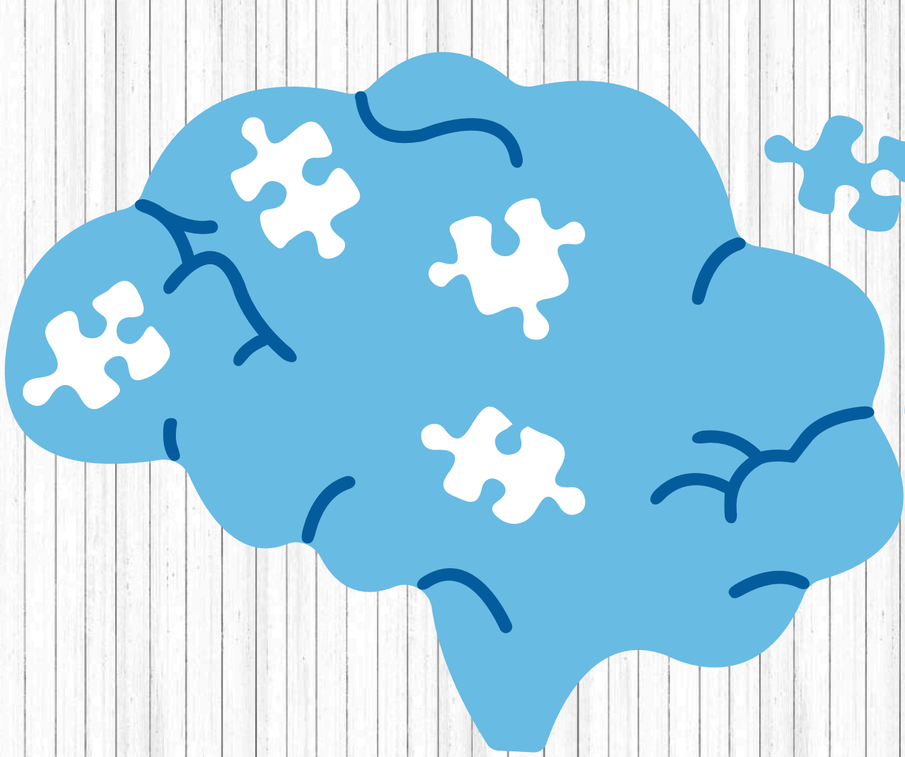
introduction



what is Alzheimer disease?

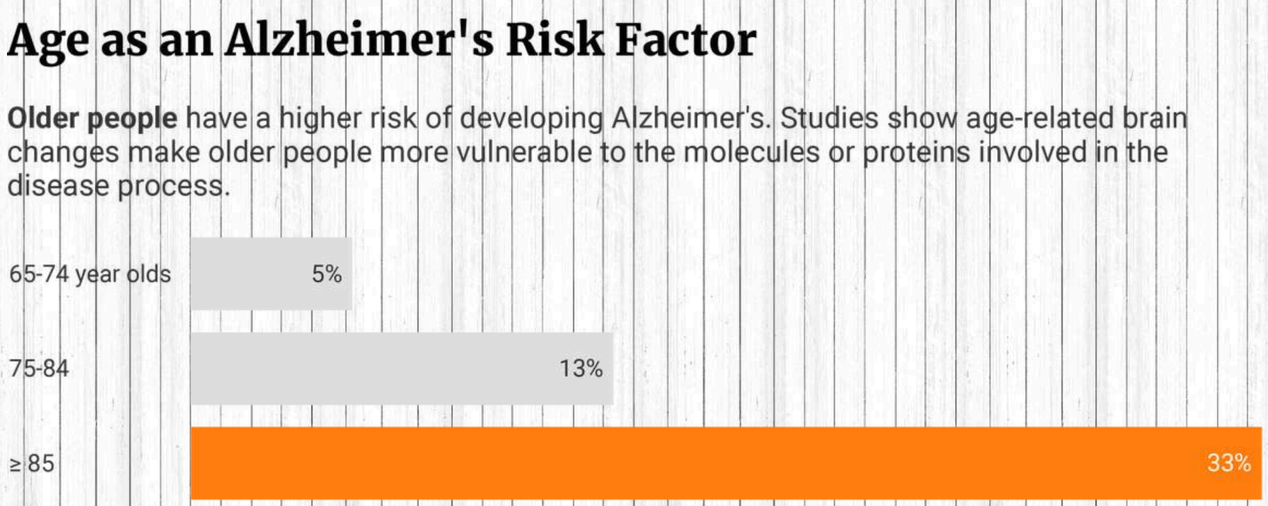
affecting over 55 million people worldwide and accounting for 60-80% of all dementia cases

What causes Alzheimer's ?

- Tau Protein: Supports brain cell structure. In Alzheimer's, it forms tangles that disrupt cell function.

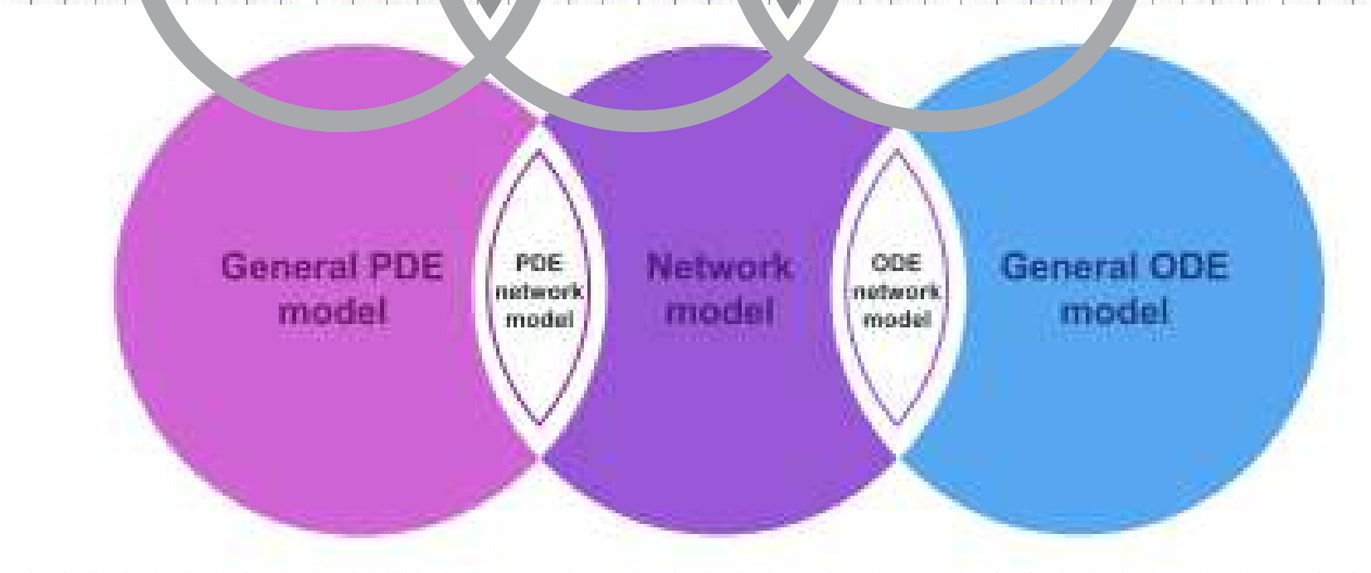
- Beta-Amyloid: Small protein pieces that clump together between brain cells, forming plaques that interfere with communication.

