A mixed pressure-velocity formulation to model flow in heterogeneous porous media with physics-informed neural networks

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Journées Transport Réactif

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Topic:

Machine learning for modeling flow and reactive transport in aquifers

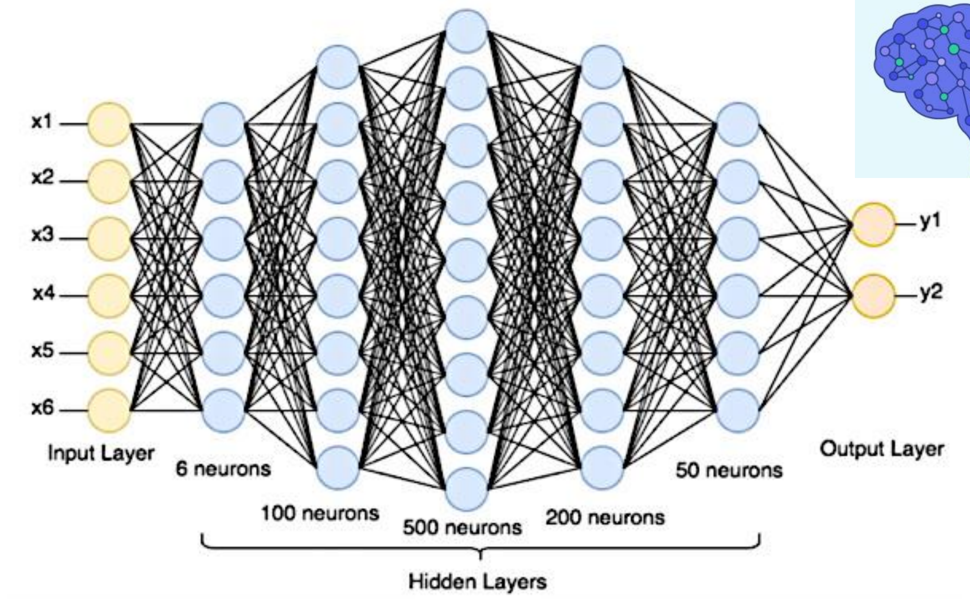
SDC, Science des Données et Connaissances

Outlines

- ❑ Deep learning neural networks (DLNNs) for modeling physical processes
- ❑ Physics informed neural networks – PINNs (2019)
- ❑ PINNs for flow in heterogeneous porous media: Mixed formulation
- ❑ Implementation and results
- ❑ Conclusions

DLNNs for modeling physical processes

Deep learning neural networks



Last evolution of machine learning

This is an interpolation technique based on specific mathematical function

This function involves parameters

Learning allows for obtaining this parameters

More accurate than other standard interpolators

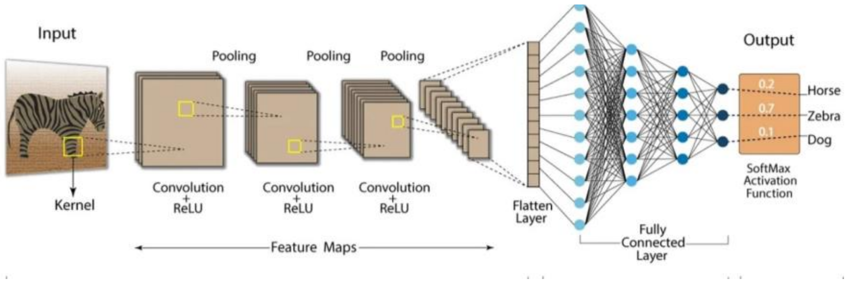
High efficiency on GPU cards

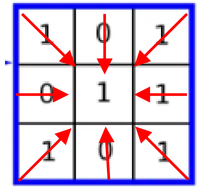
CPU: 3 hr

GPU: 3-4 minutes

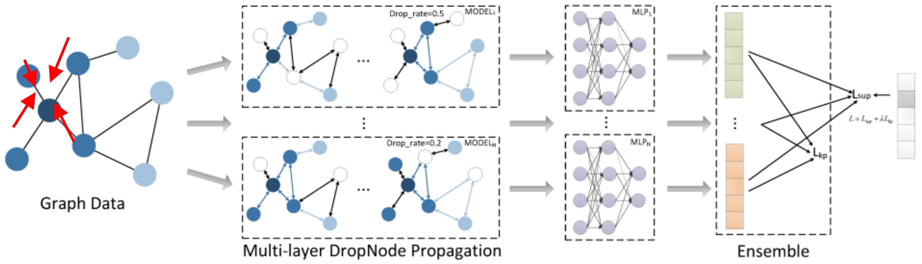
Several techniques: data and application

Convolution Neural Networks (CNN)





Graph Neural Networks (GNN)



DLNNs for modeling physical processes

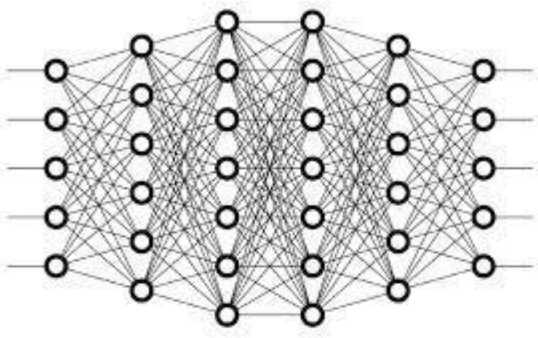
Deep learning neural networks

Fast development of computing power
graphics processing unit (GPU)

+

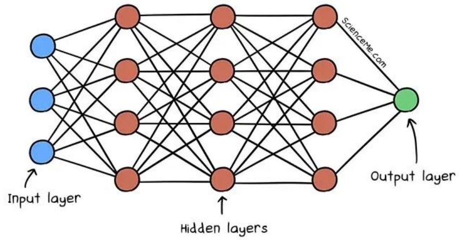
Fast growth of data availability

Deep learning neural networks
(DLNNs) as convenient tools



Several applications
autonomous vehicles,
weather forecasts
language processing
finance predictions
image or speech recognition
image colorization
.

ChatGPT



Thinking and producing text/codes… like humans

DLNNs for modeling physical processes

Applications in scientific domains and porous media

Due to their remarkable predictive capabilities:

DLNNs have gained significant attention in scientific domains such as **biomedicine, economics, chemistry, and physics**.

In addition to experimental science, model-based science, and computational science,

DLNNs are currently emerging as a novel paradigm of science

Recently, DLNNs have been used for **modeling flow and transport processes in porous media**

Surrogate modeling

Data are generated using numerical model

Data are used to train a DLNN

DLNN is used instead the numerical model

It improves CPU time

DLNNs for modeling physical processes

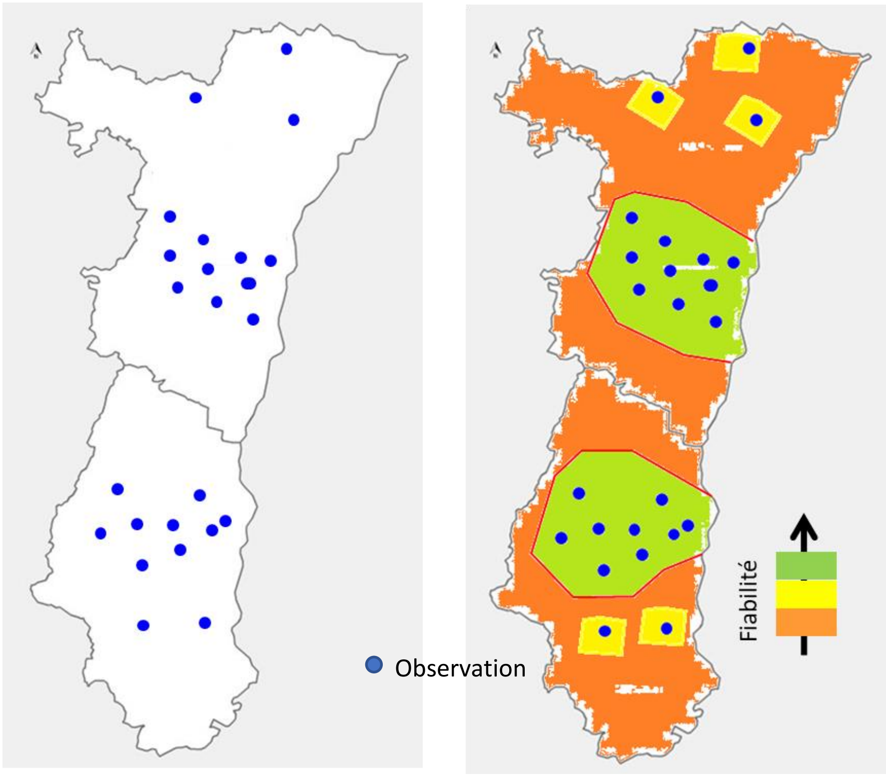
Challenges

DLNNs require a lot of data

Data are not widely available in scientific applications :
Observation or numerical data

Data availability limits the applications of DLNNs for scientific applications (Hydrogeology)

