KU LEUVEN

LMSD Mecha(tro)nic System Dynamics

FLANDERS MAKE DRIVING INNOVATION IN MANUFACTURING

GREYDIENT

Confluences Mathématiques

21 November 2024, Paris, France

A practical introduction to Physics-Informed Neural Networks (PINNs)

Damien Bonnet-Eymard

The project leading to this application has received funding from the European Union's Horizon 2020 research and innovation program under the Marie Skłodowska-Curie grant agreement No 955393.

RELIABLE & ROBUST DESIGN

About me

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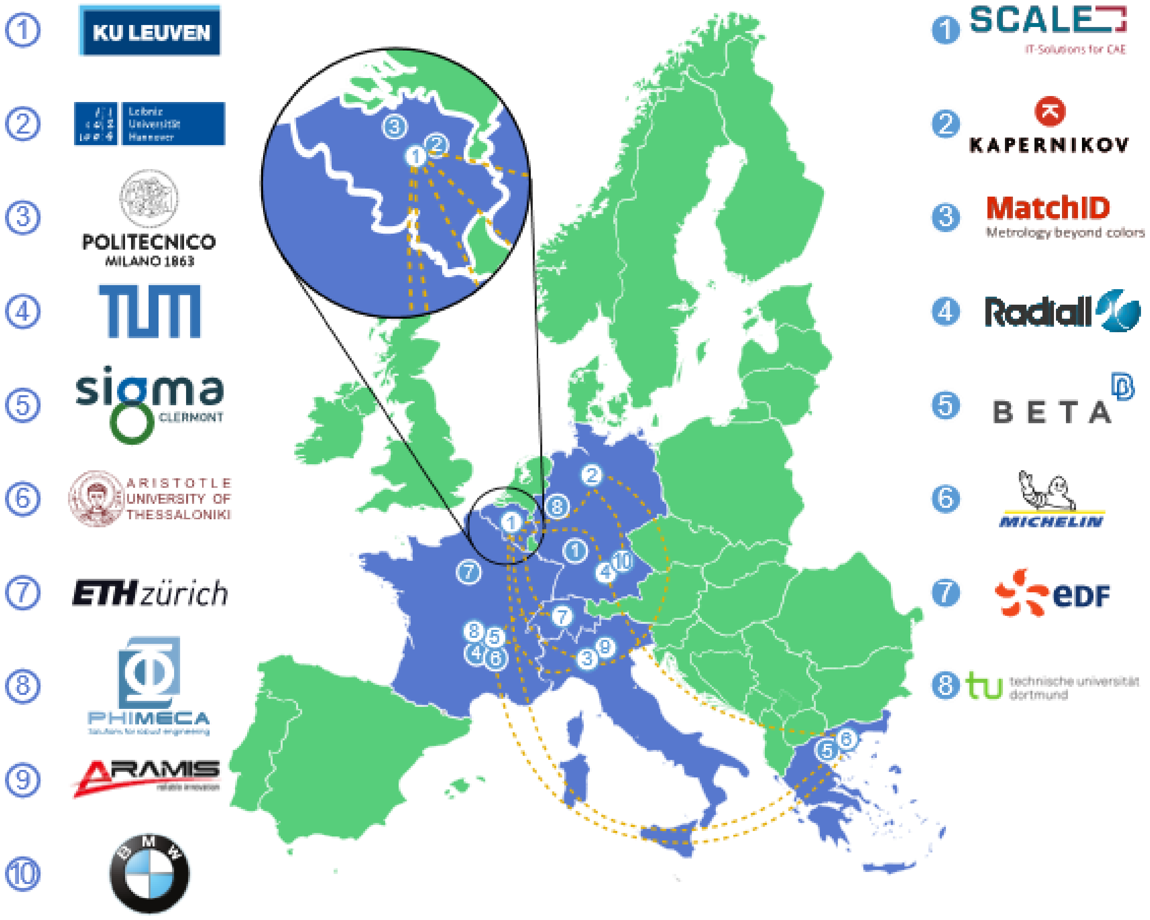
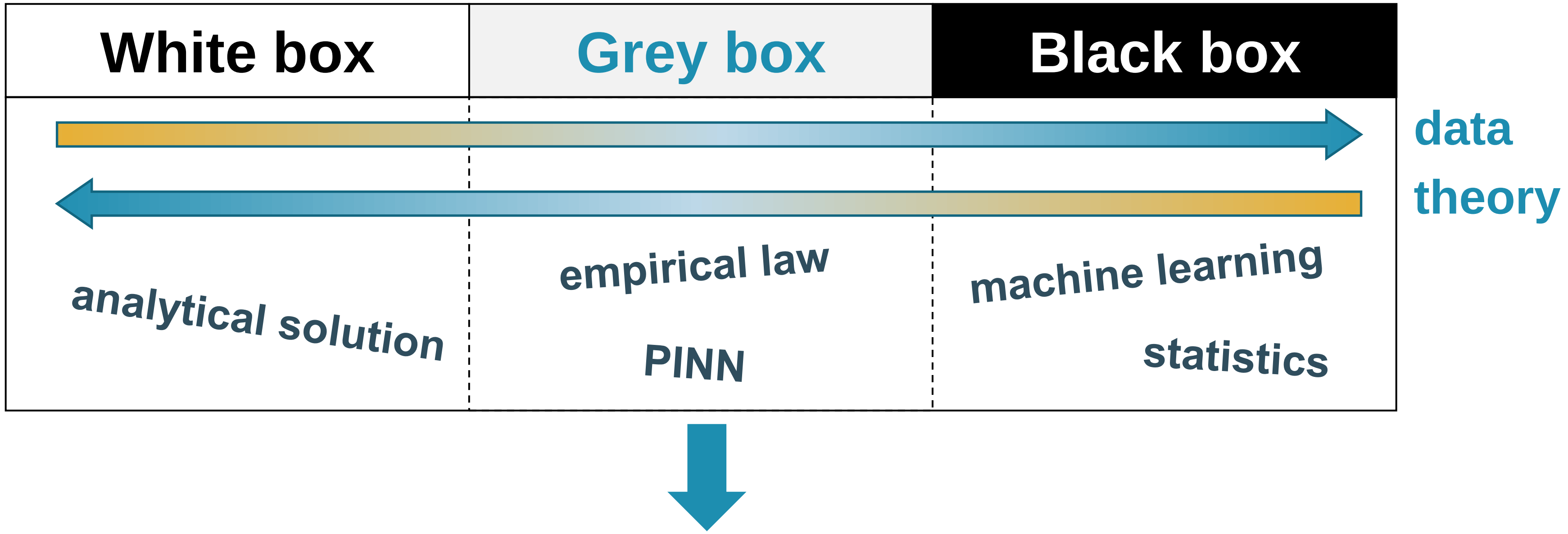
Physics-Informed neural networks for continuum mechanics applications

GREYDIENT

Marie Curie ITN project founded by the European commission



Greydient project : developing the grey-box methodology



most practical application

some physics – some data

I. Introduction to Physics-Informed Neural Networks

II. Improving the convergence of PINN

III. PINN for inverse quantification of material parameters

IV. PINN to propagate uncertainty

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Brief history of **P**hysics-**I**nformed **N**eural **N**etworks

2017

Physics Informed Deep Learning (Part I): Data-driven Solutions of Nonlinear Partial Differential Equations
Maziar Raissi, Paris Perdikaris, George Em Karniadakis

2019

Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations
Maziar Raissi, Paris Perdikaris, George Em Karniadakis

11621+ citations

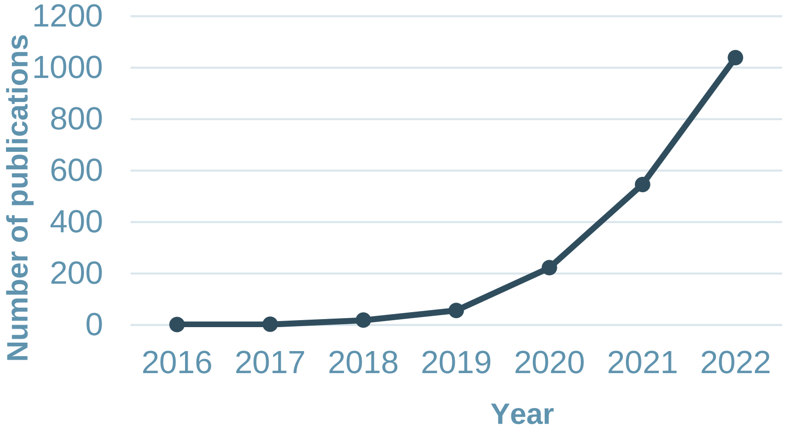


Fig.1 : Publication with title/abstract containing "Physics-Informed Neural Networks" on Dimensions (www.dimensions.ai)