“How Does Age Influence Alzheimer’s Disease Risk?“



Literature review

- The first mathematical model for Alzheimer's disease was proposed in 2001
- In 2013, a significant breakthrough applied PDE models to study the progression of Alzheimer's disease .



Problem definition

- Alzheimer's disease (AD) involves the accumulation of misfolded tau proteins in the brain.

How can we model this process mathematically?

The evolution of tau protein concentration, c(t, x), over time and space is described by a reaction-diffusion equation (PDE):

$$\frac{\partial C}{\partial t} = \nabla \cdot (D \cdot \nabla C) + f(C)$$

“Discretizing Reaction-Diffusion on Brain Networks“

To reduce the complexity, the continuous-space PDE is converted into a discrete ODE system.

We discretize the reaction-diffusion model on a weighted graph G:

- where each node i represents a brain region
- Represent axonal connections between brain regions.

This gives a discretized equation for the change in tau protein concentration ci at each region over time:

$$\frac{dc_i}{dt} = h_i^k(t, C) + f(c_i) \rightarrow i = 1, \dots, N$$

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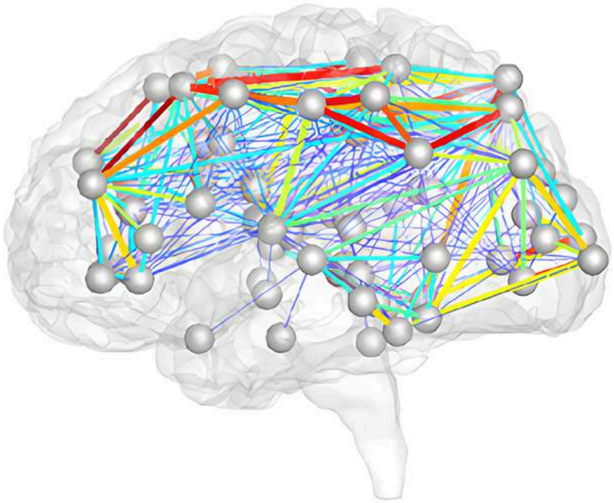


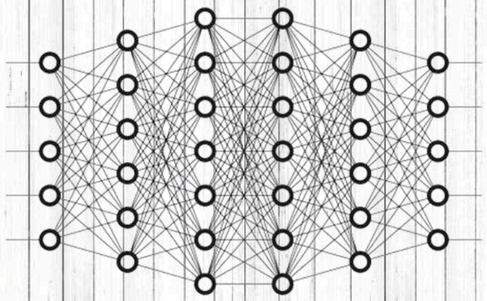
Physics-Informed Neural Network

PINNs are a class of physics-informed machine learning methods that seamlessly integrate physics knowledge with data. It used for solving PDE/ODE equation

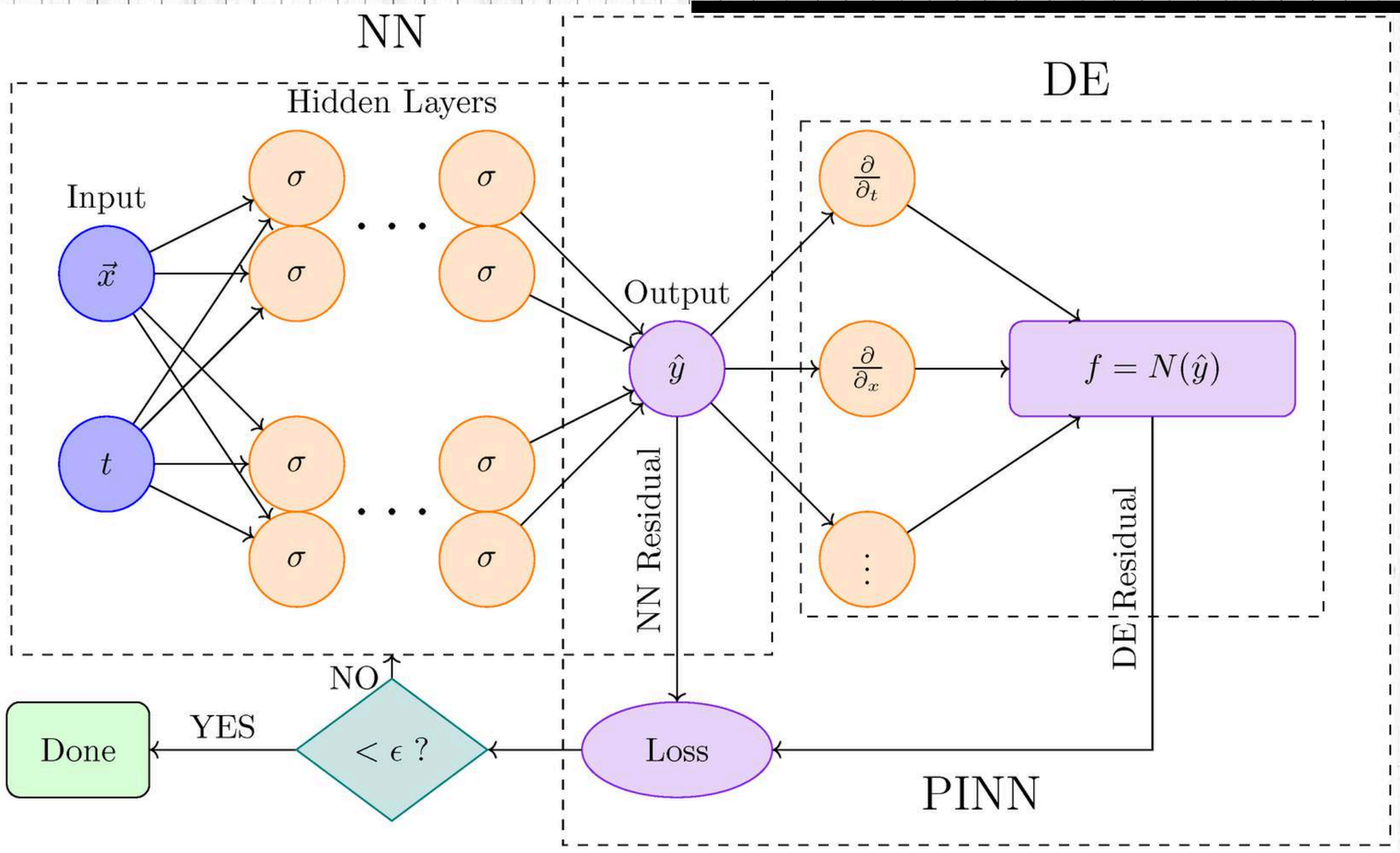
$$\partial c / \partial t = \nabla \cdot (D \cdot \nabla c) + \cancel{f(c)}$$