Example in hydrogeology: Water level in aquifers



DLNN model for interpolating the data

Predicting water level in all the domain

Unreliable predictions

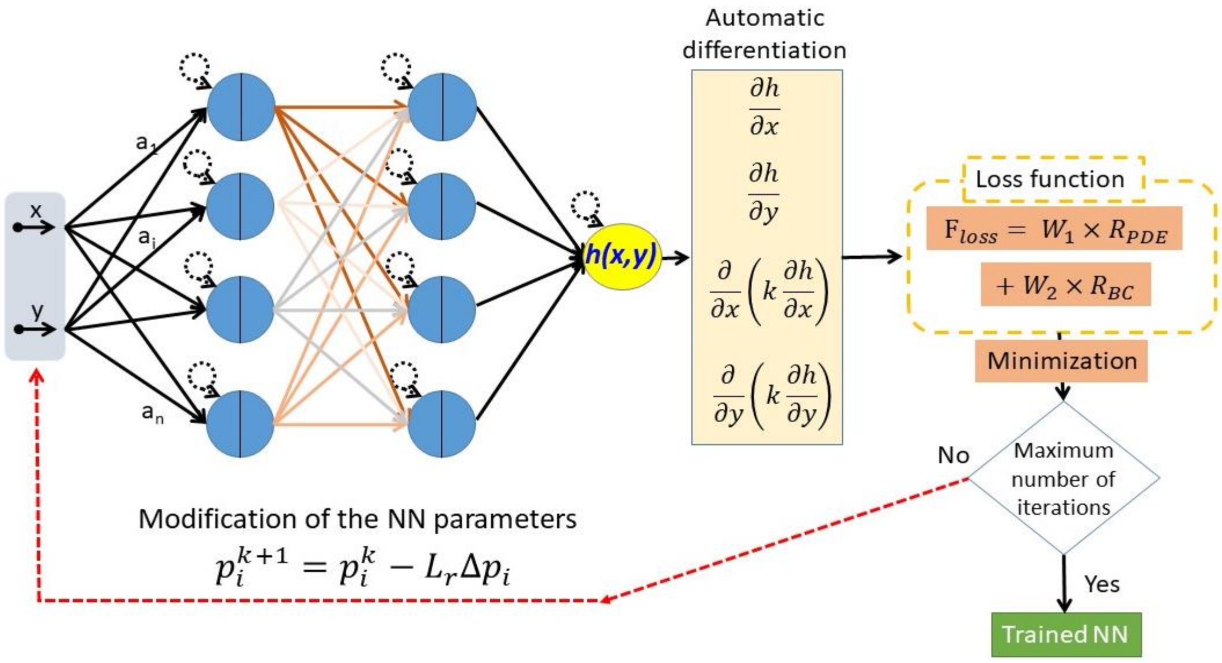
DLNNs for modeling physical processes

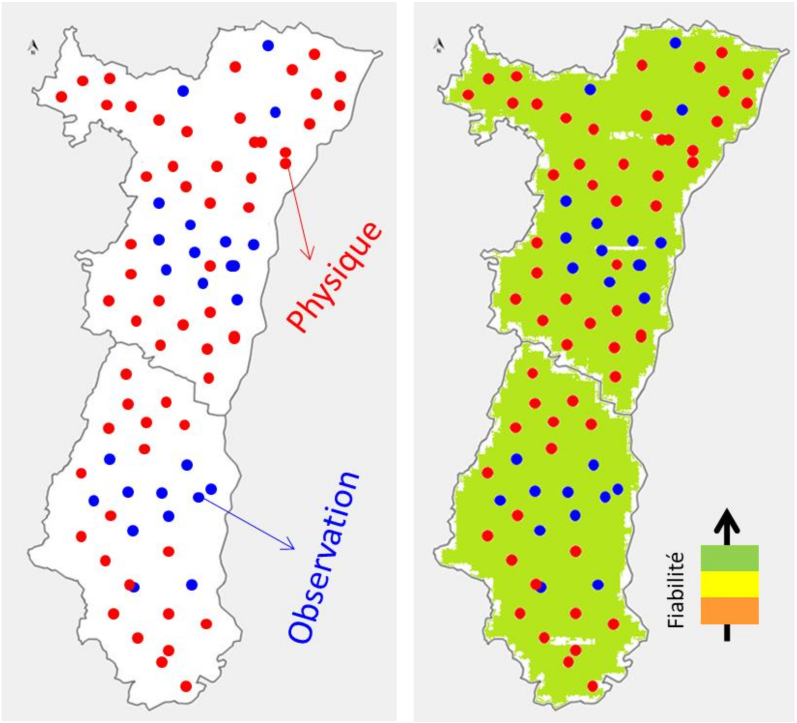
Challenges

Physics informed neural network

New technique for developed by Raissi et al., (2019)

Using DLNNs with few data or without data



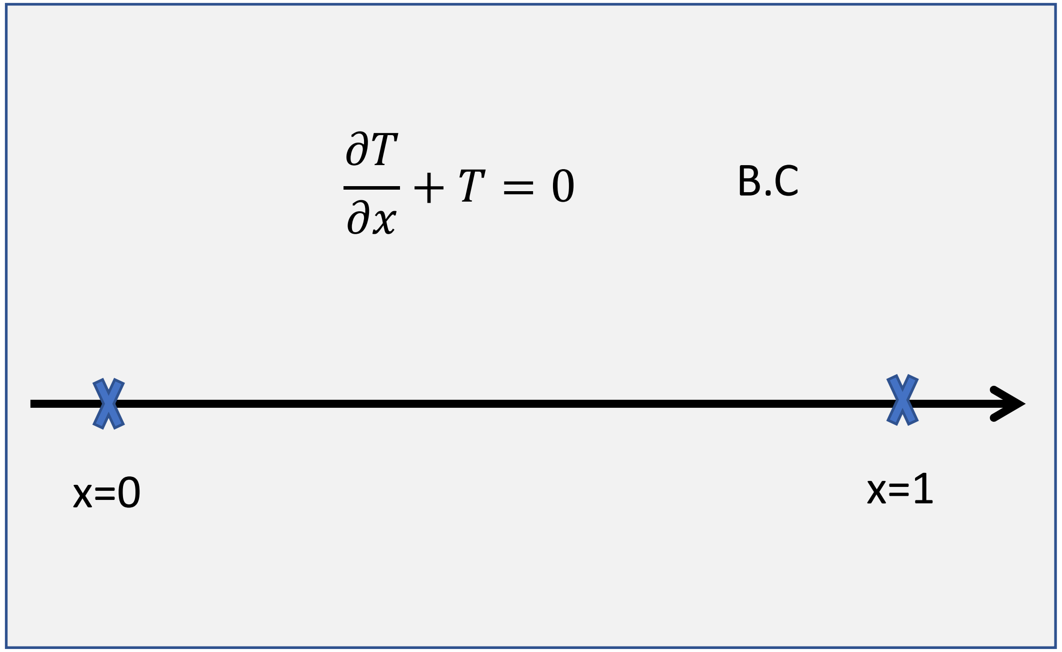


- Integration of physical laws into the "cost function".
- Calculate derivatives: automatic differentiation.
- Optimization of the cost/parameter function of the neural network.

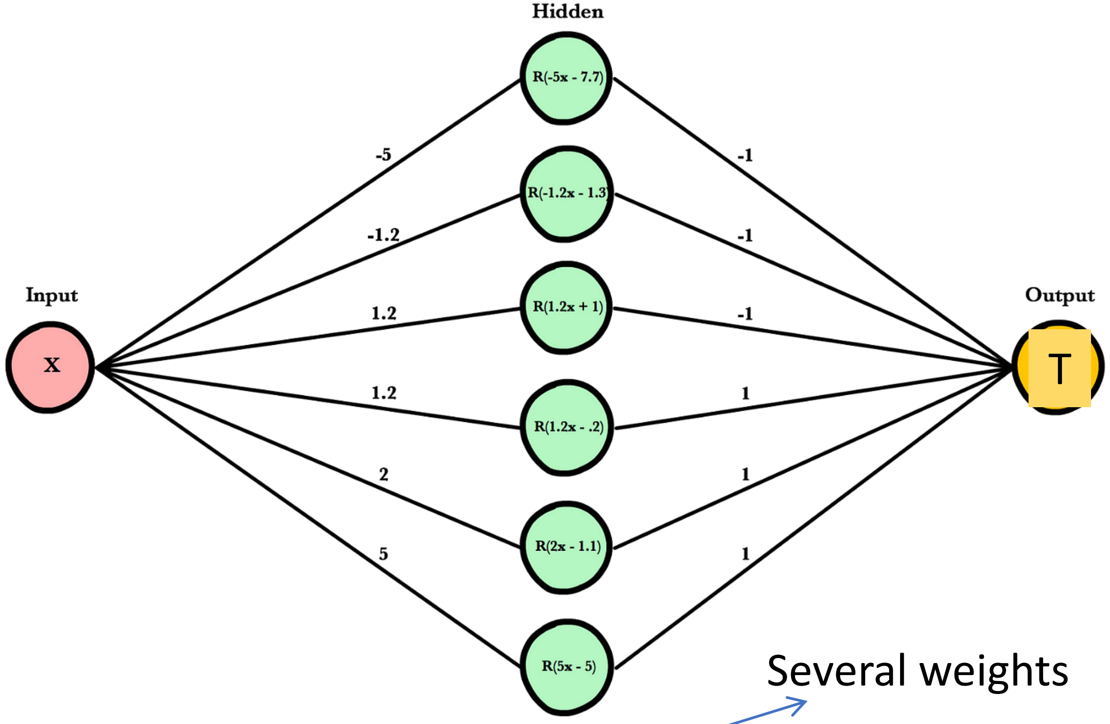
Physics informed neural networks – PINNs (2019)

Main idea of PINNs

PINNs aims at training the neural network (NN) to **fulfill the partial differential equations (PDEs)** describing the physical processes.



$$\frac{\partial T}{\partial x} + T = 0$$



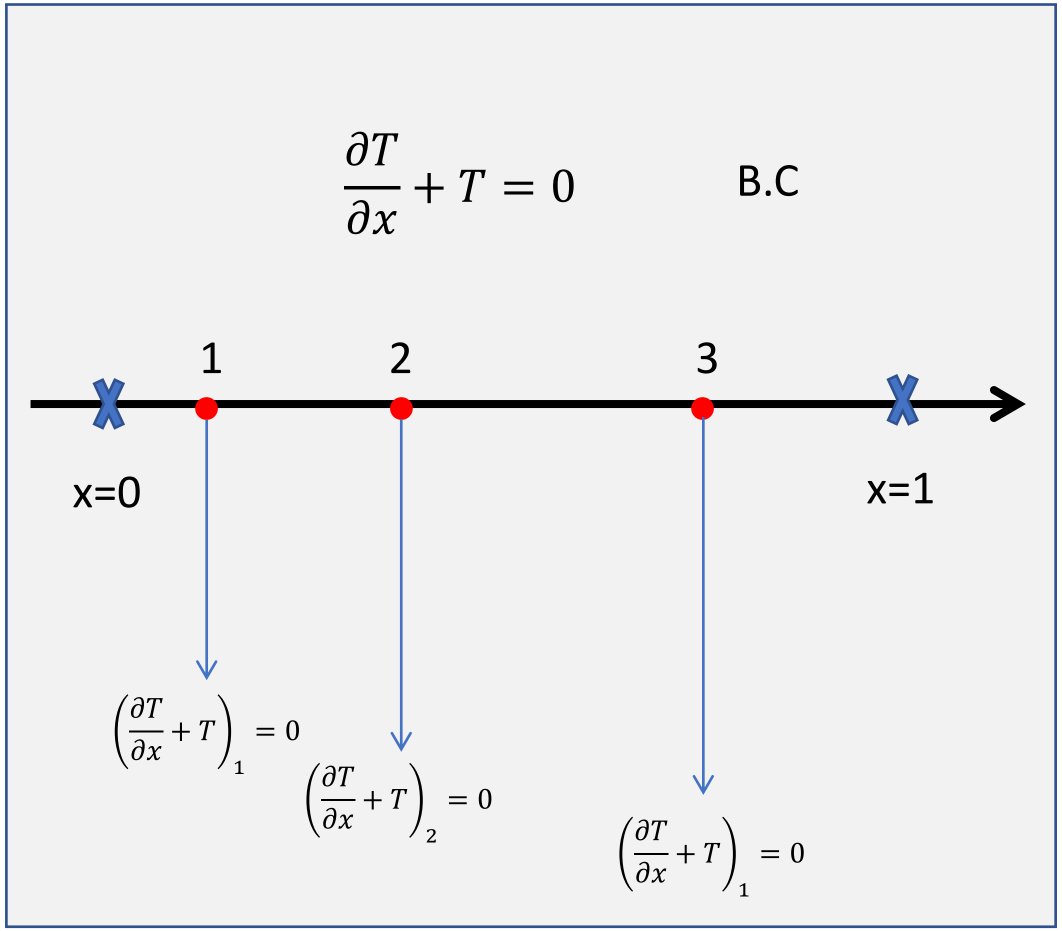
Several weights

$$T = f(x)$$

Physics informed neural networks – PINNs (2019)

Main idea of PINNs

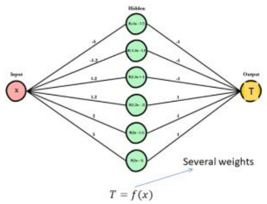
To find the weights: we use collocation points



We define a **loss function** based on the governing equations

$$Floss = \left[\left(\frac{\partial T}{\partial x} + T\right)_1\right]^2 + \left[\left(\frac{\partial T}{\partial x} + T\right)_2\right]^2 + \left[\left(\frac{\partial T}{\partial x} + T\right)_3\right]^2$$

T is approximated by the NN



$\frac{\partial T}{\partial x}$ is exactly calculated using **automatic differentiation**