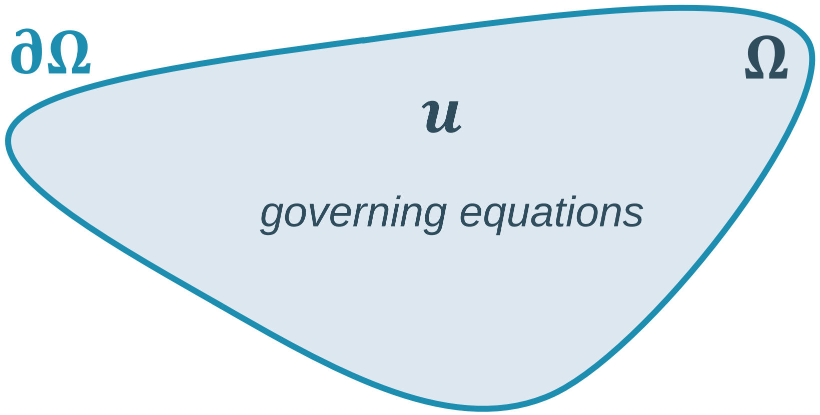
Why **PINNs** are so popular ?

- good at extrapolation/inverse problem
- benefits from late AI research
- easily applicable to any topic

⚠ *Convergence issues*

Motivation: solving a boundary value problem

Boundary **V**alue **P**roblem (**BVP**):



$$\mathbf{BC} : \partial\Omega : \ f_{BC}(u) = 0$$
$$\mathbf{IC} : u(t = 0) = u_0$$

Theory :

If well posed : *(BC well defined)*

➡ **Existence** and **uniqueness** of u[1]

The Ritz (Galerkin) method :

Discretization for numerical resolution

➡ **F**inite **E**lement **M**ethod

➡ **P**hysics-**I**nformed **N**eural **N**etworks

[1] « Picard–Lindelöf Theorem ». 2022. In *Wikipedia*.

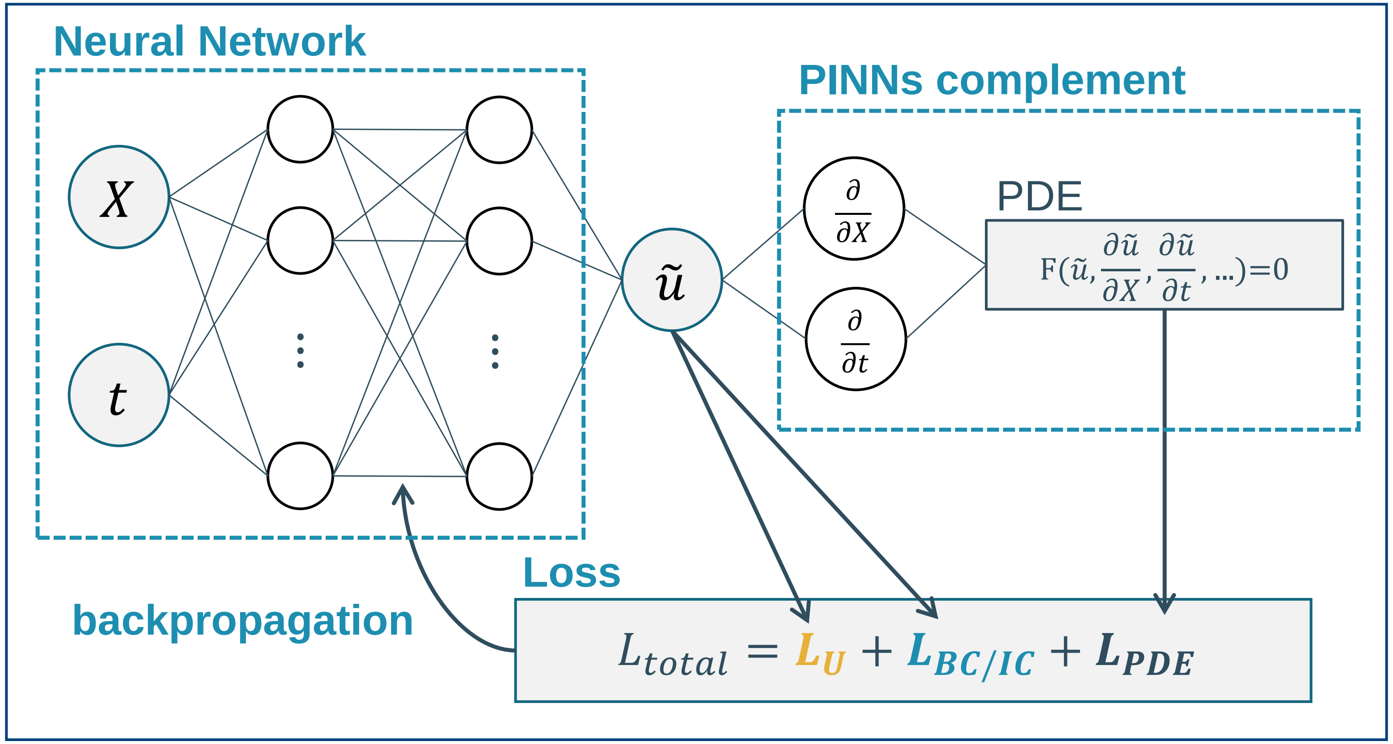
Comparing PINN and FEM : choosing the trial function space

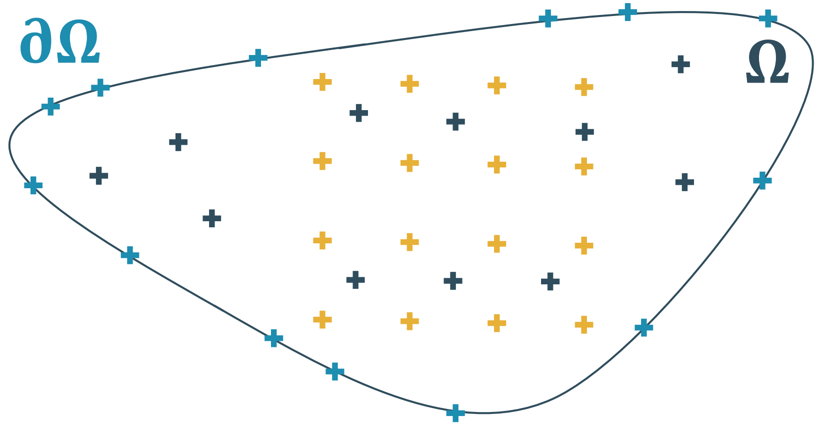
		Finite Element Method	Physics-Informed Neural Network
	Discretization	Mesh	Neural network architecture
	Trial/basis function	Piece-wise polynomials	Artificial neural network
	Parameters	Mesh nodal values	Network weight and biases
	Resolution	Matrix inversion	Stochastic optimization
	Hyper-parameter	Mesh (geometry, element)	Network, optimizer, implementation
Pros/ Cons	**Solution***	Unique	Non-unique (optimization and generalization error)
Pros/ Cons	**Boundary conditions**	All are needed (inversible matrix)	Can be missing
Pros/ Cons	**Incorporating measurement**	Can be expensive (need iterative updating)	Seamless during training (adding a residual loss term)

Hyper-parameter are crucial for the **convergence**

*of a well-posed problem for a given mesh/network

PINNs for a boundary value problem

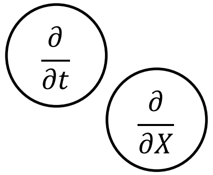




PDE evaluation : $L_{PDE} = \sum_{X \in \Omega} \left\| F(\tilde{u}, \frac{\partial \tilde{u}}{\partial X}, \frac{\partial \tilde{u}}{\partial t}, \ldots) \right\|$

BC value : $L_{BC/IC} = \sum_{X \in \partial\Omega} \| N(X) - u_{BC}(X) \|$

Ground truth data : $L_U = \sum_{X \in \Omega} \| N(X) - u \|$



performed using **A**utomatic **D**ifferentiation

Applying chain rule throw the network

PINNs for a boundary value problem

Loss

$$L_{total} = L_U + L_{BC/IC} + L_{PDE}$$

Imposing boundary condition :