Replace

NN



Physics-Informed Neural Network



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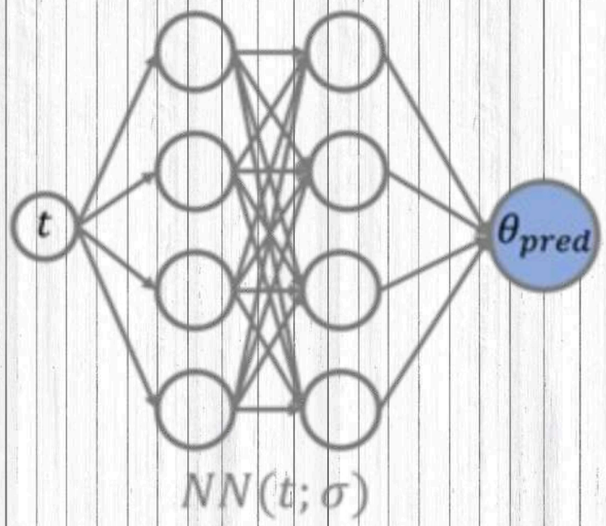
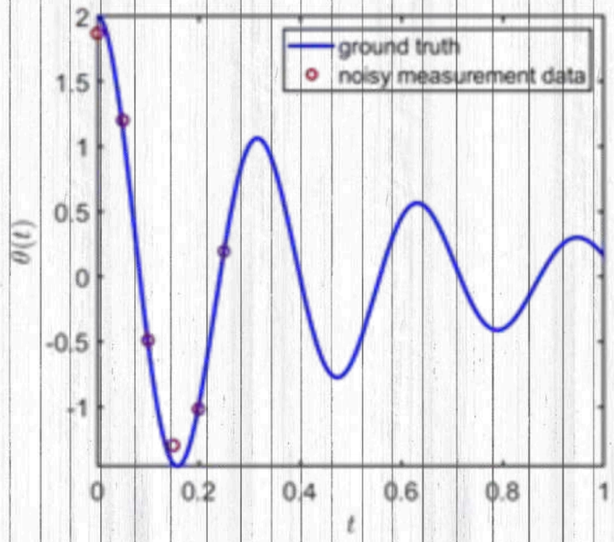
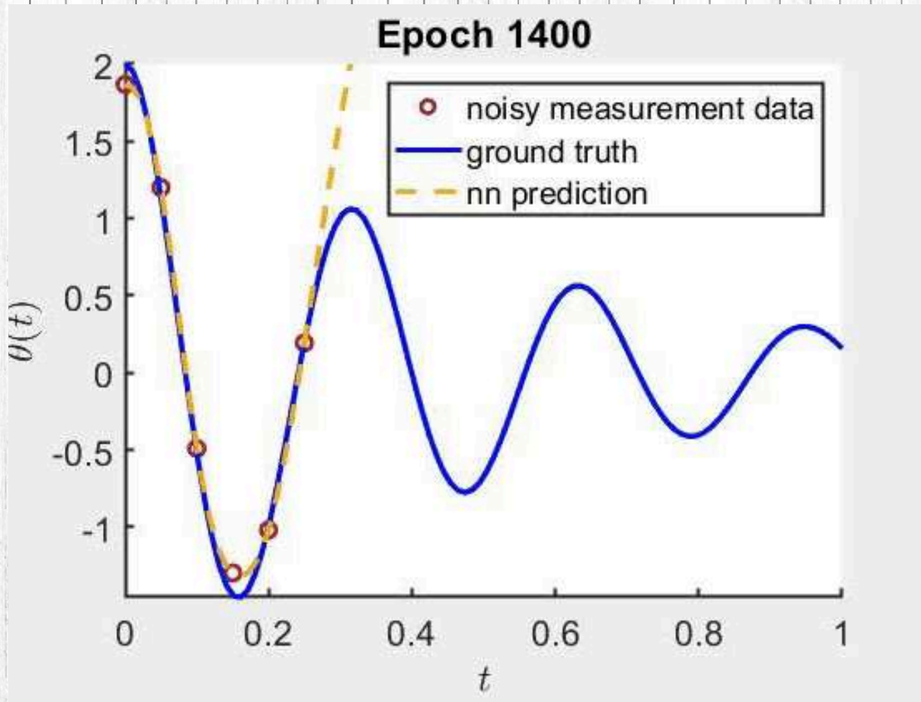


$$\theta''(t) + 2\beta\theta'(t) + \omega_0^2\theta(t) = 0$$



$$\min_{\sigma} \frac{1}{N}\sum_{i=1}^{N} \left|\theta_{pred}(t_i;\sigma) - \theta_{meas}(t_i)\right|^2$$



Physics-Informed Neural Network

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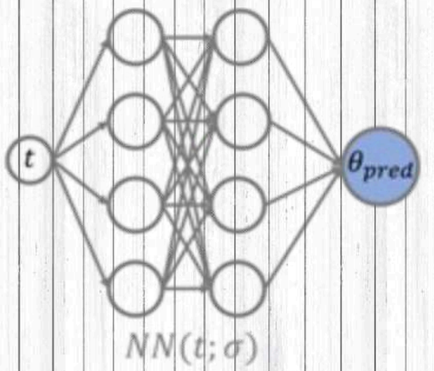

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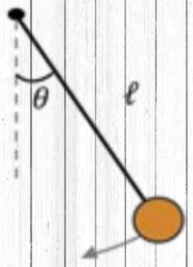

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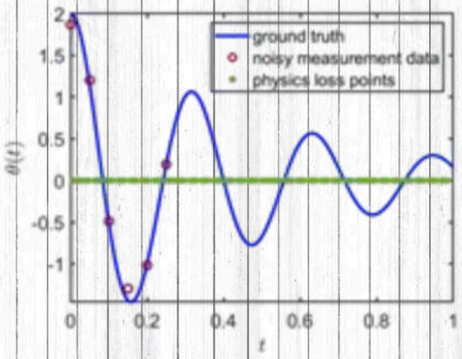
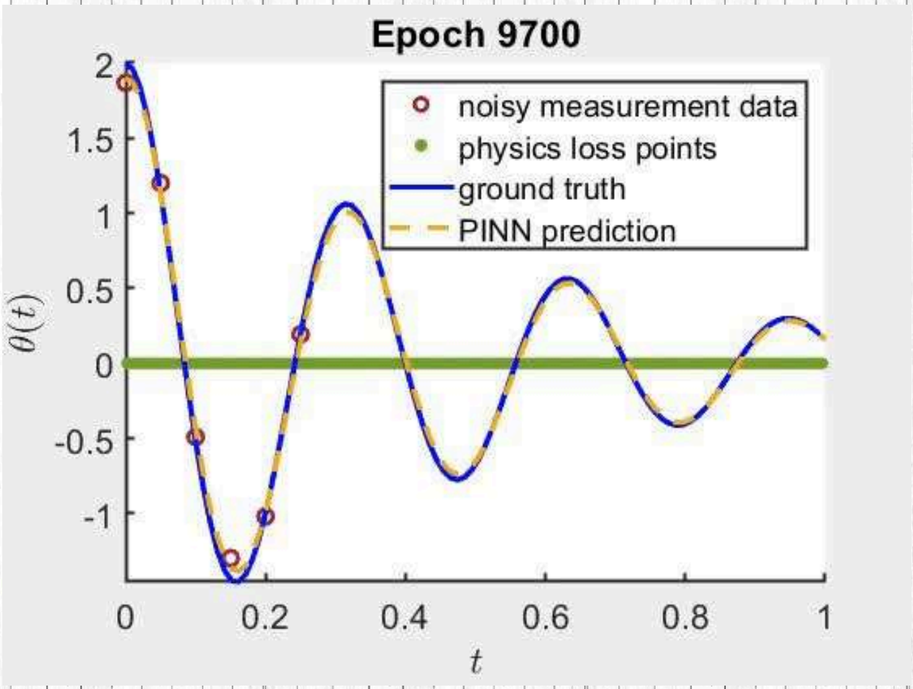


$$\min_{\sigma} \frac{1}{N}\sum_{i=1}^{N}\left|\theta_{pred}(t_i;\sigma) - \theta_{meas}(t_i)\right|^2$$

$$+\frac{1}{M}\sum_{j=1}^{M}\left|\frac{\partial^2}{\partial t^2}\theta_{pred}(t_j;\sigma) + 2\beta\frac{\partial}{\partial t}\theta_{pred}(t_j;\sigma) + \omega_0^2\theta_{pred}(t_j;\sigma)\right|^2$$