The loss function is optimized to find the weights of the NN

Result: a NN that represents the solution of this equation

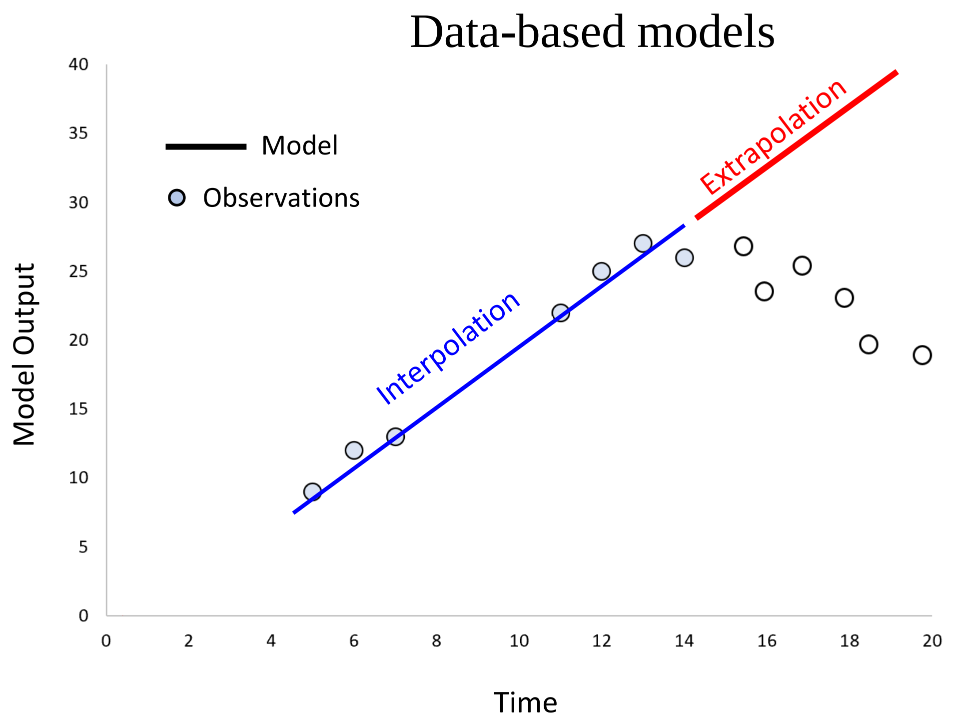
Physics informed neural networks – PINNs (2019)

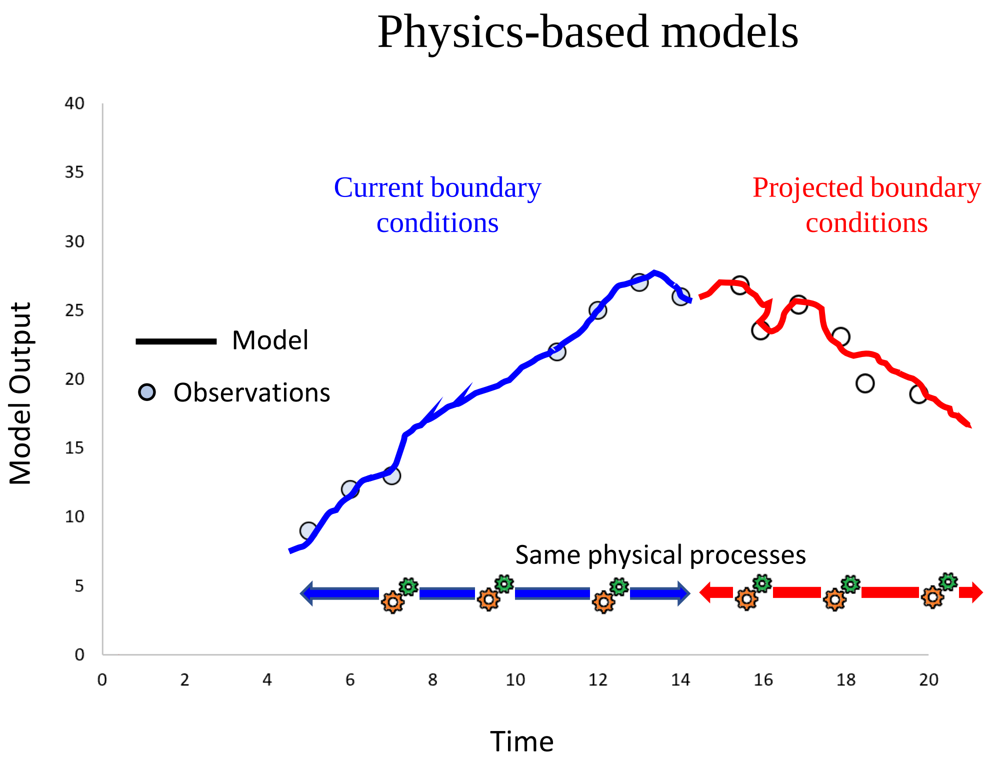
Advantages of PINNs

- **Fast training of the NN:** Physics constraint the solution and help the convergence of the algorithm
- Generating reliable model with **few data**
- Solving the PDR **without mesh and time discretization**
- Improving the computational time
- **PINNs can be also used for inverse problem where parameters of the physical equations have to be estimated**.

Physics informed neural networks – PINNs (2019)

Advantages of PINNs: prediction – extrapolation – climate change





Data- based model are accurate for interpolation but less accurate for extrapolation

« Physics Informed Neural Networks » PINNs

Physics informed neural networks – PINNs (2019)

PINNs for porous media

First applications of PINNs for fluid mechanics (Navier stockes)

Extending PINNs to other applications is a hot topic

The utilization of PINNs for modeling flow in porous media is currently receiving increased attention

Saturated subsurface flow (Wang et al., 2020)
Unsaturated flow (Tartakovsky et al., 2020)
subsurface flow and mass transport (He et al., 2020)
Seepage equation (Daolun et al., 2021)
Coupled Stokes–Darcy equations (Pu and Feng 2022)
Thermo–hydro–mechanical processes (Amini et al., 2022)
Two-phase flow (Zhang et al., 2023)

All the existing applications are limited to homogeneous domains

PINNs is facing **convergence issues** in heterogeneous domains

Heterogeneity plays **key role** in flow processes in porous media

Developing new implementation of PINNS for flow in heterogeneous porous media is a challenge

PINNs for flow in heterogeneous porous media: Mixed formulation

Why PINNs are facing problems for heterogeneous domains?

- ❑ Governing equation: 2D pressure head form

$$\frac{\partial}{\partial x}\left(K\frac{\partial h}{\partial x}\right)+\frac{\partial}{\partial y}\left(K\frac{\partial h}{\partial y}\right)=0$$

- ❑ PINNs cannot ensure accurate solutions when dealing with the flow in heterogeneous domains,
- ❑ Particularly when the properties of the heterogeneous domains are discontinuous

$$\frac{\partial}{\partial x}\left(K\frac{\partial h}{\partial x}\right)=\boldsymbol{\frac{\partial K}{\partial x}\frac{\partial h}{\partial x}}+K\frac{\partial}{\partial x}\left(\frac{\partial h}{\partial x}\right)$$

This term cannot be calculated with automatic differentiation

PINNs for flow in heterogeneous porous media: Mixed formulation

New implementation of PINNs: pressure head-velocity form

- Governing equation: **pressure head-velocity form**

$$\frac{\partial q_x}{\partial x} + \frac{\partial q_y}{\partial y} = 0$$

$$q_x + \boldsymbol{K}\frac{\partial h}{\partial x} = 0 \quad \text{and } q_y + \boldsymbol{K}\frac{\partial h}{\partial y} = 0$$

- With the new implementation: PINNs is used for solving the pressure head-velocity form of the governing equations

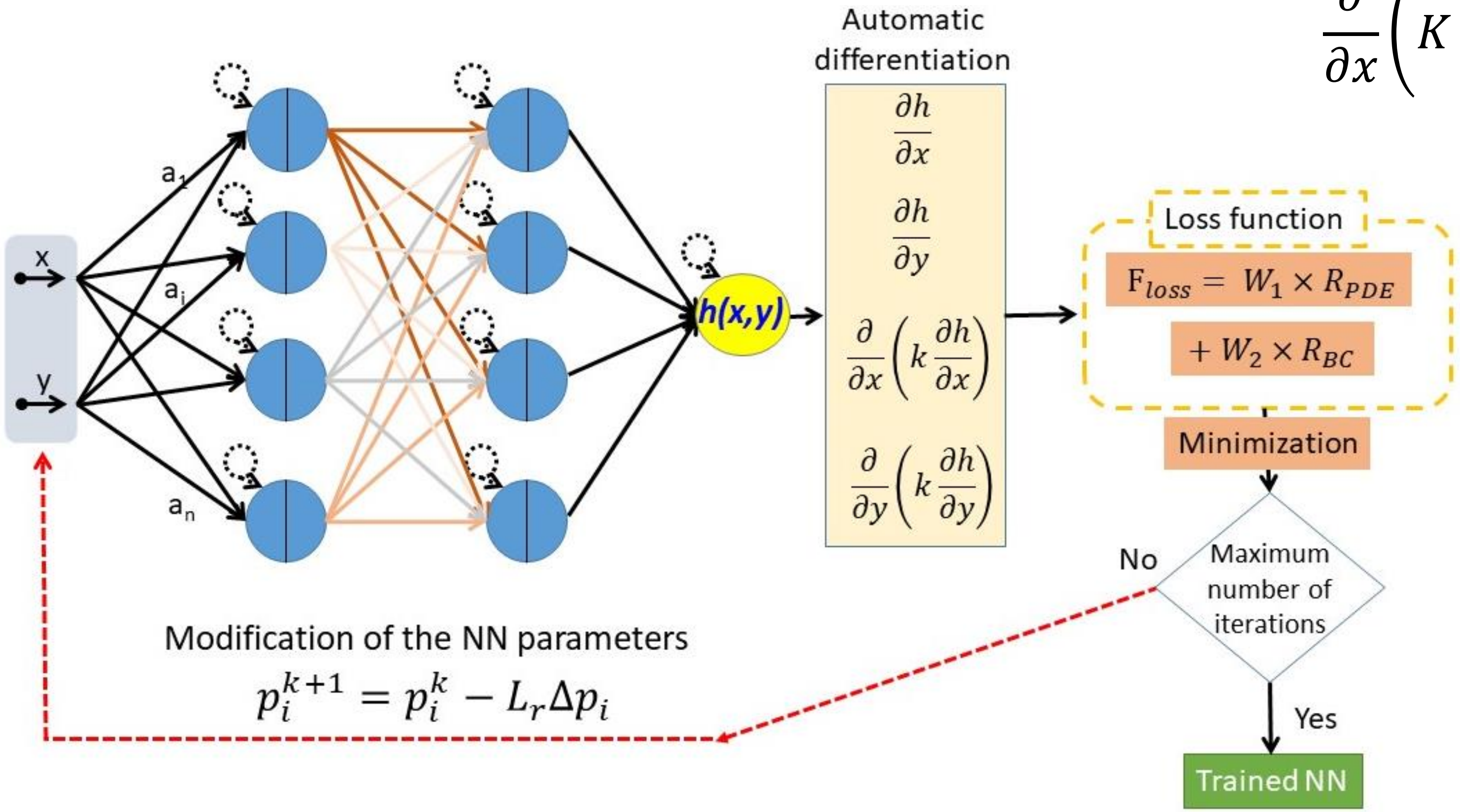
- This form does not require the derivative of K with respect to the space direction