SOFT

Adding a loss term :

$$L_{BC/IC} = \sum_{X \in \partial\Omega} \|N(X) - u_{BC}(X)\|$$

penalize non-respect of boundary conditions

HARD

Applying a mask function on the output :

$$u = F_{mask}[N(X)]$$

directly enforce boundary conditions

PINNs for a boundary value problem

Loss

$$L_{total} = L_U + \cancel{L_{BC/IC}} + L_{PDE}$$

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directly enforce boundary conditions

Hard BC example :

$u_{x=0} = u_{x=1} = 0$

$u_{y=0} = u_{y=1} = \cos(2\pi x)$

NN output

Mask function

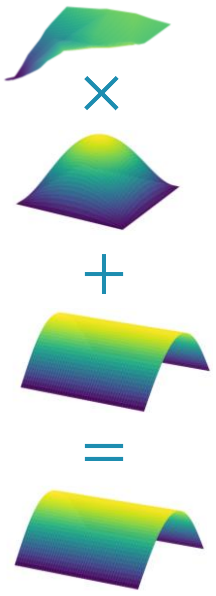
$= 0 \; on \; \partial\Omega_{BC}$

$\neq 0 \; elswhere$

BC function

$= U_{BC} \; on \; \partial\Omega_{BC}$

BC compliant output



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Relaxed constraint	Exact imposition
General and seamless to implement	Specific to every problem (generalization possible)
Multi-term optimization (make convergence harder)	Better convergence

Hard BC example :

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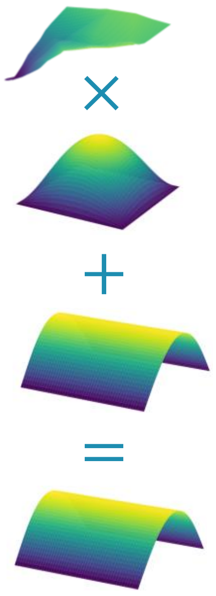

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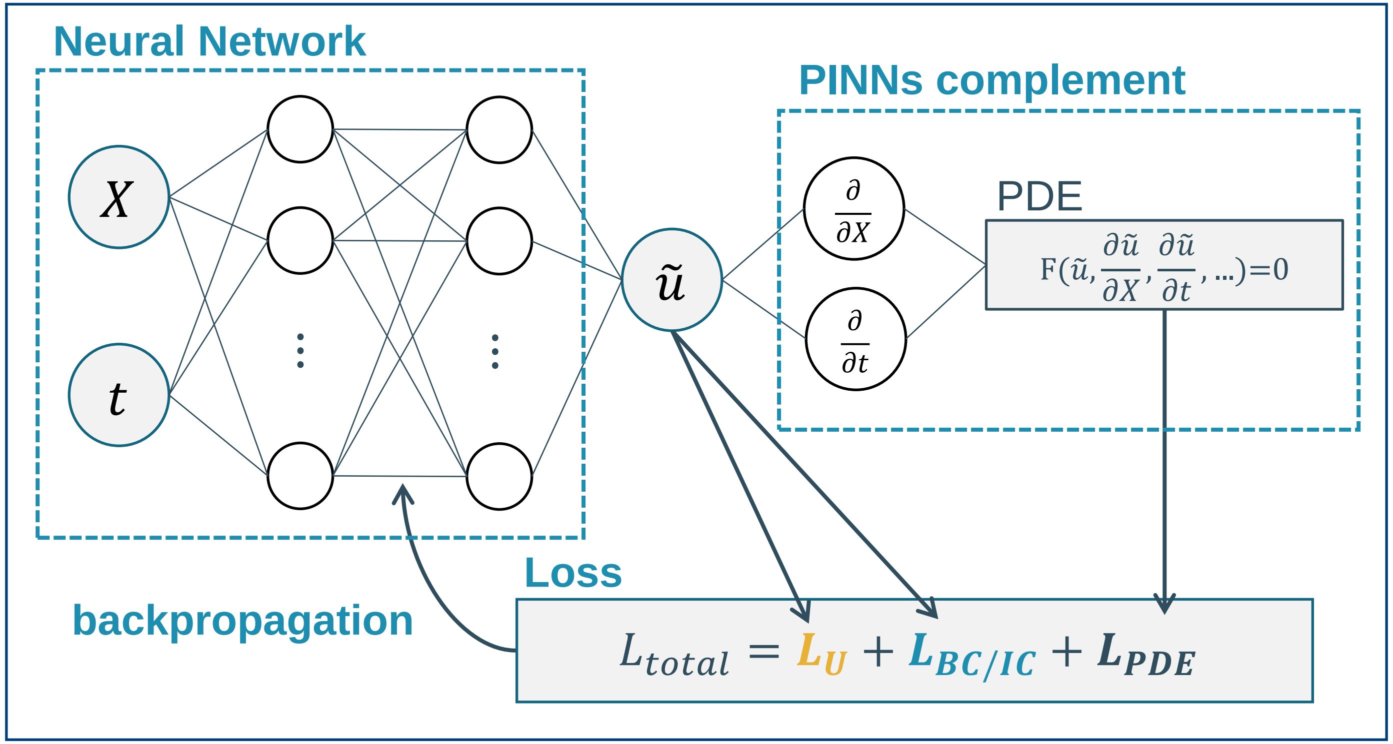
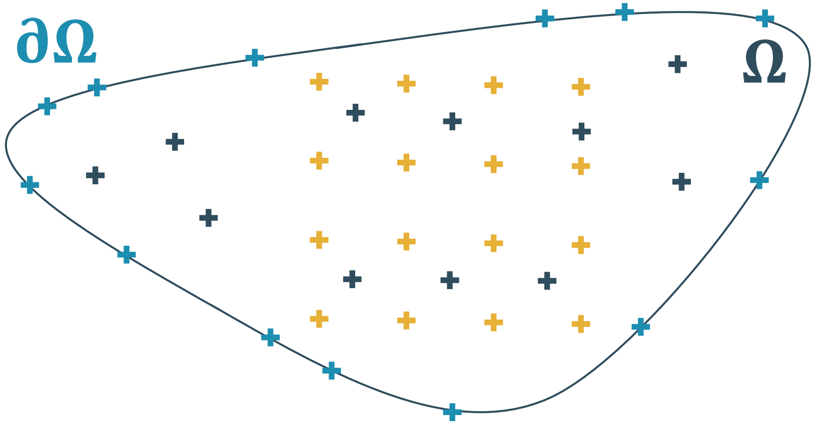
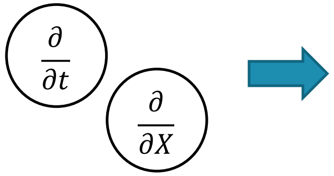
PINNs for a boundary value problem





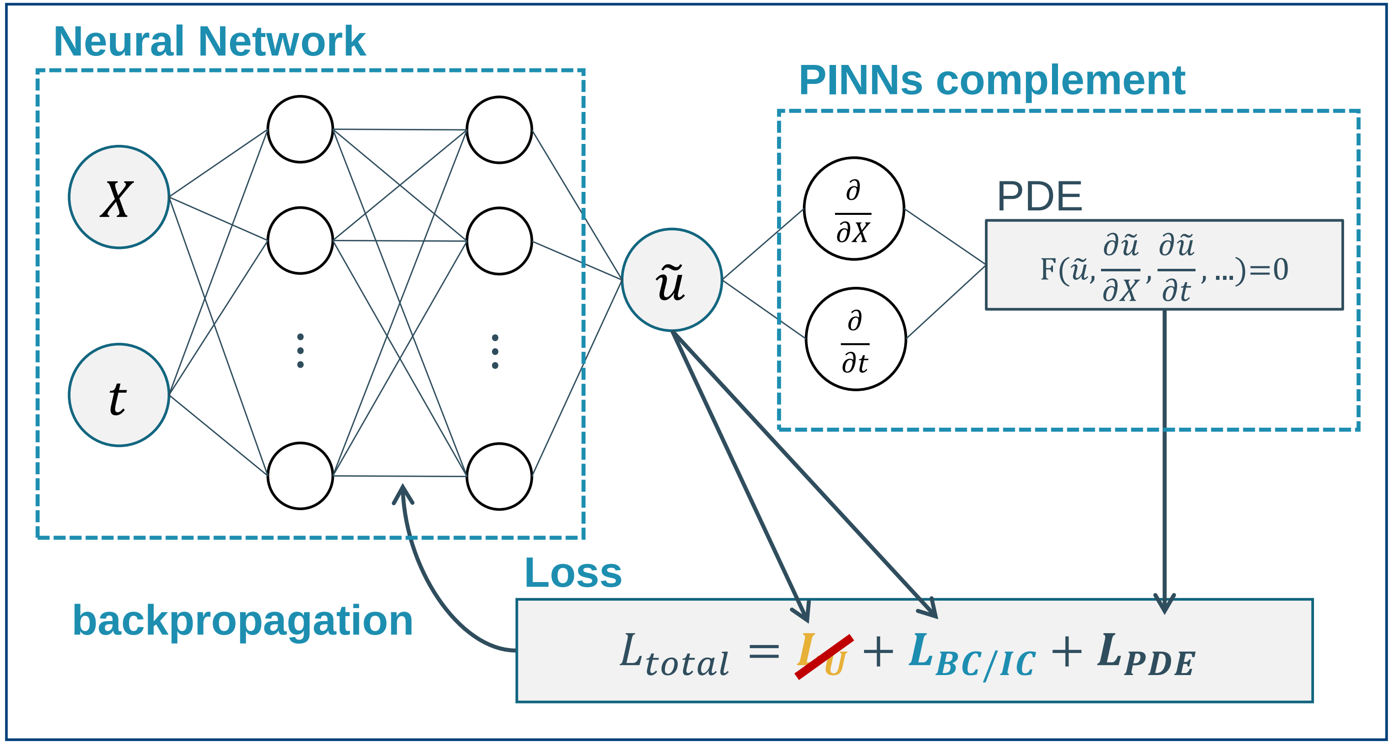
- *PDE evaluation :* $L_{PDE} = \sum_{X \in \Omega} \left\| F(\tilde{u}, \frac{\partial \tilde{u}}{\partial X}, \frac{\partial \tilde{u}}{\partial t}, \dots) \right\|$
- *BC value :* $L_{BC/IC} = \sum_{X \in \partial\Omega} \| N(X) - u_{BC}(X) \|$
- *Ground truth data :* $L_U = \sum_{X \in \Omega} \| N(X) - u \|$