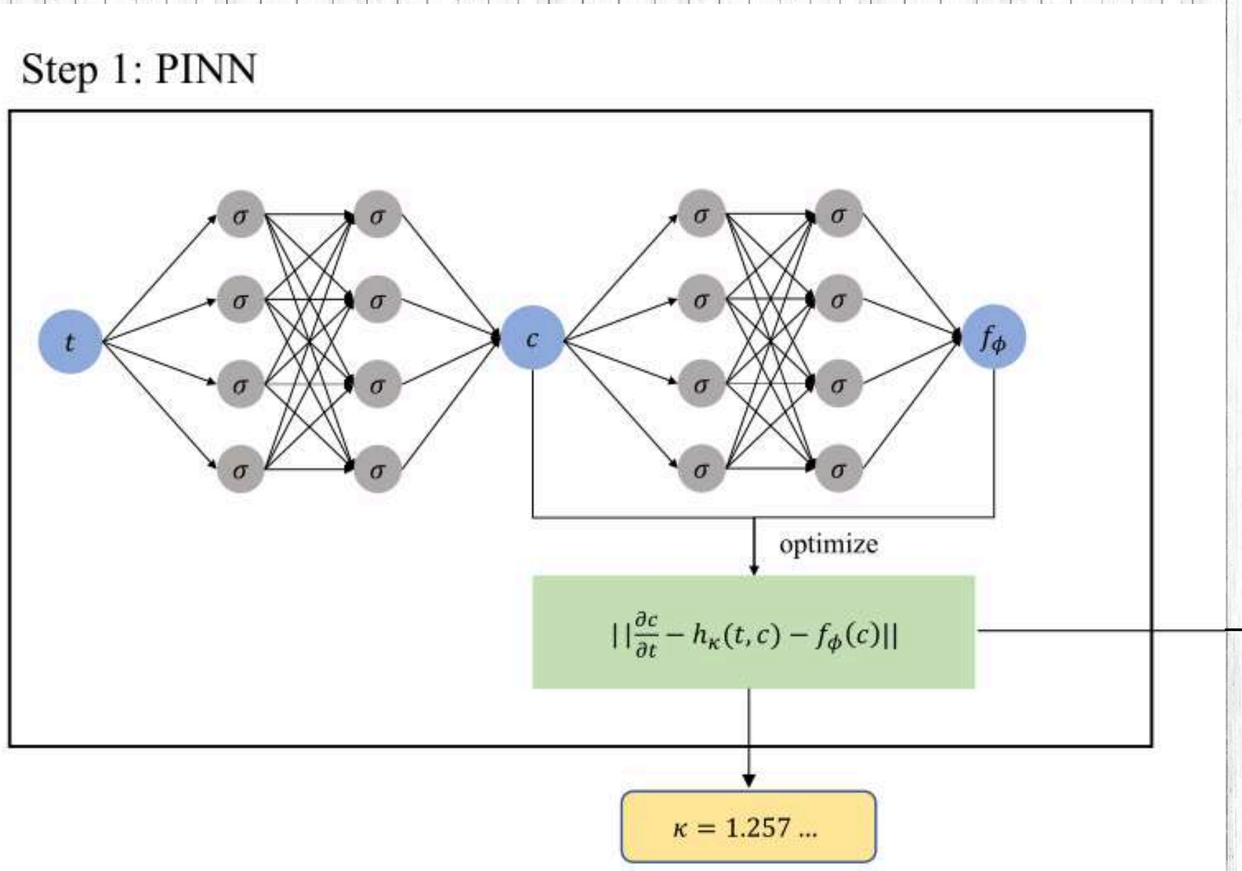
PINN for RDE

$$L(\Theta) = L_{\text{data}}(\theta) + L_{\text{res}}(\theta, \phi, \kappa)$$

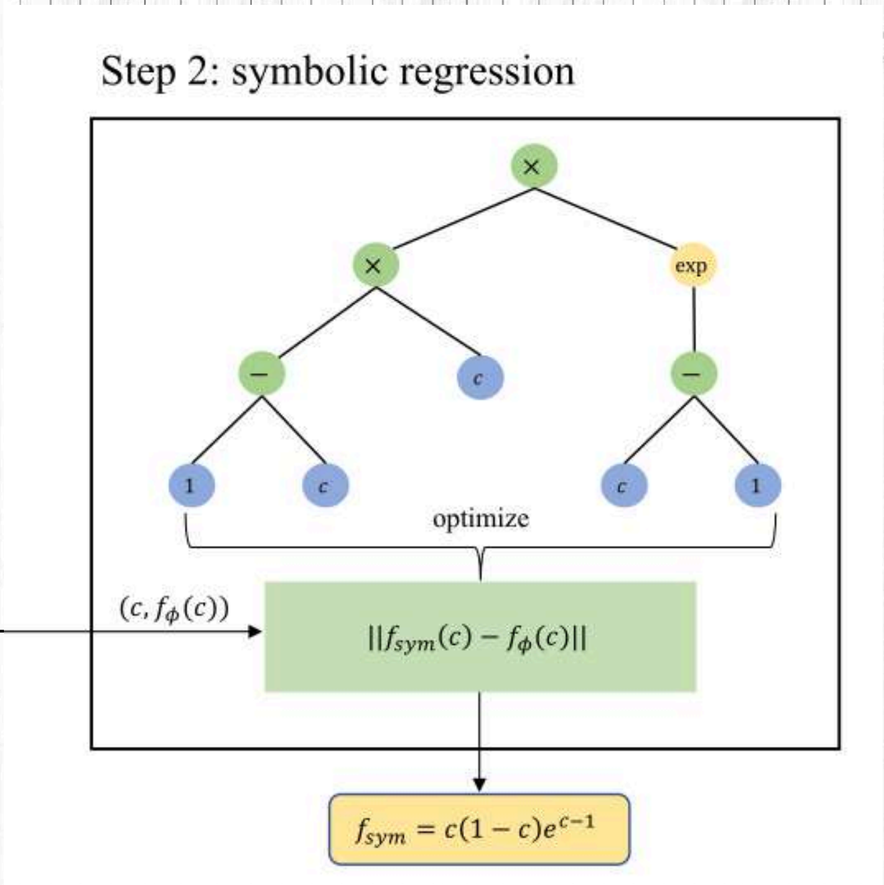
with respect to $\Theta := \{\theta, \phi, \kappa\}$, where

$$L_{\text{data}}(\theta) = \frac{1}{|T_D|} \sum_{t \in T_D} \|c(t) - c_\theta(t)\|_2^2,$$

$$L_{\text{res}}(\theta, \phi, \kappa) = \frac{1}{|T_R|} \sum_{t \in T_R} \left\| \frac{dc_\theta}{dt}(t) - h_\kappa(c_\theta) - f_\phi(c_\theta) \right\|_2^2$$