Implementation and results

4 implementations have been tested

Standard PINNS: Pressure form

$$\frac{\partial}{\partial x}\left(K\frac{\partial h}{\partial x}\right)+\frac{\partial}{\partial y}\left(K\frac{\partial h}{\partial y}\right)=0$$

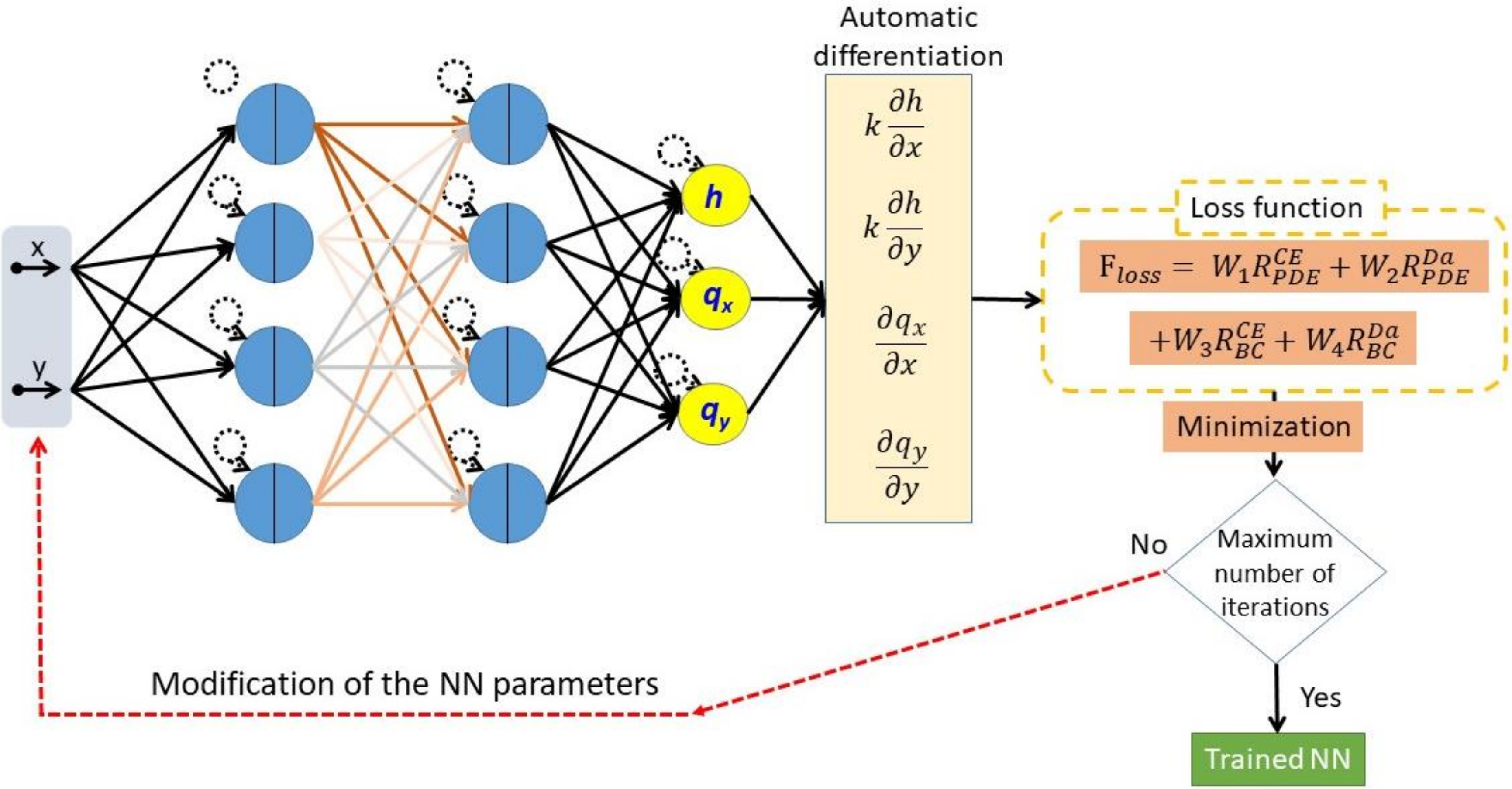


Implementation and results

4 implementations have been tested

New PINNS: Pressure-velocity form

H-V-1-PINN



$$\frac{\partial q_x}{\partial x} + \frac{\partial q_y}{\partial y} = 0$$

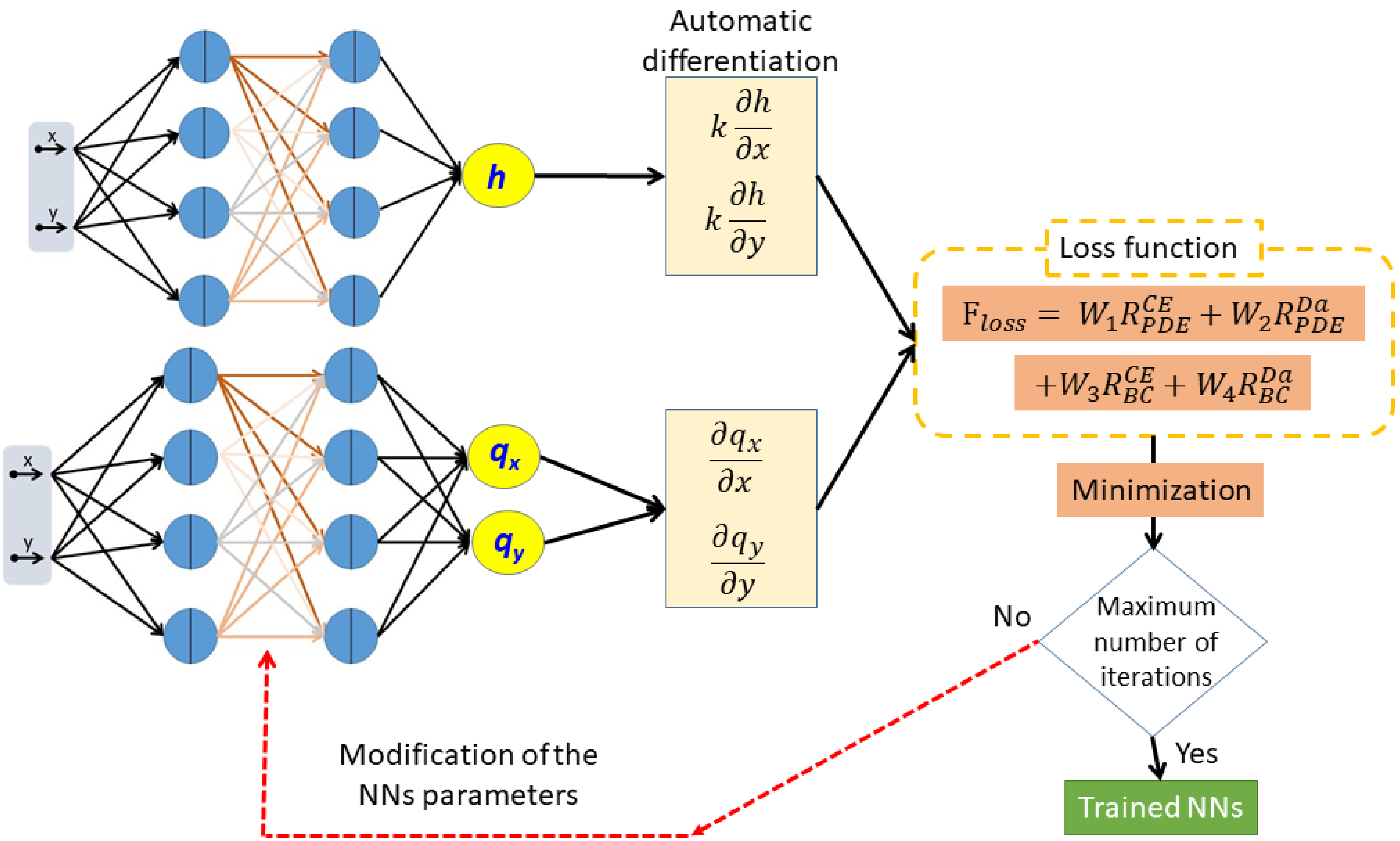
$$\boldsymbol{K}\frac{\partial h}{\partial x} = 0 \quad \text{and } q_y + \boldsymbol{K}\frac{\partial h}{\partial y} = 0$$

Implementation and results

4 implementations have been tested

New PINNS: Pressure-velocity form

H-V-2-PINN



$$\frac{\partial q_x}{\partial x} + \frac{\partial q_y}{\partial y} = 0$$

$$K\frac{\partial h}{\partial x} = 0 \quad \text{and} \quad q_y + K\frac{\partial h}{\partial y} = 0$$