performed using **A**utomatic **D**ifferentiation

Applying chain rule throw the network

PINNs for a boundary value problem



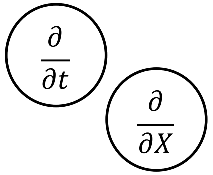
$$L_{PDE} = \sum_{X \in \Omega} \left\| F\left(\tilde{u}, \frac{\partial \tilde{u}}{\partial X}, \frac{\partial \tilde{u}}{\partial t}, \ldots\right) \right\|$$

$$L_{BC/IC} = \sum_{X \in \partial\Omega} \| N(X) - u_{BC}(X) \|$$

~~$$L_U = \sum_{X \in \Omega} \| N(X) - u \|$$~~

Forward problem :

➡ *no need for labeled data*



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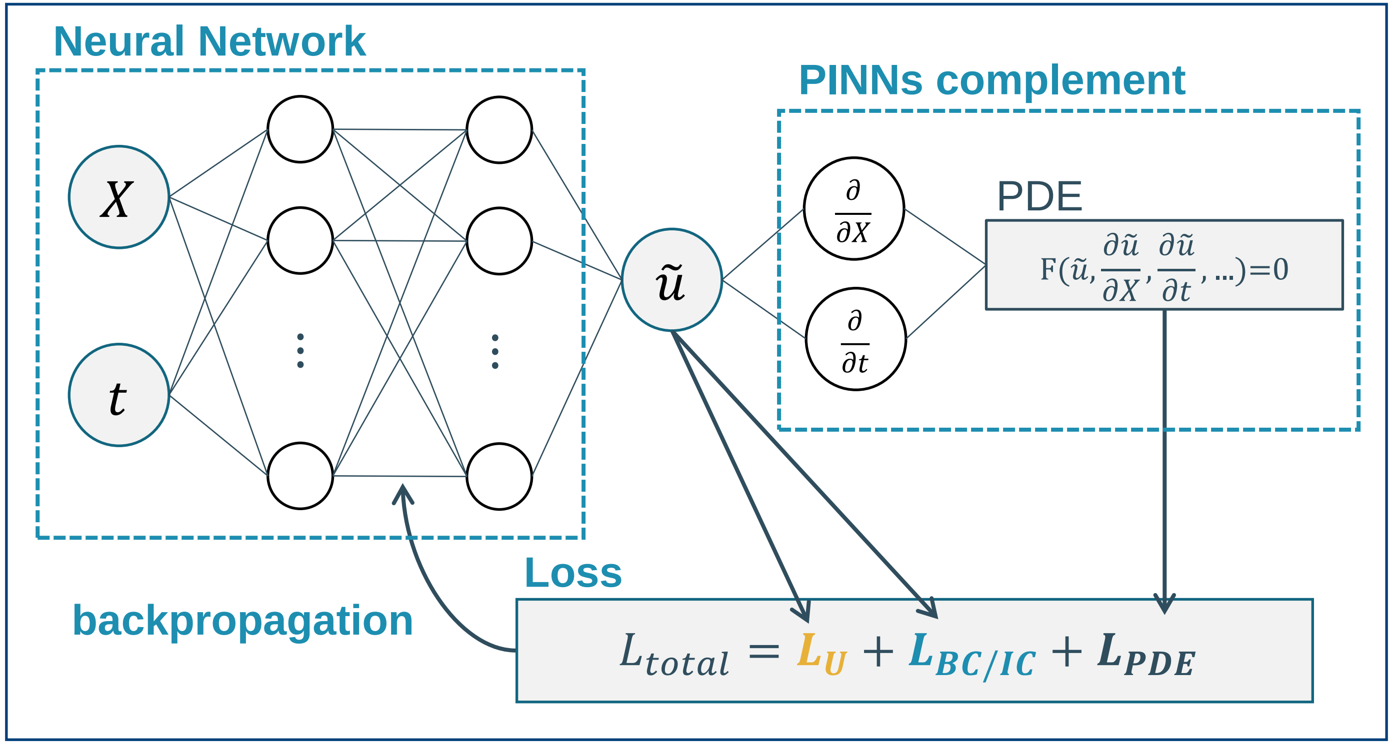
PINNs for a boundary value problem



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Forward problem :

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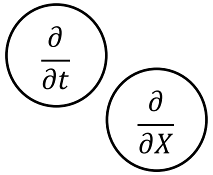


➡ performed using **A**utomatic **D**ifferentiation

Applying chain rule throw the network

Inverse problem :

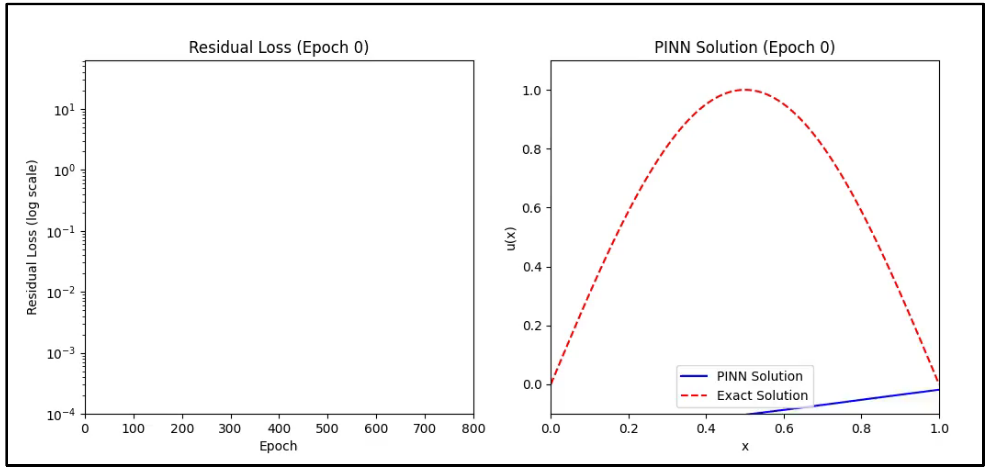
Determining PDE parameters

$F_{p_i}(\tilde{u}, \frac{\partial \tilde{u}}{\partial X}, \frac{\partial \tilde{u}}{\partial t}, \ldots)$ p_i : *model parameters*

PINN to solve 1D Poisson equation

$$\begin{cases} -\frac{\partial^2 u}{\partial x^2} = \pi^2 \sin(\pi x), \quad x \in [0,1] \\ u(0) = u(1) = 0 \end{cases}$$