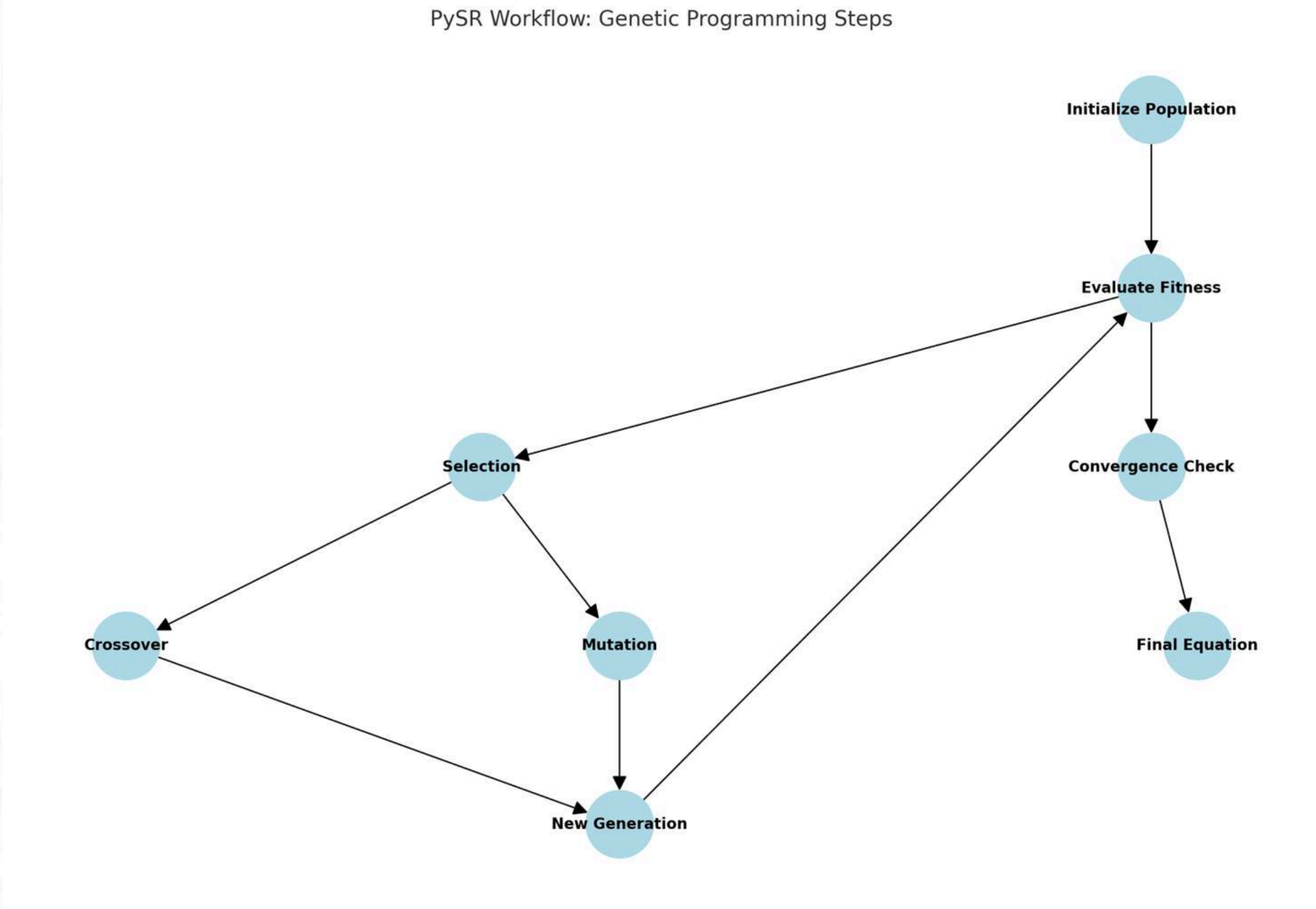


Symbolic Regression



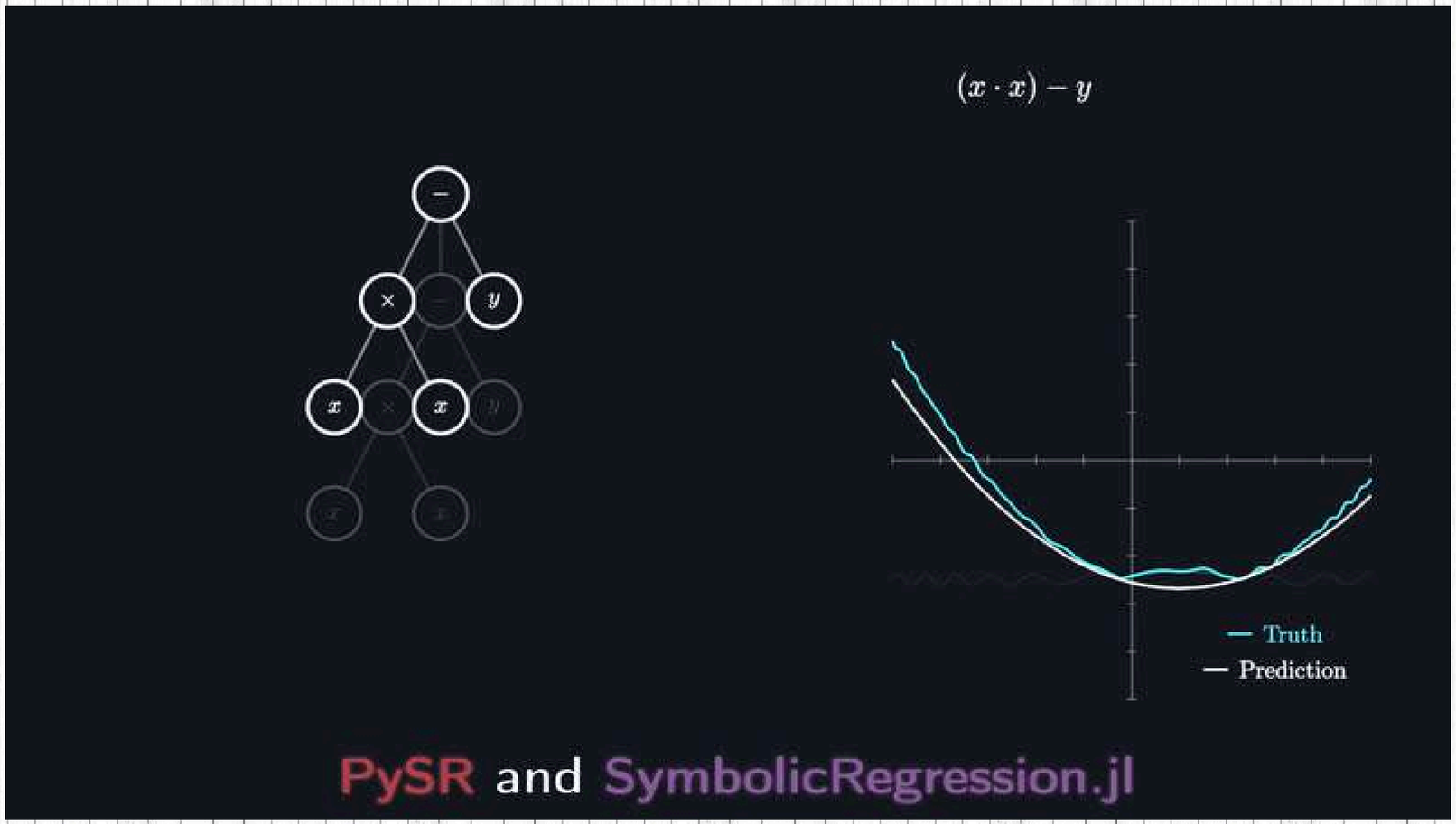
Symbolic regression is a regression analysis that searches for the best mathematical formula to describe the relationship between input data (features) and output data (target).

Symbolic Regression



Symbolic Regression

Julia?