Implementation and results

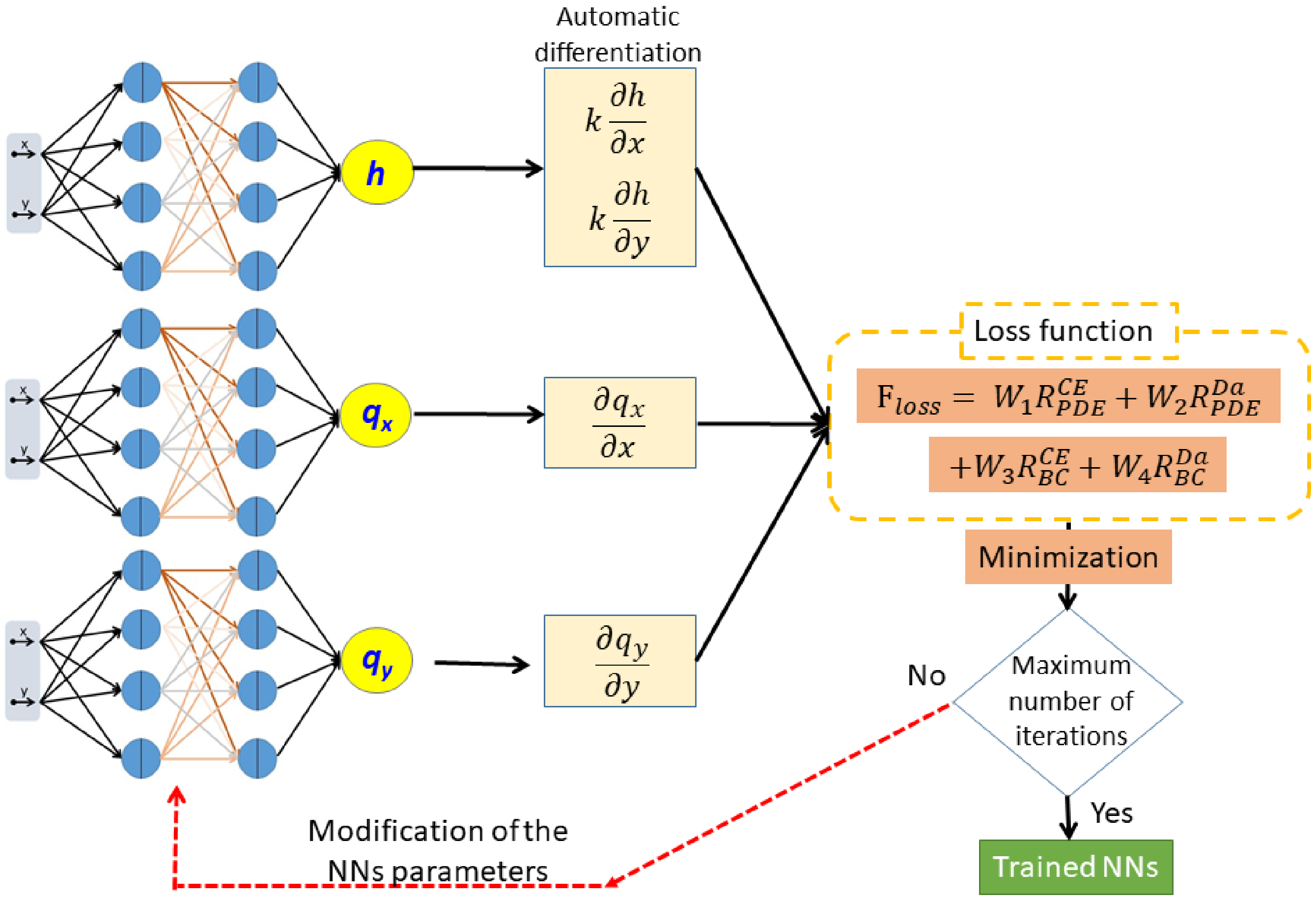
4 implementations have been tested

New PINNS: Pressure-velocity form

H-V-3-PINN

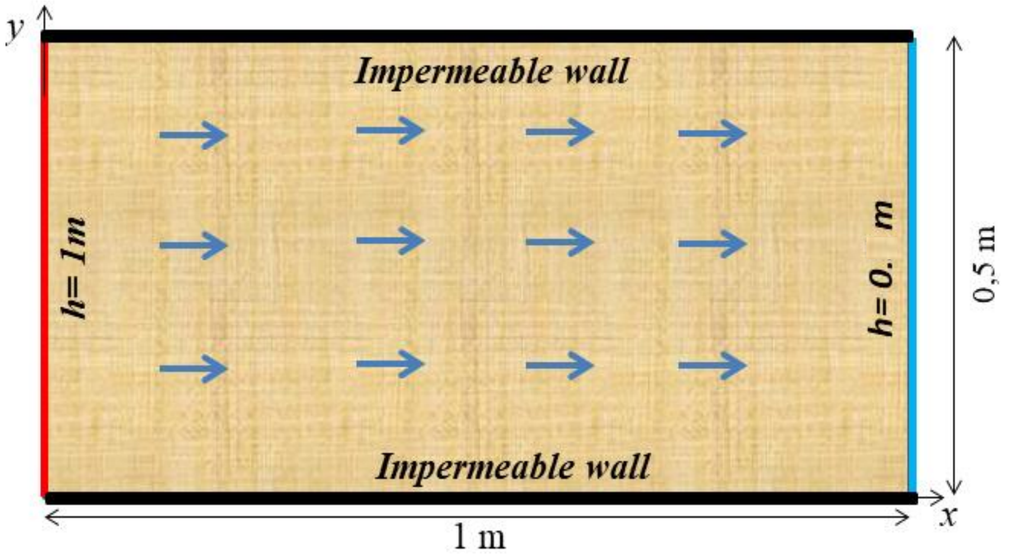
$$\frac{\partial q_x}{\partial x} + \frac{\partial q_y}{\partial y} = 0$$

$$\boldsymbol{K}\frac{\partial h}{\partial x} = 0 \quad \text{and } q_y + \boldsymbol{K}\frac{\partial h}{\partial y} = 0$$

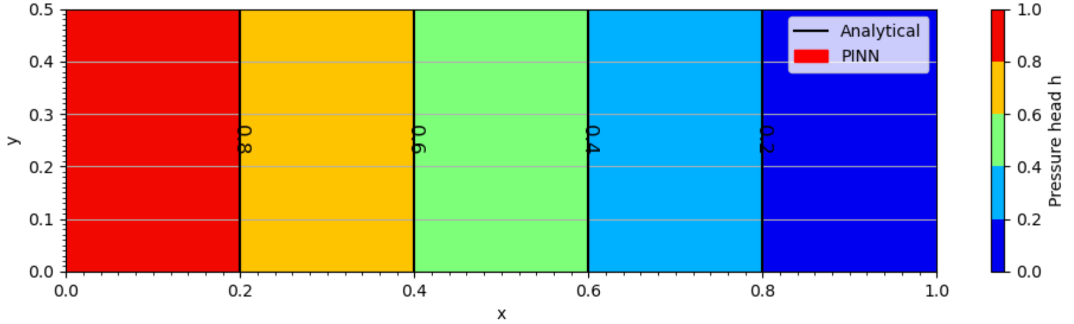


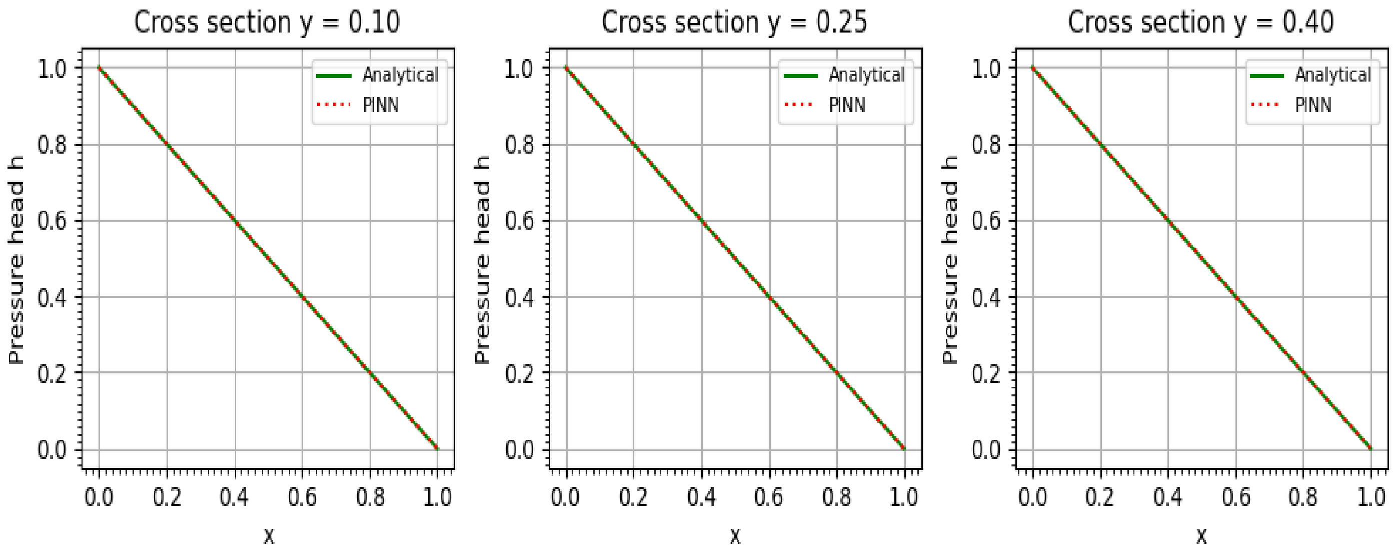
Implementation and results

Test case 1: homogenous domain



Analytical solution

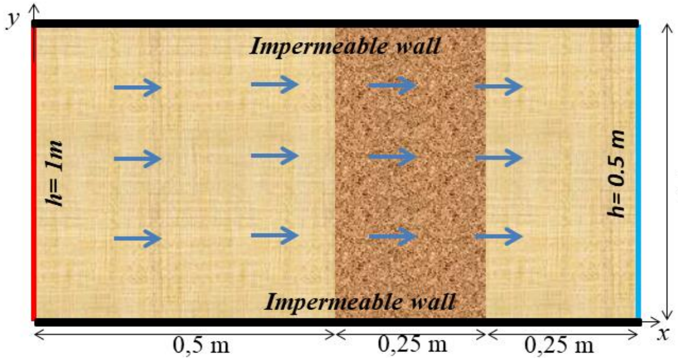


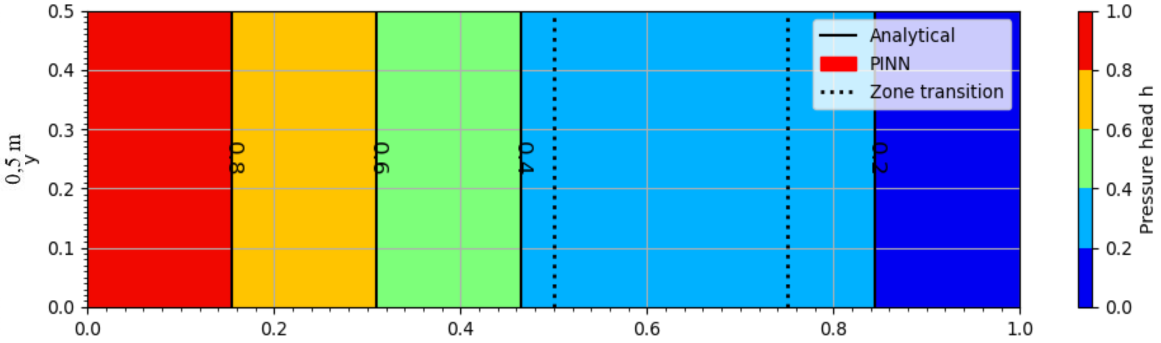


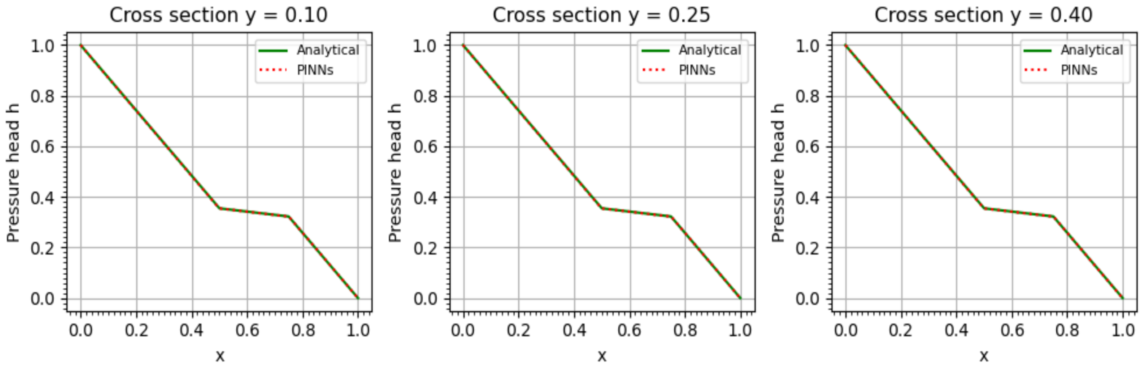
Standard and new PINNs provide the same results