Exact solution : $u(x) = \sin(\pi x)$



PyTorch

```python
import torch
import torch.nn as nn
import torch.optim as optim

class PINN(nn.Module):
    def __init__(self):
        super().__init__()
        self.net = nn.Sequential(
            nn.Linear(1, 20), nn.Tanh(),
            nn.Linear(20, 20), nn.Tanh(),
            nn.Linear(20, 1)
        )

    def forward(self, x):
        return self.net(x)

def poisson_residual(x, model):
    u = model(x)
    u_x = torch.autograd.grad(u, x, torch.ones_like(u), create_graph=True)[0]
    u_xx = torch.autograd.grad(u_x, x, torch.ones_like(u_x), create_graph=True)[0]
    f = torch.pi**2*torch.sin(torch.pi * x)
    return (-u_xx - f).pow(2).mean()  # Residual loss

def boundary_loss(model):
    return model(torch.tensor([[0.0]]))**2 + model(torch.tensor([[1.0]]))**2  # Enforce u(0)=u(1)=0

# Initialize model and optimizer
model = PINN()
optimizer = optim.Adam(model.parameters(), lr=0.001)

# Training loop
for epoch in range(1000):
    x = torch.rand(100, 1, requires_grad=True)
    loss = poisson_residual(x, model) + boundary_loss(model)
    optimizer.zero_grad()
    loss.backward()
    optimizer.step()
    if epoch % 100 == 0:
        print(f"Epoch {epoch}, Loss: {loss.item()}")
```

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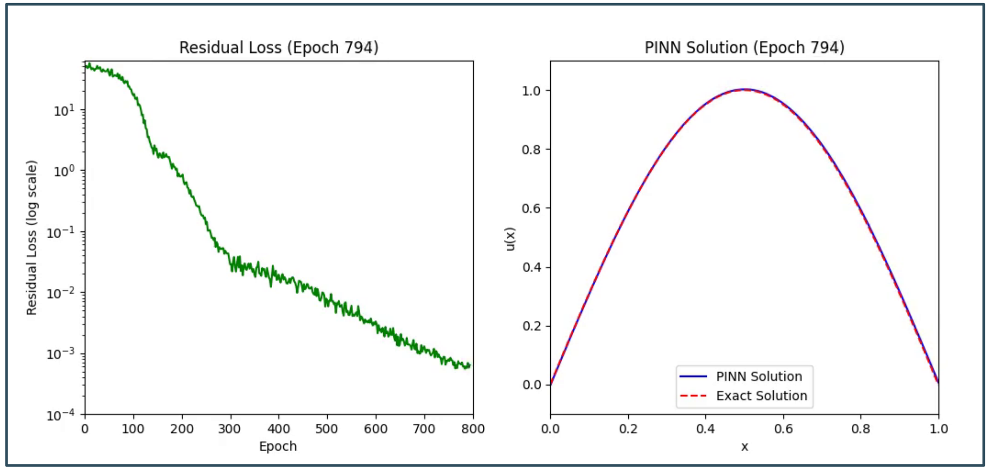

DeepXDE

```python
import deepxde as dde
import torch

def pde(x, y):
    dy_xx = dde.grad.hessian(y, x)
    return -dy_xx - np.pi ** 2 * torch.sin(np.pi * x)

def boundary(x, on_boundary):
    return on_boundary

def func(x):
    return np.sin(np.pi * x)

geom = dde.geometry.Interval(-1, 1)
bc = dde.icbc.DirichletBC(geom, func, boundary)
data = dde.data.PDE(geom, pde, bc, 16, 2, solution=func, num_test=100)

layer_size = [1] + [50] * 3 + [1]
activation = "tanh"
initializer = "Glorot uniform"
net = dde.nn.FNN(layer_size, activation, initializer)

model = dde.Model(data, net)
model.compile("adam", lr=0.001, metrics=["l2 relative error"])

losshistory, train_state = model.train(iterations=10000)
```

PINN software

Python

- ***DeepXDE*[1]**
- *SciANN*
- *NeuroDiffEq*
- *IDRLnet*
- …

Julia

- *NeuralPDE.jl*

Nvidia

- *Modulus*

DeepXDE

A library for scientific machine learning and physics-informed learning

- ➢ Multi-backend : Tensorflow, Pytorch, JAX…
- ➢ Simplified implementation, lot of features
- ➢ Very active community, latest research implemented
- ➢ Well documented with a lot of examples

[1] Lu, Lu, Xuhui Meng, Zhiping Mao, et George E. Karniadakis. 2021. « DeepXDE: A deep learning library for solving differential equations ». *SIAM Review* 63 (1): 208-28. https://doi.org/10.1137/19M1274067

Literature review of PINN

Review papers

- **2021** Physics-informed machine learning
- **2022** Scientific Machine Learning through Physics-Informed Neural Networks: Where we are and What's next
- **2024** From PINNs to PIKANs: Recent Advances in Physics-Informed Machine Learning

Github repository

bitzhangcy/Neural-PDE-Solver

1000+ papers by category

- **Application papers**
  __Mechanics__, Chemistry, Robotics,…
- **Network architecture**
  Convolution, Graph Network, __Separable-PINN__, KAN…
- **New implementation**
  Variational form, __Mixed PINN__…
- **Extension**
  __Uncertainty Quantification__…
- **Improving training**
  Sampling strategy, Fourier features, Loss balance…

⚠ *Convergence issues*

[1] Karniadakis, George Em, Ioannis G. Kevrekidis, Lu Lu, Paris Perdikaris, Sifan Wang, and Liu Yang. "Physics-Informed Machine Learning." Nature Reviews Physics 3, no. 6 (June 2021): 422–40. https://doi.org/10.1038/s42254-021-00314-5.
[2] Cuomo, Salvatore, Vincenzo Schiano di Cola, Fabio Giampaolo, Gianluigi Rozza, Maziar Raissi, and Francesco Piccialli. "Scientific Machine Learning through Physics-Informed Neural Networks: Where We Are and What's Next." arXiv, June 7, 2022. https://doi.org/10.48550/arXiv.2201.05624
[3] Toscano, Juan Diego, Vivek Oommen, Alan John Varghese, Zongren Zou, Nazanin Ahmadi Daryakenari, Chenxi Wu, and George Em Karniadakis. "From PINNs to PIKANs: Recent Advances in Physics-Informed Machine Learning." arXiv, October 22, 2024. https://doi.org/10.48550/arXiv.2410.13228.

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Techniques from the literature

An Expert's Guide to Training Physics-informed Neural Networks

Sifan Wang, Shyam Sankaran, Hanwen Wang, Paris Perdikaris

- Non-dimensionalization
- Fourier features
- Causal/curriculum training
- Loss weighting strategies

Problem implementation

- Maximizing hard constraints
- Mixed-PINN formulation

Network architecture

- **S**eparable **PINN**
- **K**olmogorov-**A**rnold **N**etwork

Optimization algorithm

- Adam + LBFGS
- Adaptative sampling

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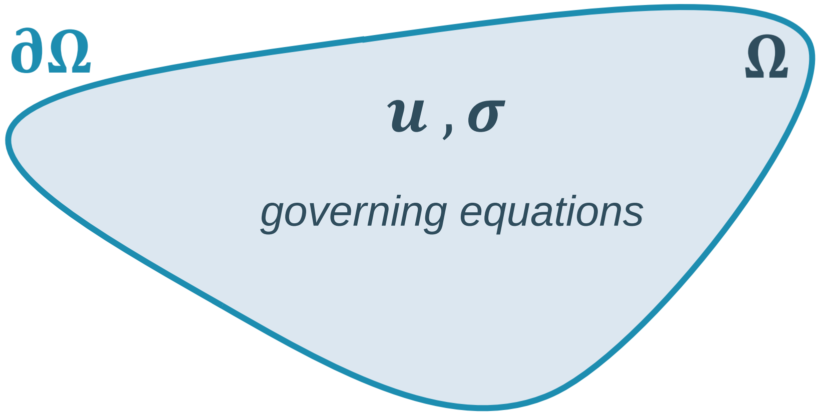
PINNs framework for continuum mechanics

Boundary **V**alue **P**roblem (**BVP**):



Boundary conditions :

$\partial\Omega_u \,:\, u = u_{BC}$	*in displacement*
$\partial\Omega_f \,:\, \sigma.\vec{n} = \vec{F}_{BC}$	*in stress*

Fields :

u	*displacement*
ε	*strain tensor*
σ	*stress tensor*

→ *Which output for the network ?*

Equations :