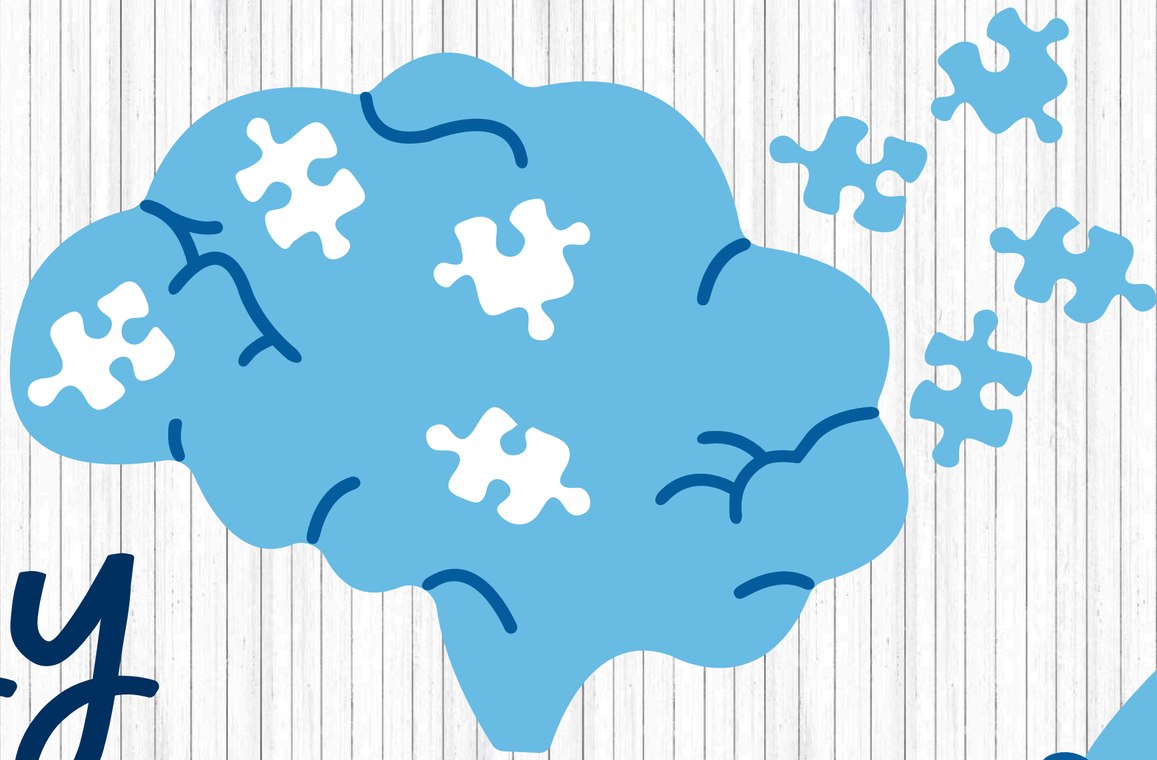
Genetic Programming?

MilesCranmer/PySR: High-Performance Symbolic Regression in Python and Julia

High-Performance Symbolic Regression in Python and Julia - MilesCranmer/PySR

GitHub

Our Methodology



How it works

Analyze Data

- Initialize parameters: Time (20 years)
- Calculate diffusion coefficient.

Create PINN Model

- Predict concentration (C).
- Predict reaction terms f(c)

Solve Tau Equation

- Substitute parameters.
- Use `scipy.integrate.odeint`
- Calculate tau concentration over 20 years.

Symbolic Regression

- Derive the best reaction term equation.

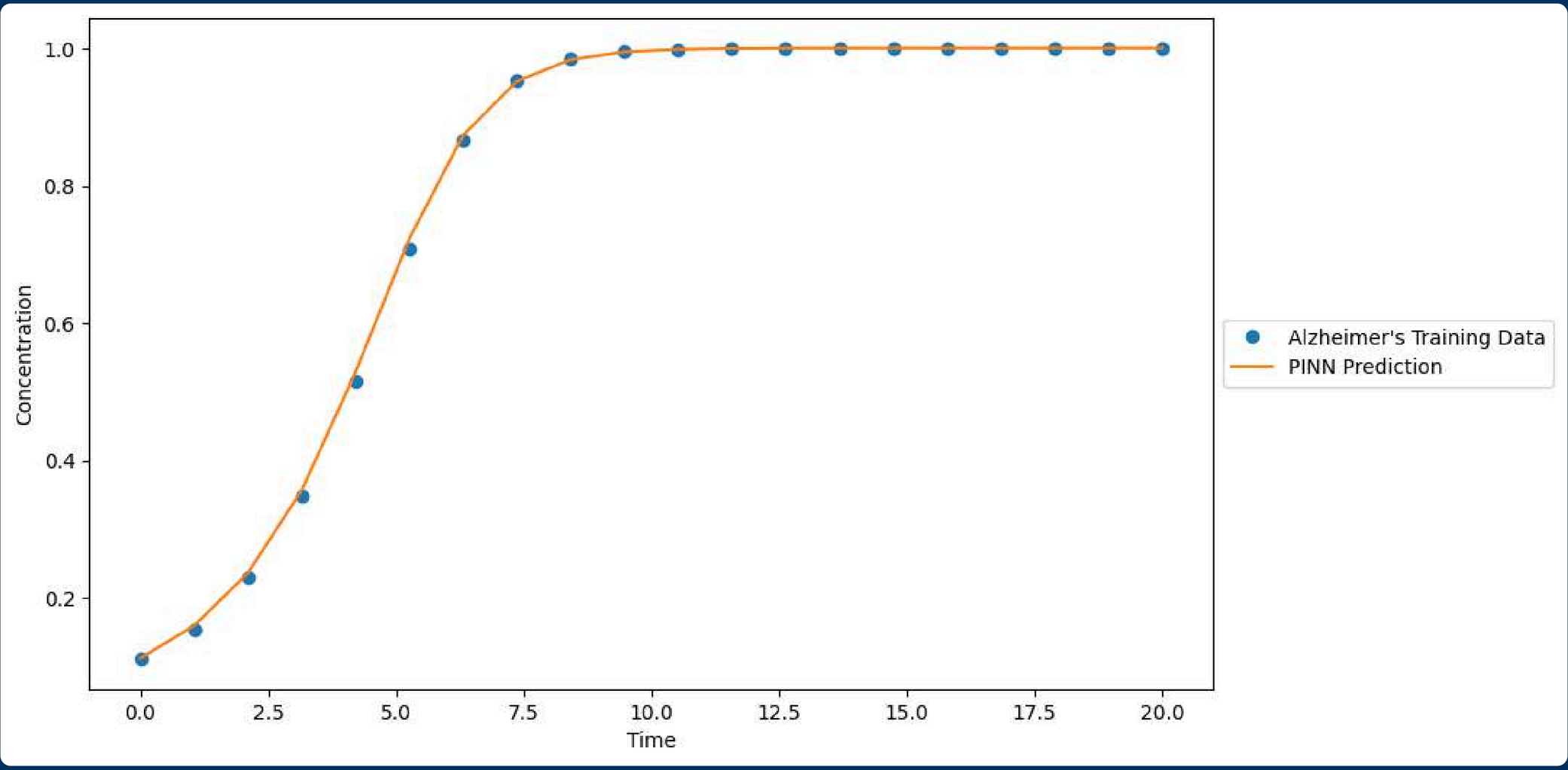
Train PINN

- Use ADAM optimizer.
- Fine-tune with L-BFGS.

Visualize Results

- Plot tau concentration.