Implementation and results

Test case 2: heterogeneous domain





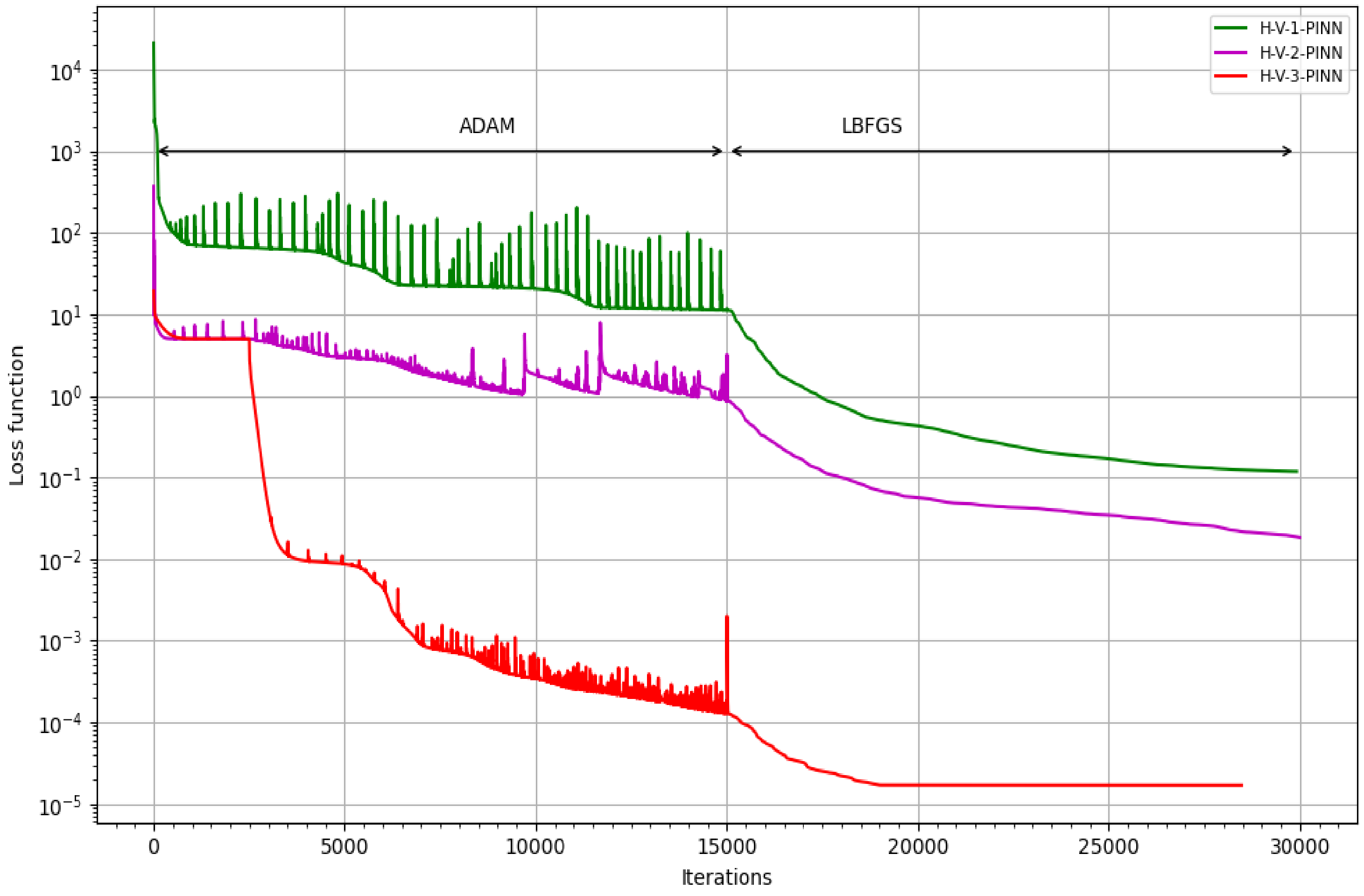


1D Heterogeneous	Number of parameters	Adam Loss	LBFGS Loss
H-PINN	-	-	-
H-V-1-PINN	9915	$1.11 \times 10^{+1}$	1.18×10^{-1}
H-V-2-PINN	9736	8.60×10^{-1}	1.84×10^{-2}
H-V-3-PINN	9893	1.52×10^{-4}	1.68×10^{-5}

Implementation and results

Test case 2: heterogeneous domain

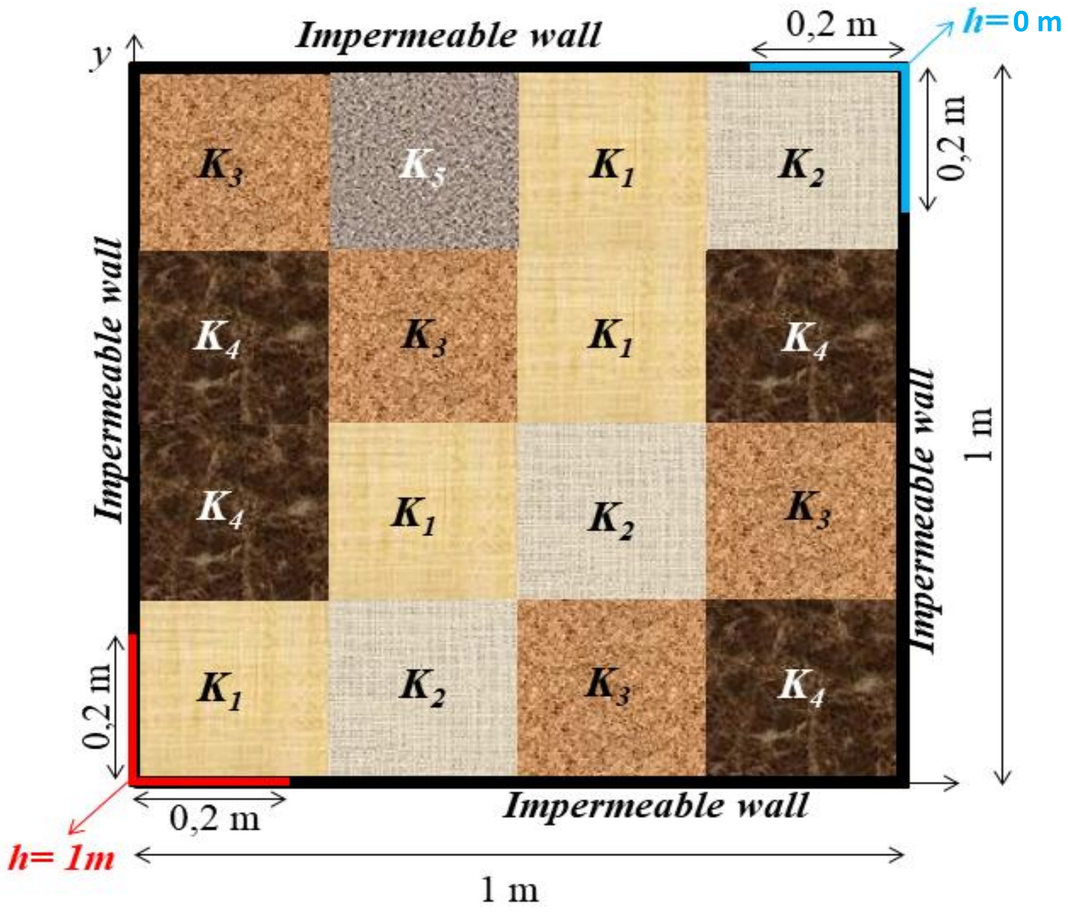
Convergence of the loss function



Model with 3 NN is providing the best results

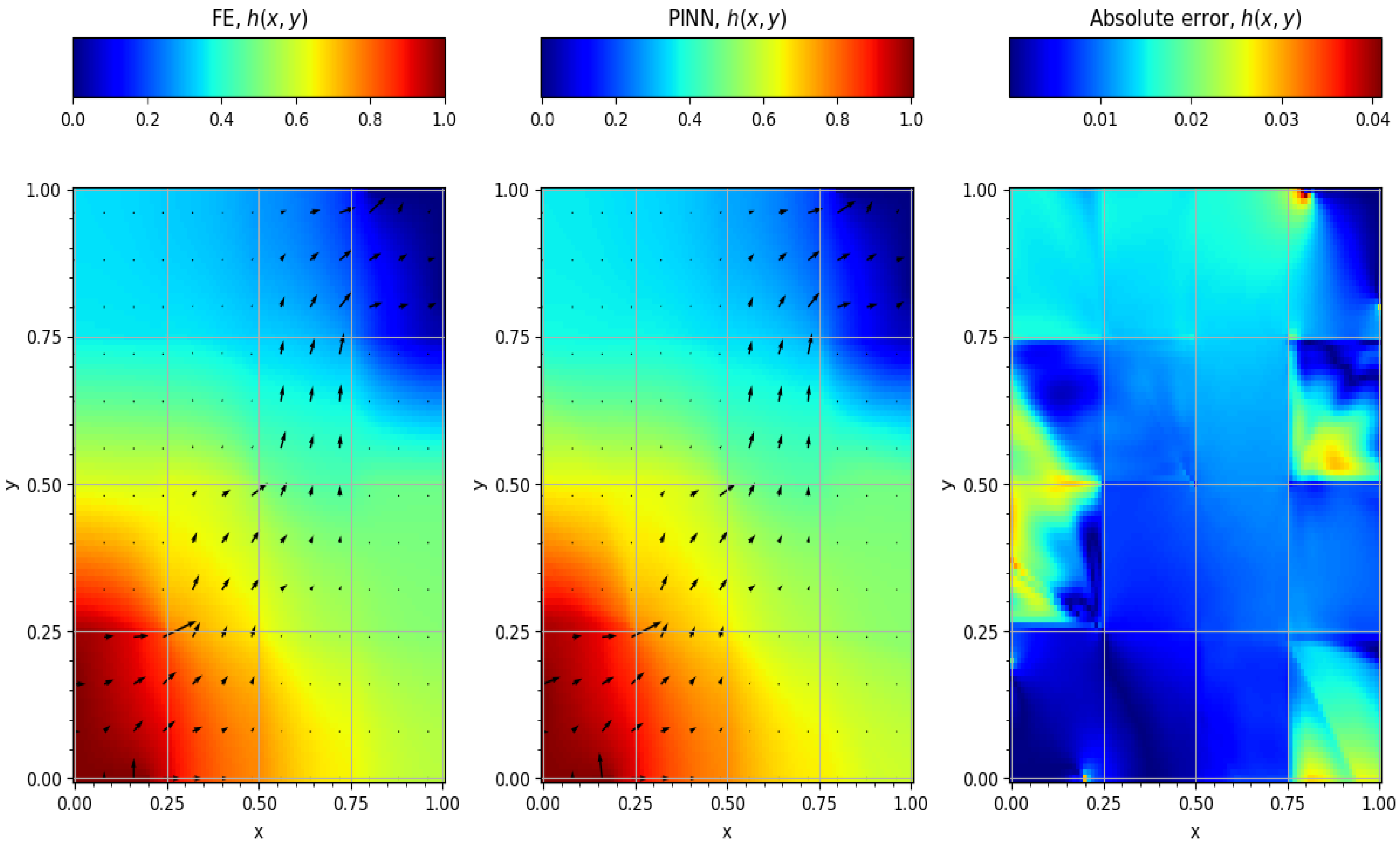
Implementation and results

Test case 3: High heterogeneous domain with 16 regular blocks

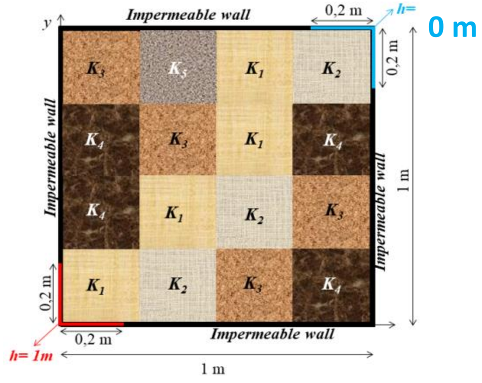


Implementation and results

Test case 3: High heterogeneous domain with 16 regular blocks



COMSOL PINNs Discrepancy



Good agreement between COMSOL and PINNS

Conclusion

- Current implementation of PINNs are facing convergence issues for flow in heterogeneous domain.

- A new implementation is suggested here by using the mixed pressure-velocity form of the governing equations.