$\varepsilon_{ij} = \frac{1}{2}\left(u_{i,j} + u_{j,i}\right)$	*small deformation*
$\sigma_{ij} = f(\varepsilon_{ij})$	*material law*
$\sigma_{ij,j} + f_i = 0$	*momentum balance*

$$\rightarrow \quad L_{PDE} = \sum_{\tilde{\sigma}\in\Omega} \left\| \widetilde{\sigma_{ij,j}} + f_i \right\|$$

PINNs framework for continuum mechanics

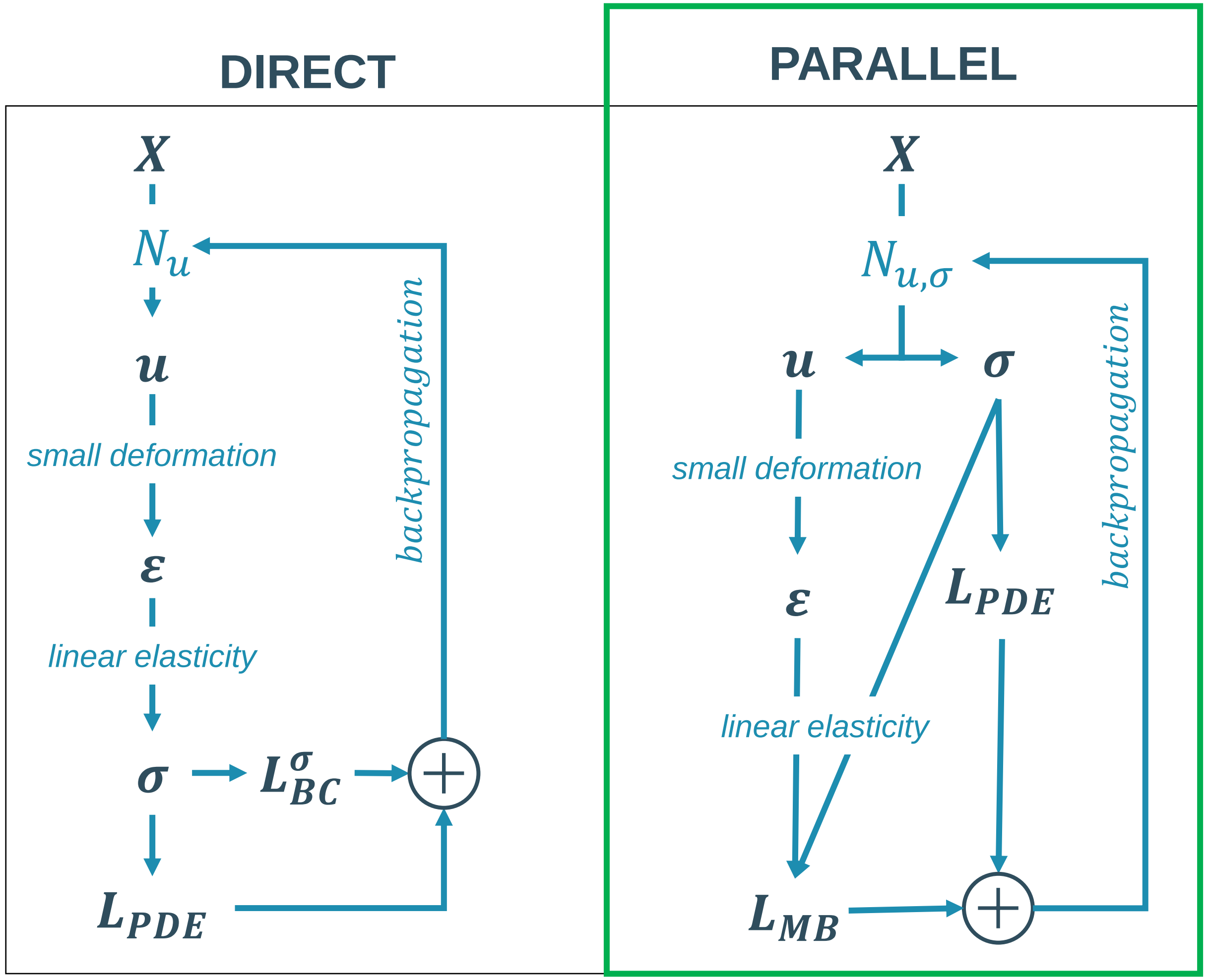
Which output for the network ? $\boldsymbol{u}$? $\boldsymbol{\sigma}$? $\boldsymbol{both}$?

Goal : maximise the number of **hard constraint**

Hard boundary condition only on the output of a neural network

	DIRECT	PARALLEL
$\boldsymbol{BC_u}$	Hard	Hard
$\boldsymbol{BC_\sigma}$	Soft	Hard
Material law	Hard	Soft

+ limit the order of the derivatives



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Introduction to Separable-PINN

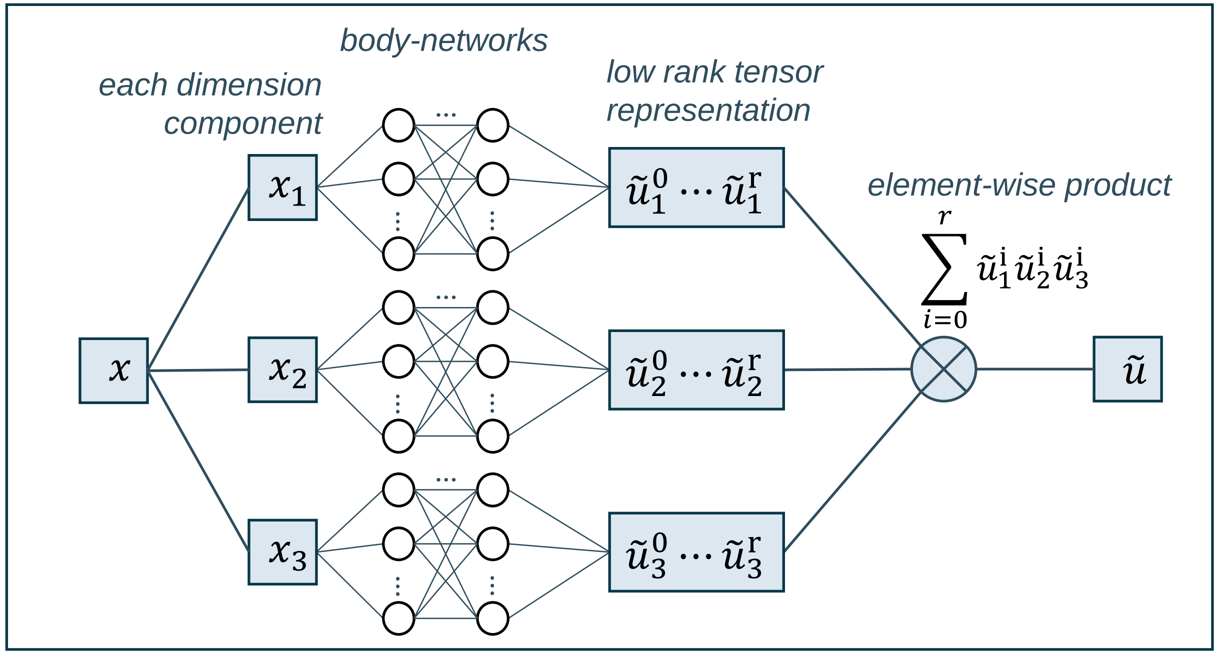


Fig. 1: SPINN architecture for a 3D problem

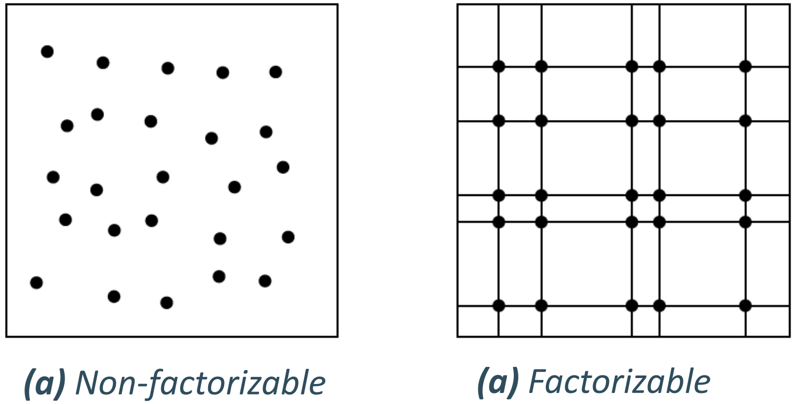


Fig. 2: Illustrative example of factorizable-coordinates constraint required for SPINN sampling