Tau concentration for 1 reigon over 20 years



4

Synthetic Data Preparation

A 76 Subjects

C KPP Equations

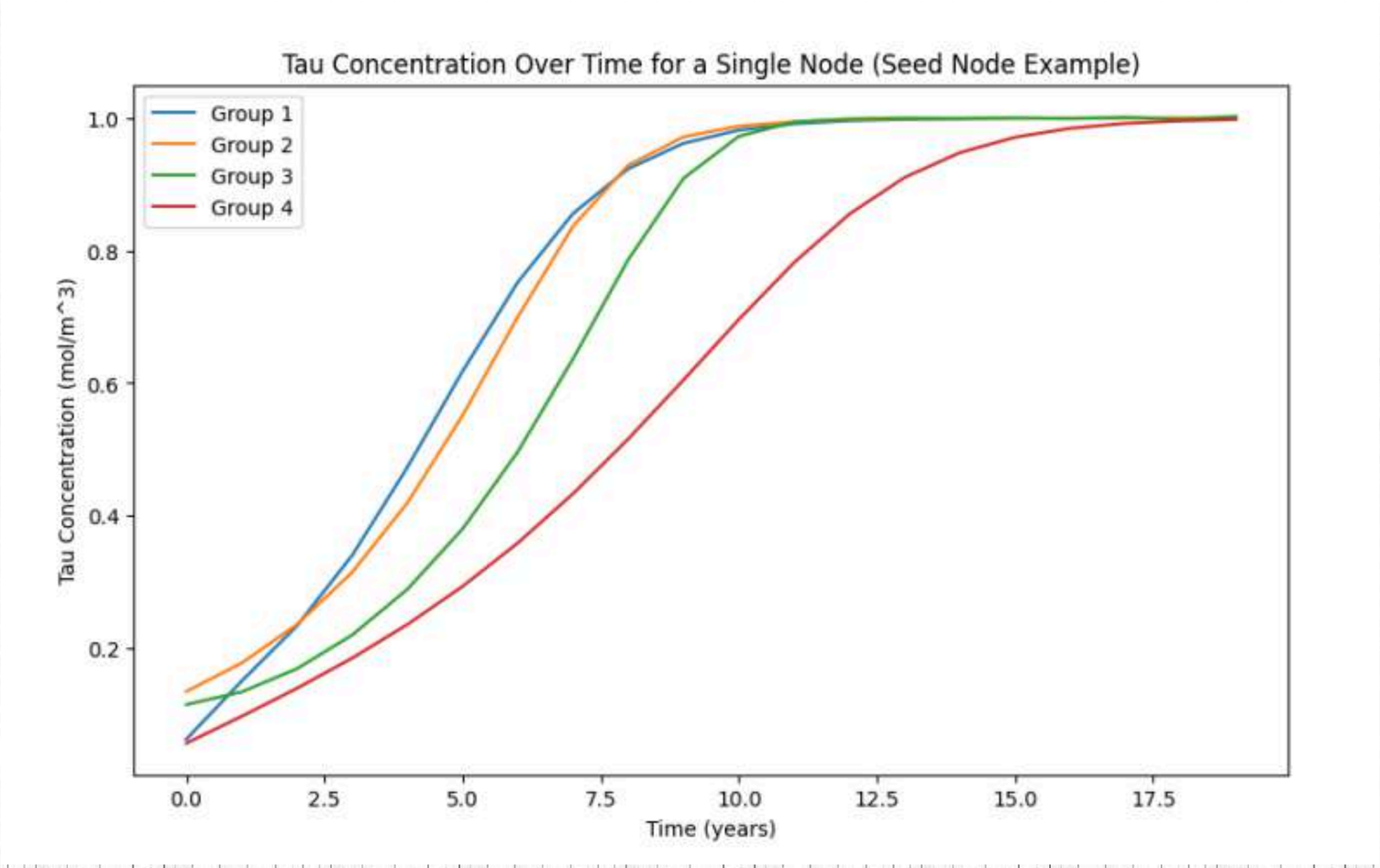
B Brain Discretization

D ADNI

KPP Equations

Equation	General Form
Fisher	$kc(1 - c)$
Newell-Whitehead-Segel	$kc(1 - c^q)$ $kc(1 - c^3)$
Zeldovich-Frank-Kamenetskii	$kc(1 - c)e^{(\beta(c-1))}$

Graphical Representation



2

COMSOL Multiphysics Simulation

A Geometry

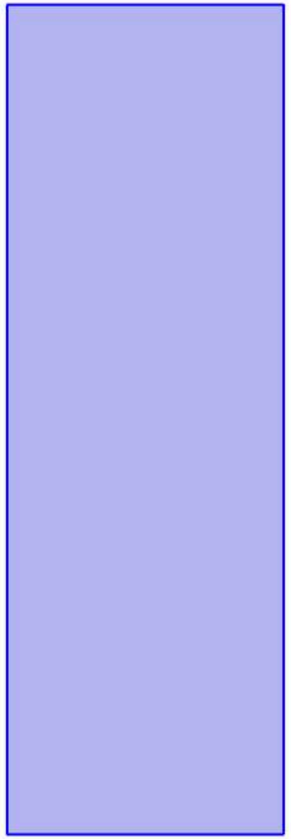
C Physics

B Study

D Results

2

Geometry



2

Physics & Study

Transport of diluted species

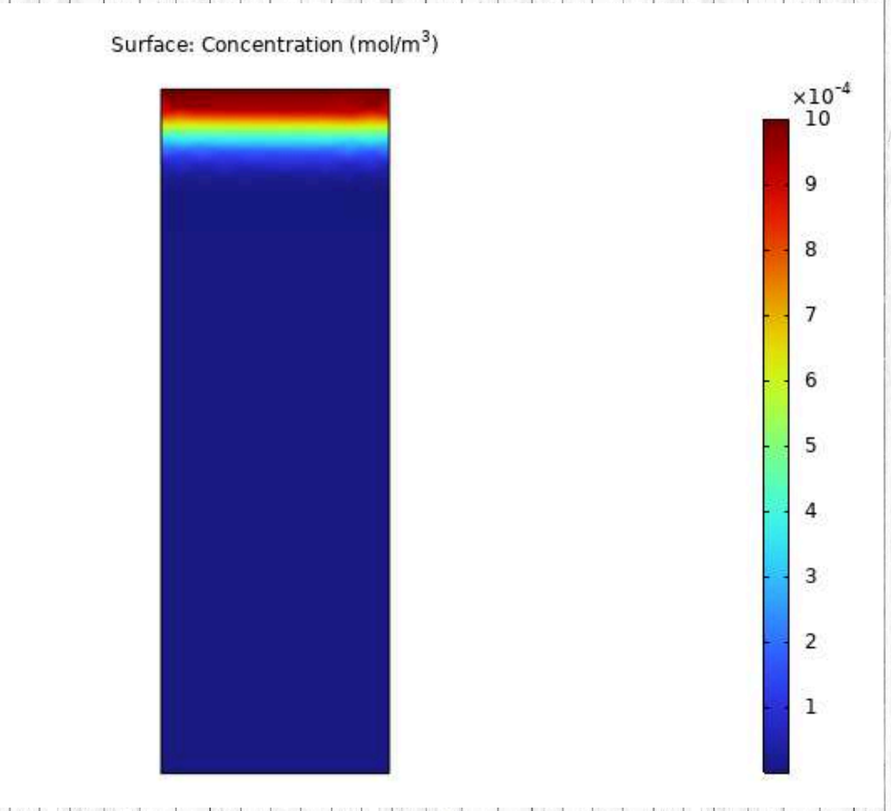
No Flux (Neumann)