- The new implementation extend the applicability of PINNs to heterogeneous domains

- It is generic and can be applied for different types of heterogeneity

- Perspectives: Fractured domains, coupled mass, heat and flow processes

Further applications

Weighting techniques

$$\mathcal{L}_{PDE} = \lambda_{Dx}\mathrm{R}_{Dx} + \lambda_{Dy}\mathrm{R}_{Dy} + \lambda_{CE}\mathrm{R}_{CE}$$

Selecting these weights has important impact on the convergence of the optimizer

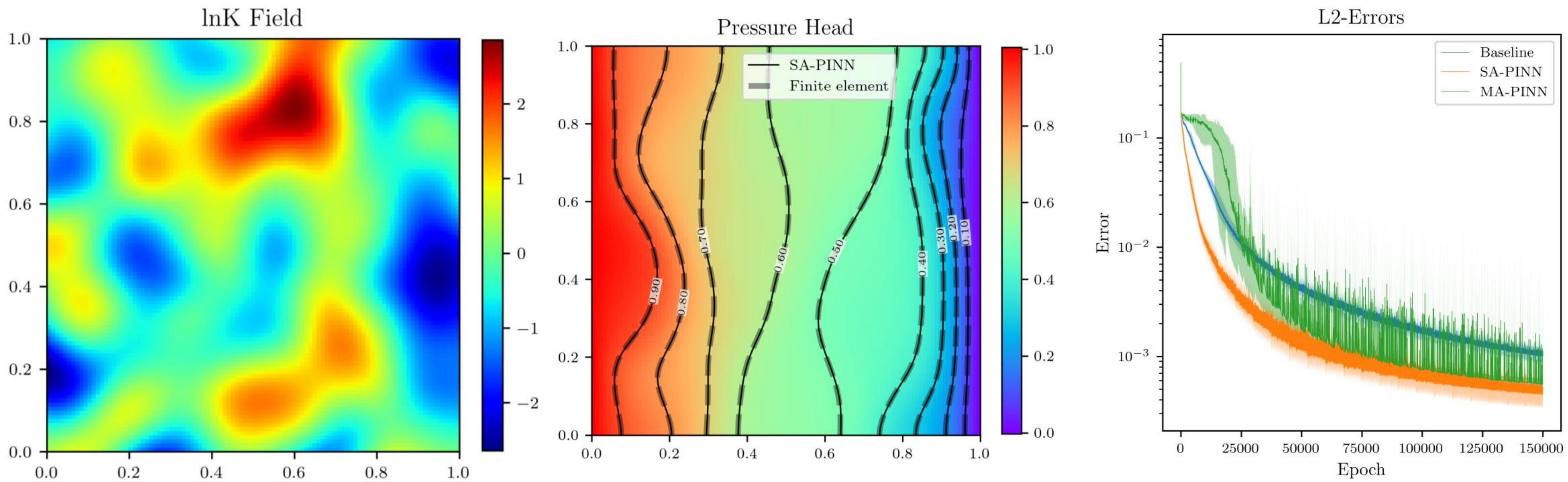
Max-Average Weighting Technique

$$\hat{\lambda}_k^n = \frac{max\{|\nabla_\theta \mathcal{L}_1|\}}{\lambda_k^{n-1}\overline{|\nabla_\theta \mathcal{L}_k|}}$$

Further applications

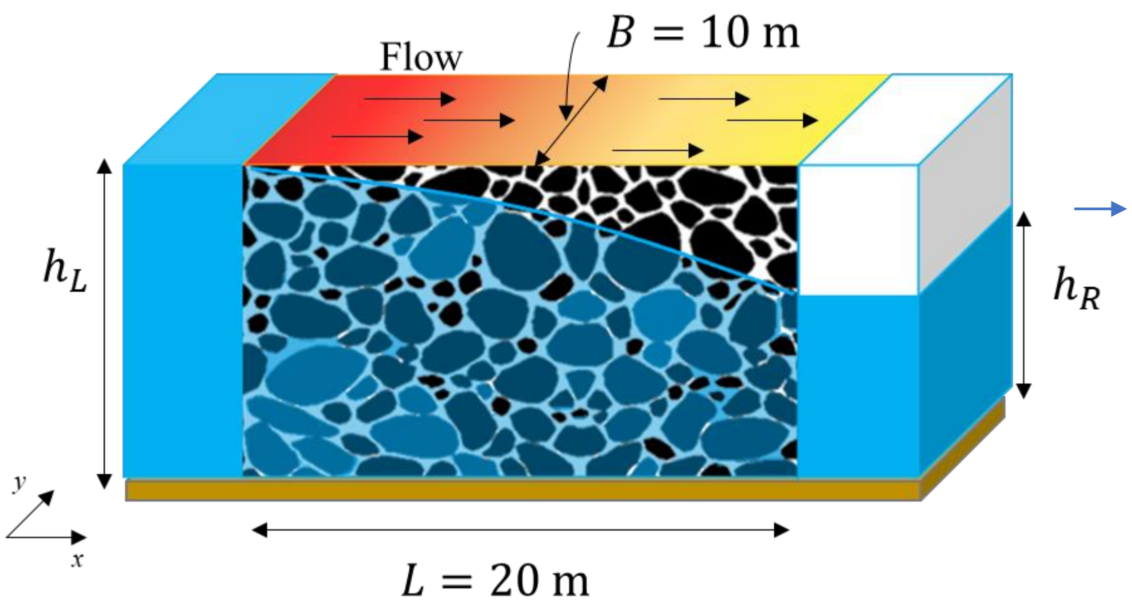
Weighting techniques

Max-Average Weighting Technique



Further applications

Flow in unconfined aquifers: time variability



Level of water variable over 7 days

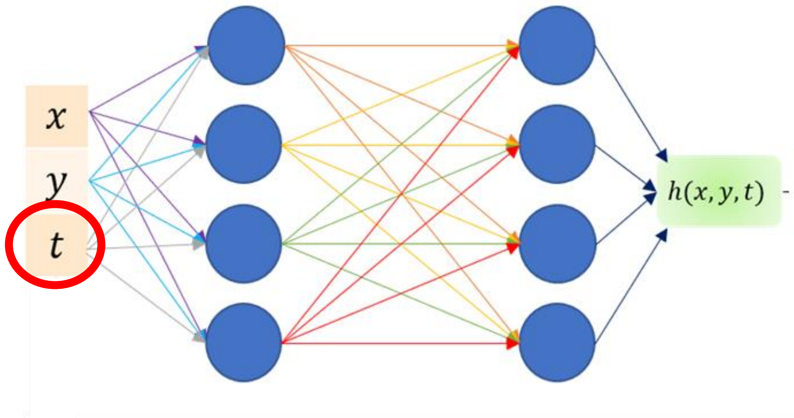
Experimental Site (SCERES)

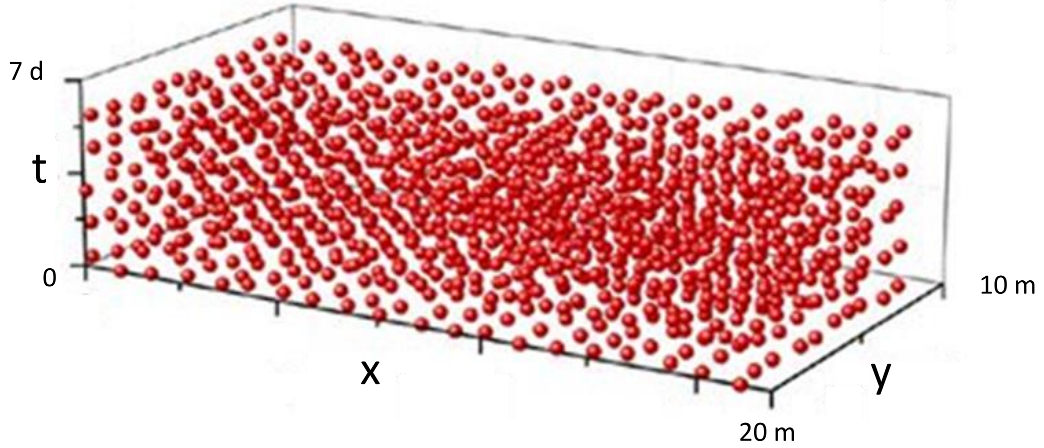
Equation of flow in unconfined aquifers

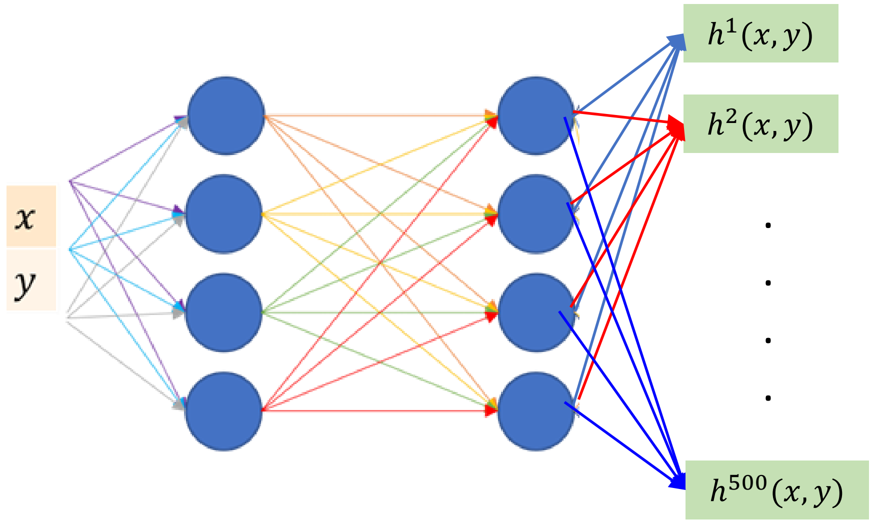
$$S\frac{\partial h}{\partial t} - \frac{\partial}{\partial x}\left(kh\frac{\partial h}{\partial x}\right) - \frac{\partial}{\partial y}\left(kh\frac{\partial h}{\partial y}\right) = 0$$