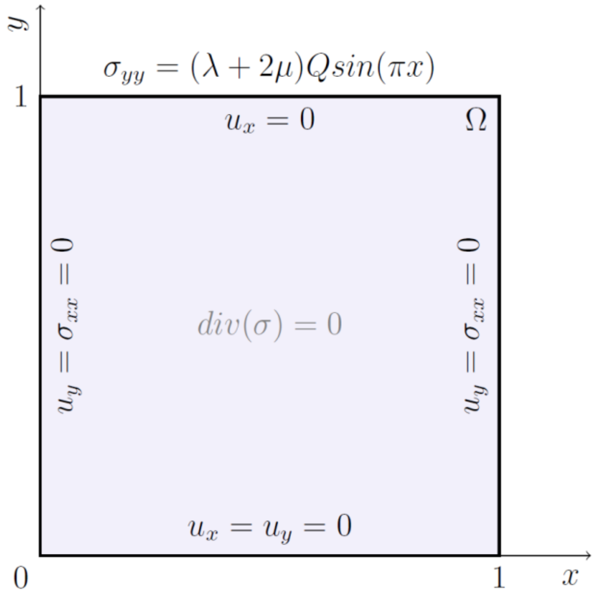
- A different network for each dimension
- Low-rank tensor approximation
- Expressive enough

- Faster computation
- N^d points for the price of $N \times d$
- Bring limitations in the geometry

[1] Cho, Junwoo, Seungtae Nam, Hyunmo Yang, Seok-Bae Yun, Youngjoon Hong, et Eunbyung Park. 2023. « Separable Physics-Informed Neural Networks ». arXiv. https://doi.org/10.48550/arXiv.2306.15969.

PINN for continuum mechanics : example from literature[1]

Domain and boundary condition :



Volumic forces :

$$f_x = \lambda \left[4\pi^2 \cos(2\pi x)\sin(\pi y) - \pi \cos(\pi x) Q y^3\right] + \mu \left[9\pi^2 \cos(2\pi x)\sin(\pi y) - \pi \cos(\pi x) Q y^3\right]$$

$$f_y = \lambda \left[-3\sin(\pi x) Q y^2 + 2\pi^2 \sin(2\pi x)\cos(\pi y)\right] + \mu \left[-6\sin(\pi x) Q y^2 + 2\pi^2 \sin(2\pi x)\cos(\pi y) + \pi^2 \sin(\pi x) Q y^4/4\right].$$

Exact solution :

$$u_x(x,y) = \cos(2\pi x)\sin(\pi y),$$
$$u_y(x,y) = \sin(\pi x) Q y^4/4.$$

Parameters :

$\lambda = 1$
$\mu = 0{,}5$

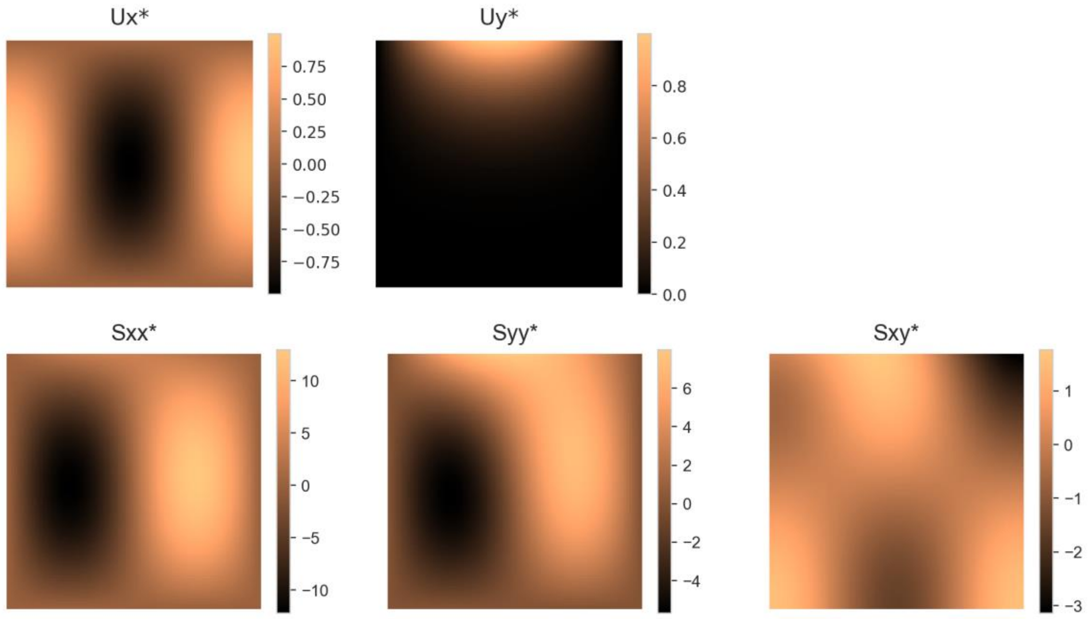
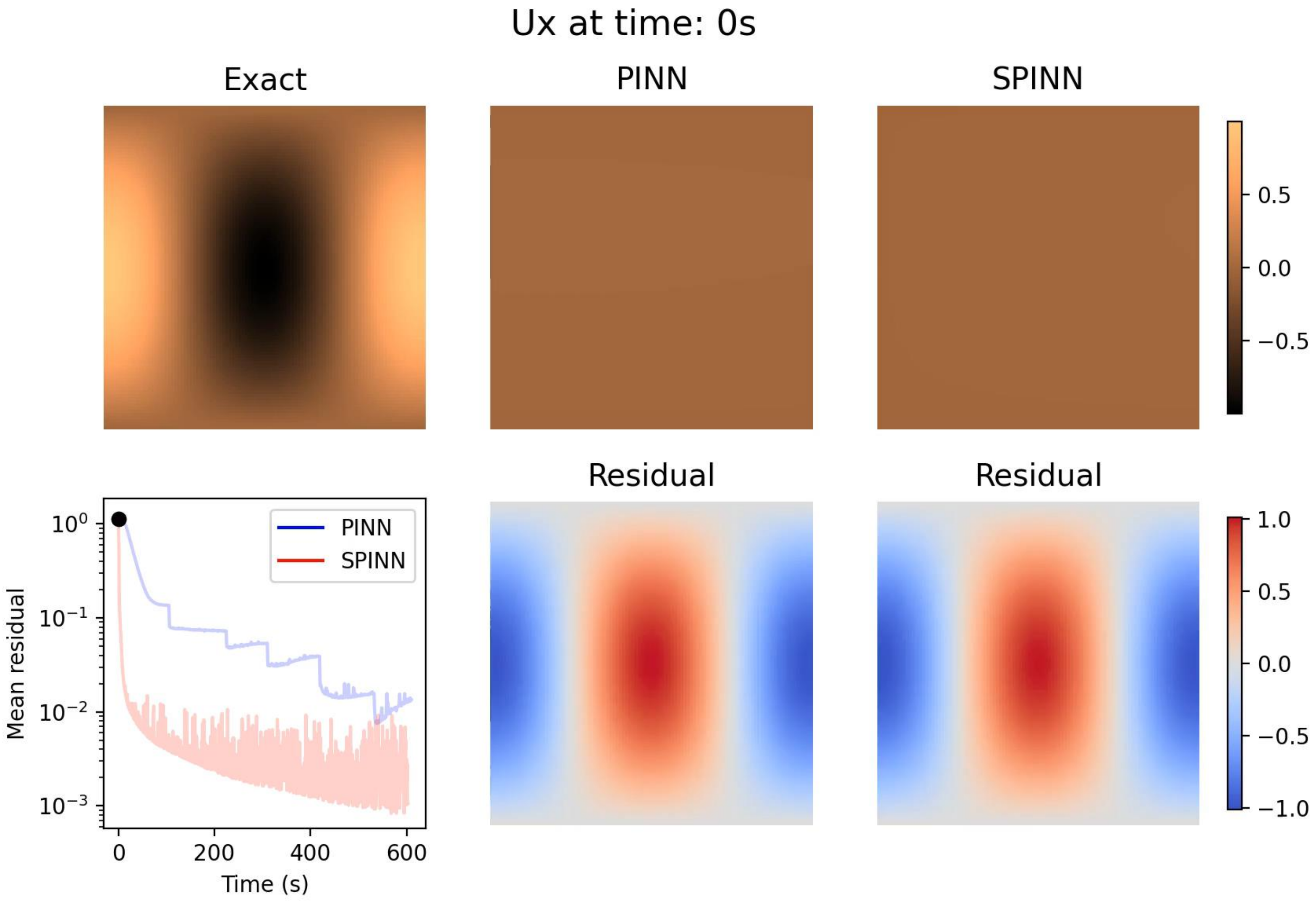


Fig. 2 : Exact displacement and stress solution of the problem

[1] Haghighat, Ehsan, Maziar Raissi, Adrian Moure, Hector Gomez, and Ruben Juanes. “A Deep Learning Framework for Solution and Discovery in Solid Mechanics.” *ArXiv:2003.02751 [Cs, Stat]*, May 6, 2020.