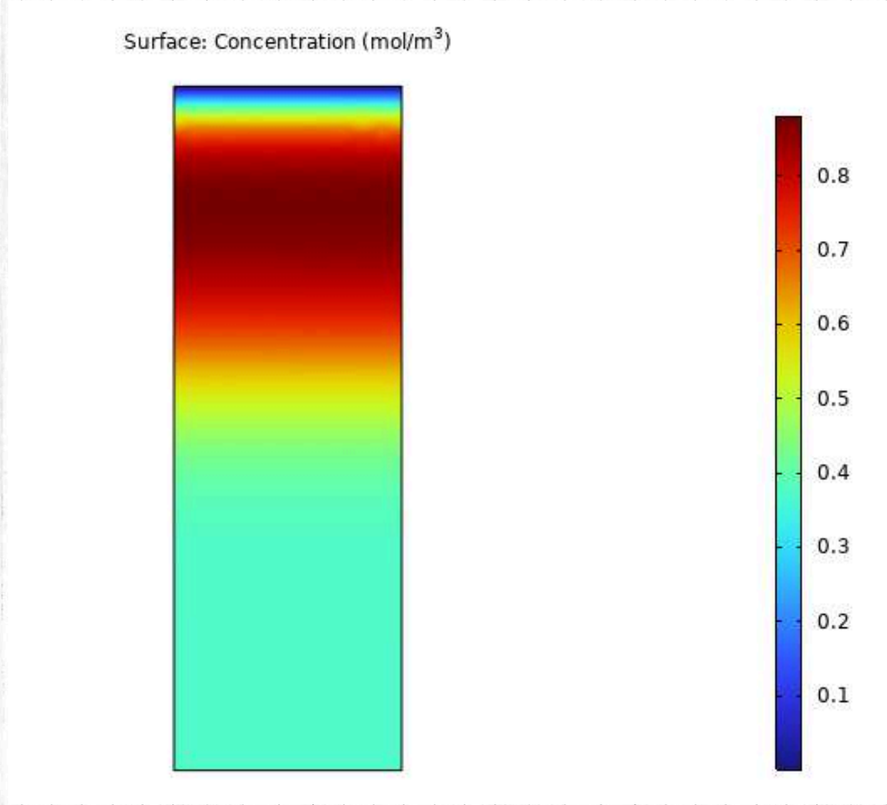
Fixed Concentration dirichlet

Time Dependent Study

2

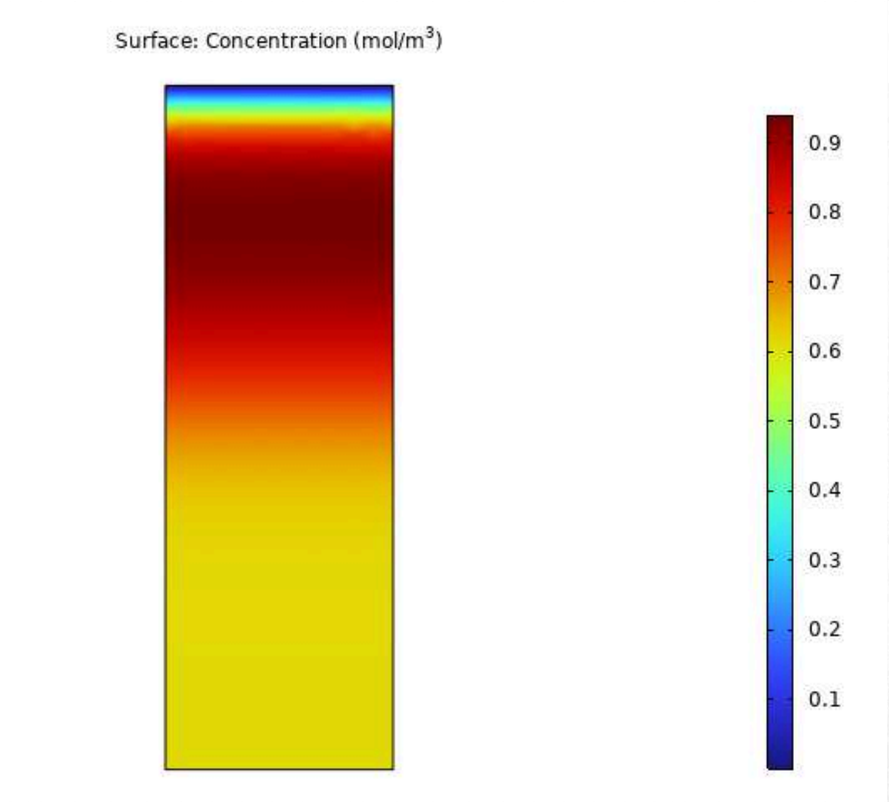
Geometry

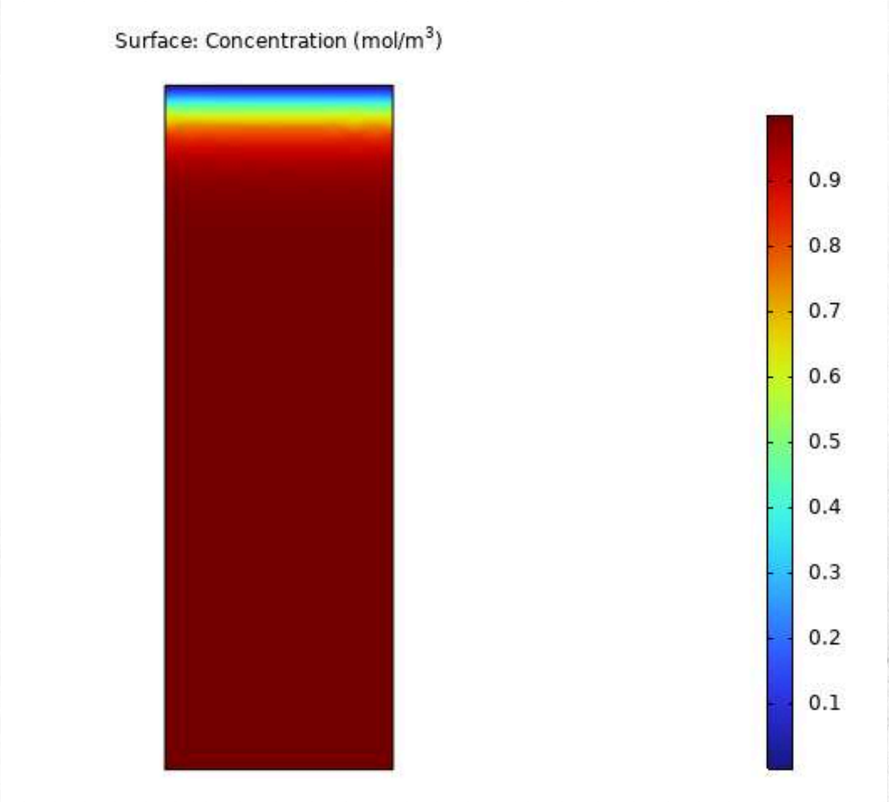

Surface: Concentration (mol/m3)
×10-4
10
9
8
7
6
5
4
3
2
1


Surface: Concentration (mol/m3)
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1

2

Geometry


Surface: Concentration (mol/m3)
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1


Surface: Concentration (mol/m3)
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1

Future work

Future work

- Enhance tau dynamics model with PET and MRI data.
- Visualize tau trends and disease progression using a web-based platform.

our web

HTML

CSS

JAVA SCRIPT