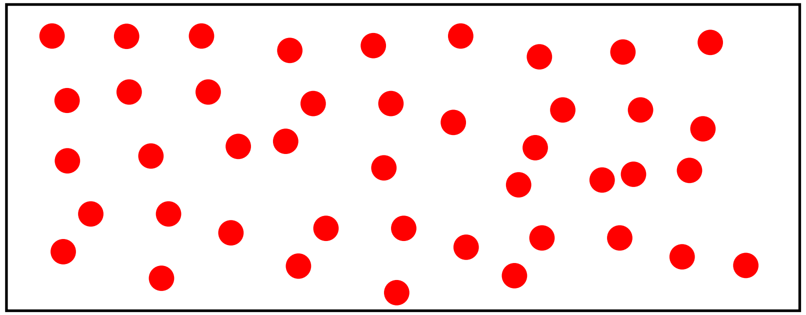
Further applications

Flow in unconfined aquifers: RK 500



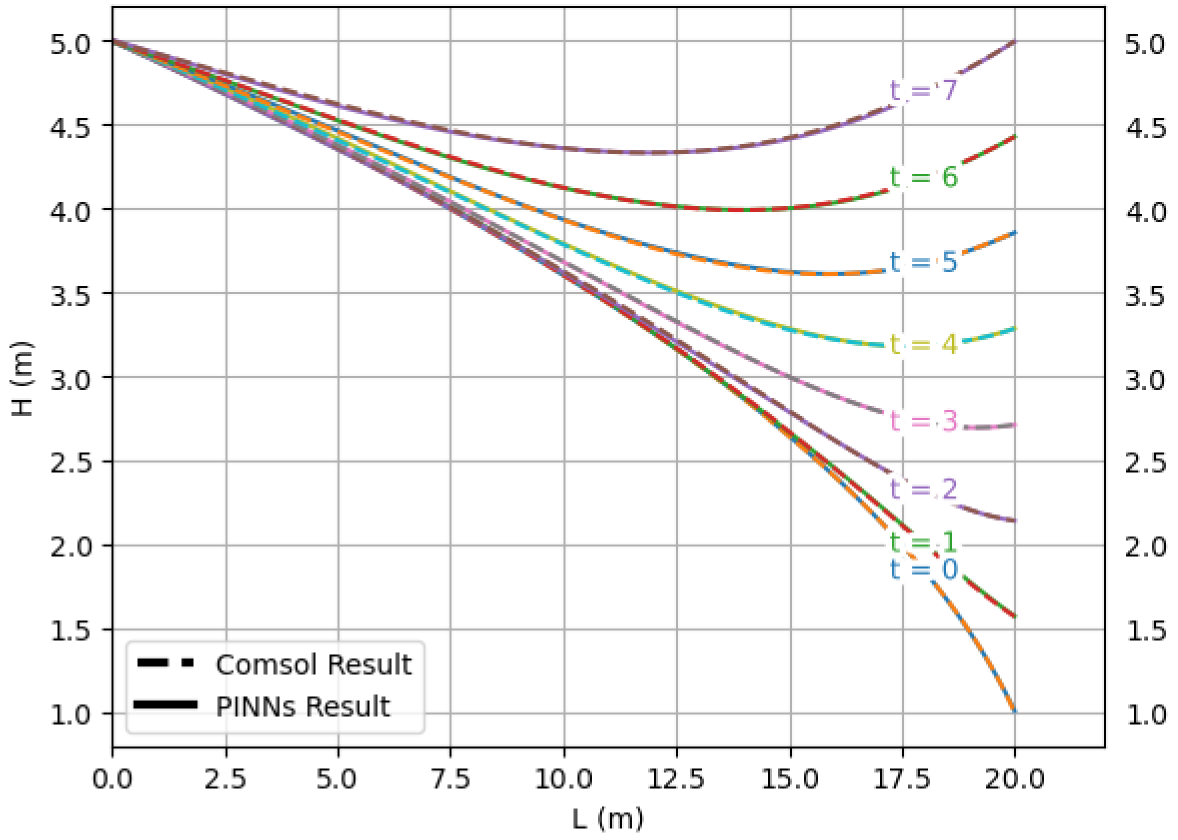






Further applications

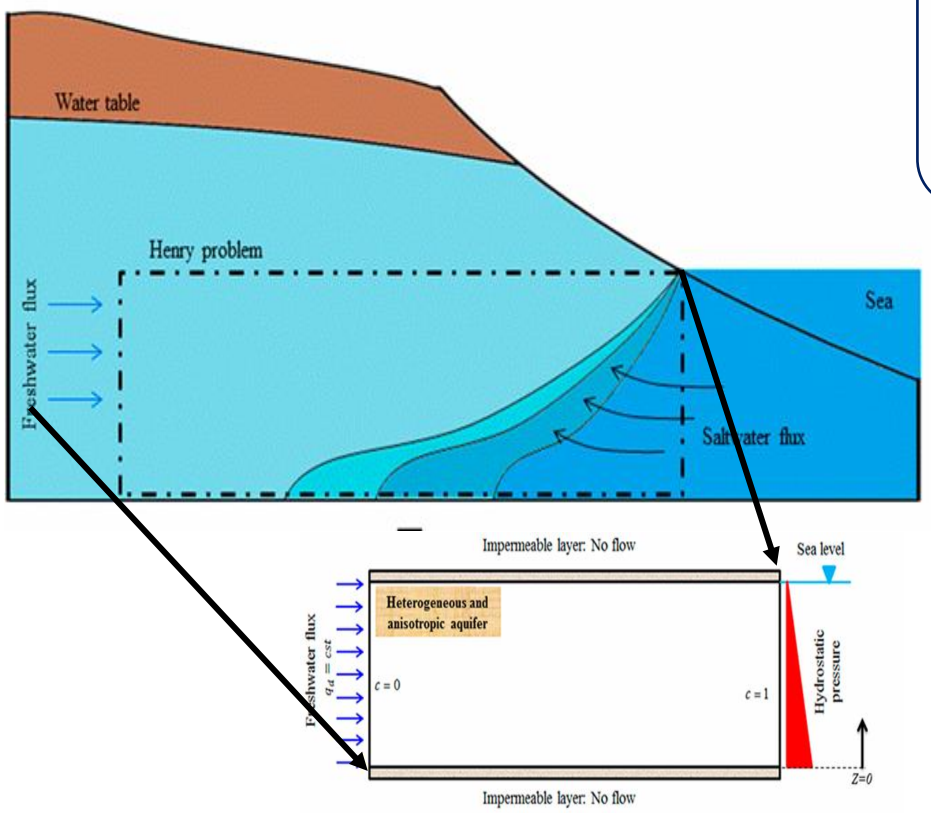
Flow in unconfined aquifers: RK 500



	Inputs	Adam Iterations	LBFGS Iterations	Final Loss	Time
Continuous Time	Space and time coordinates (x, y, t)	30,000	30,000	0.00012851	2:38:24
Time Discretization	Space coordinates (x, y)	30,000	4000	0.00002325	00:11:09

Further applications

Seawater intrusion

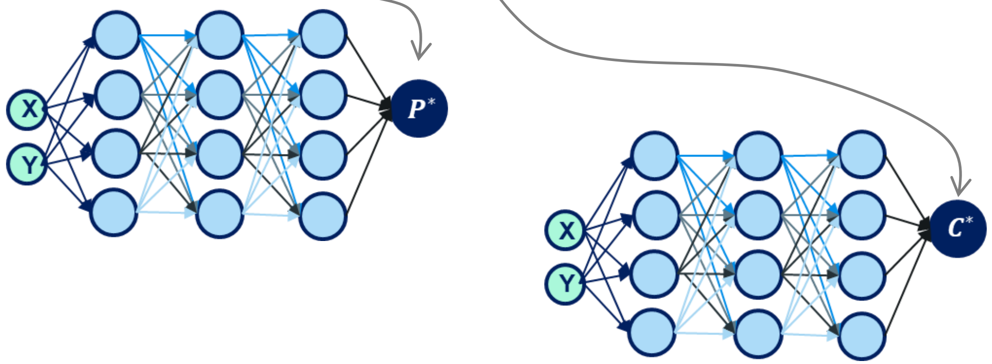


Water flow

$$\frac{\partial^2 p^*}{\partial x^{*2}} + \frac{\partial^2 p^*}{\partial z^{*2}} + Ra\,.\frac{\partial c^*}{\partial z^*} = 0$$

Salinity transp

$$u^*.\frac{\partial c^*}{\partial x^*} + v^*.\frac{\partial c^*}{\partial z^*} - Pe\left(\frac{\partial^2 c^*}{\partial x^{*2}} + \frac{\partial^2 c^*}{\partial z^{*2}}\right) = 0$$



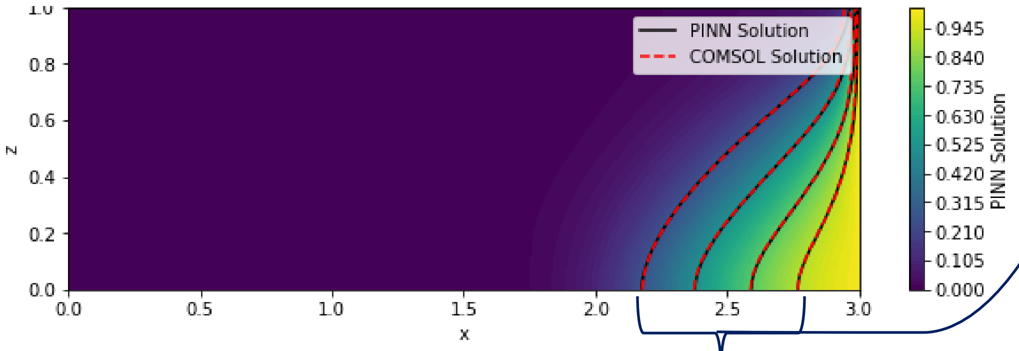
3 layers with 64 neurons
Tanh activation function

Further applications

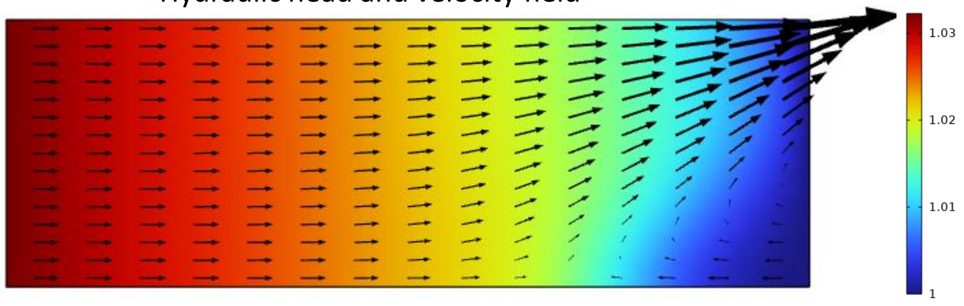
Seawater intrusion

Results for wide mixing zone

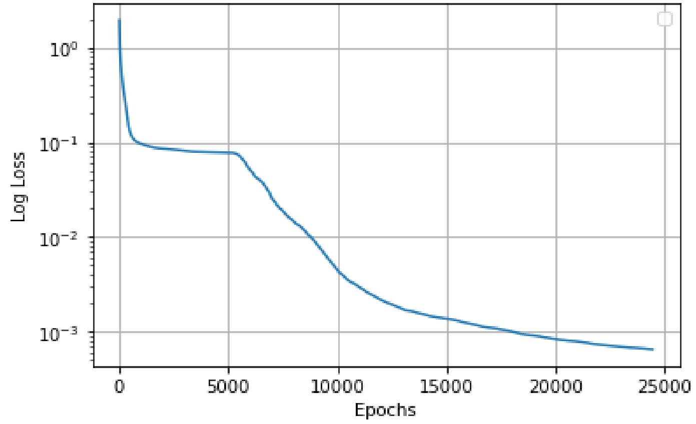
Salinity distribution in the aquifer

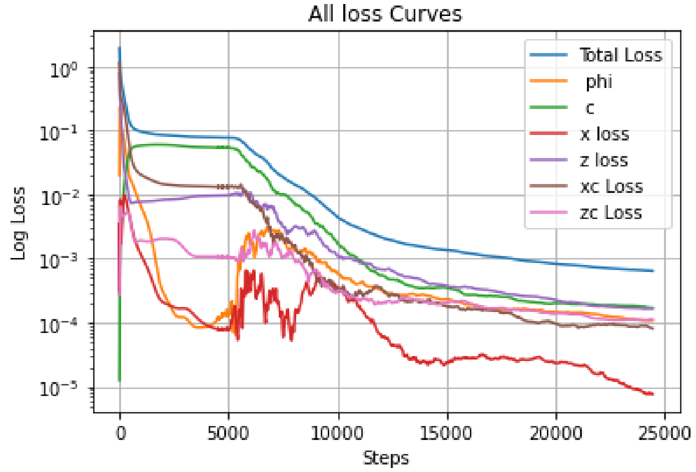


Hydraulic head and velocity field



Convergence of the training algorithm





Thank you for you attention