PINN vs SPINN on a continuum mechanics example



SPINN outperforms in both speed and accuracy

KU LEUVEN

Techniques from the literature

An Expert's Guide to Training Physics-informed Neural Networks
Sifan Wang, Shyam Sankaran, Hanwen Wang, Paris Perdikaris

- non-dimensionalization
- Fourier feature
- causal/curriculum training
- loss weighting strategies

Problem implementation

- Maximizing hard constraints
- Mixed-PINN formulation

Network architecture

- **S**eparable **PINN**
- **K**olmogorov-**A**rnold **N**etwork

Optimization algorithm

- Adam + LBFGS
- Adaptative sampling

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Resources

Separable Physics-Informed Neural Networks for Robust Inverse Quantification in Solid Mechanics

Damien Bonnet-Eymard, Augustin Persoons, Matthias Faes, and David Moens

Presented at ISRERM 2024 conference - Available on ResearchGate

Code and results are available online :

www.github.com/bonneted/ISRERM2024

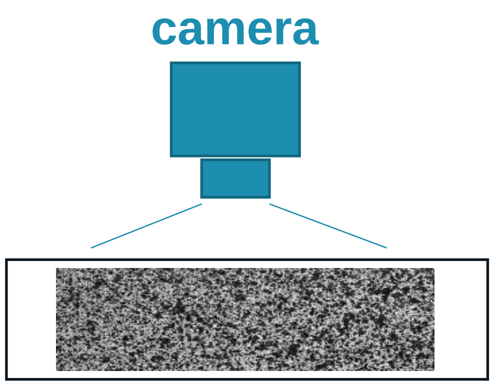
relies on

SPINN branch of DeepXDE

- bonneted/deepxde at SPINN (github.com)
- still under development

Inverse quantification from full field measurements

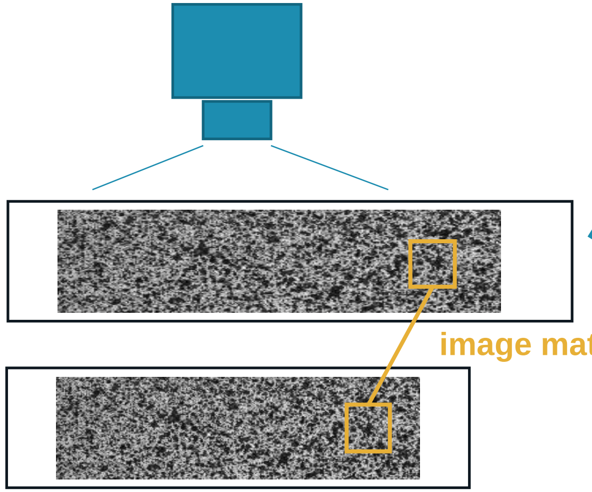
Digital **I**mage **C**orrelation



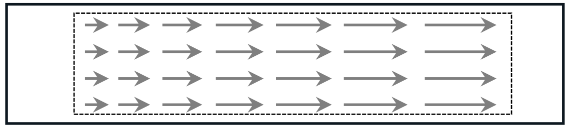
Inverse quantification from full field measurements

Digital **I**mage **C**orrelation

camera



Full field measurement



Inverse quantification :

- ***V**irtual **F**ield **M**ethod*
- ***F**inite **E**lement **M**ethod **U**pdating*
- …

Can struggle on complex geometry or material behavior

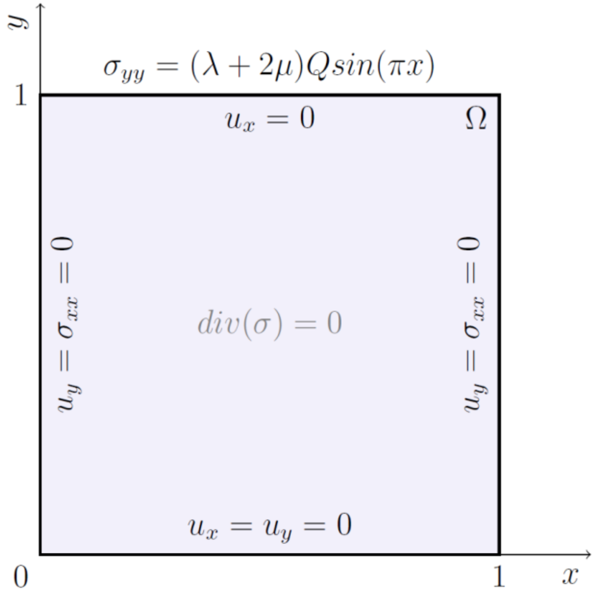
Use **P**hysics **I**nformed **N**eural **N**etworks as an alternative inverse method

Material properties

?

PINNs for continuum mechanics : case study from literature[1]

Domain and boundary condition :



Volumic forces :

$$
\begin{aligned}
f_x &= \lambda \left[4\pi^2 \cos(2\pi x)\sin(\pi y) - \pi \cos(\pi x) Q y^3\right] \\
&\quad + \mu \left[9\pi^2 \cos(2\pi x)\sin(\pi y) - \pi \cos(\pi x) Q y^3\right] \\
f_y &= \lambda \left[-3\sin(\pi x) Q y^2 + 2\pi^2 \sin(2\pi x)\cos(\pi y)\right] \\
&\quad + \mu \left[-6\sin(\pi x) Q y^2 + 2\pi^2 \sin(2\pi x)\cos(\pi y) + \pi^2 \sin(\pi x) Q y^4/4\right].
\end{aligned}
$$

Exact solution :

$$
\begin{aligned}
u_x(x,y) &= \cos(2\pi x)\sin(\pi y), \\
u_y(x,y) &= \sin(\pi x) Q y^4/4.
\end{aligned}
$$

Parameters :

$\lambda = 1$
$\mu = 0{,}5$

Find elasticity parameters

+ measurements

ground truth displacement

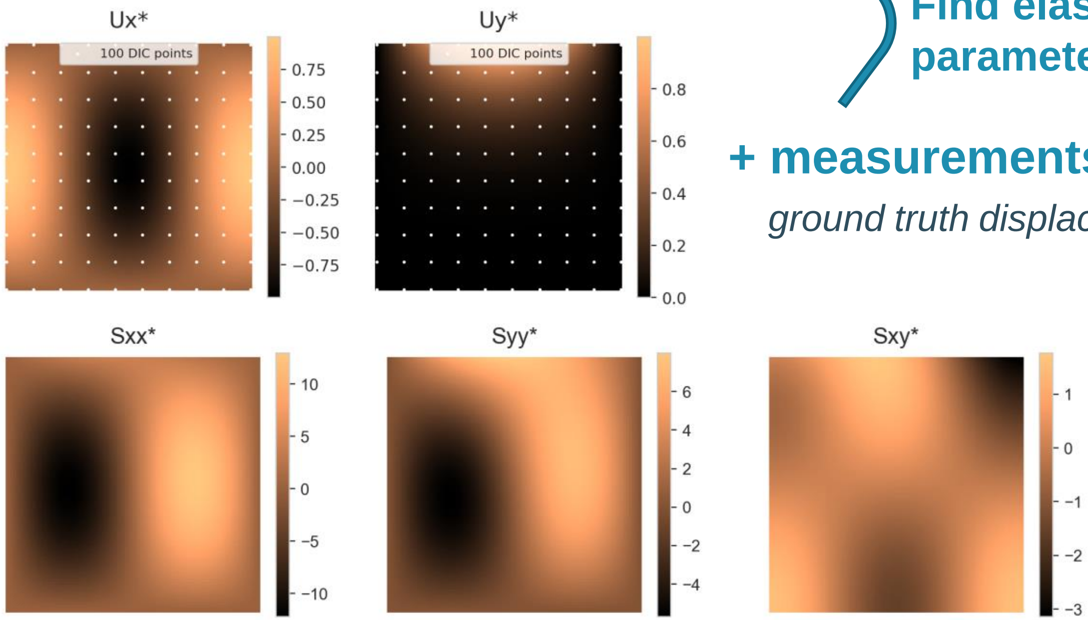
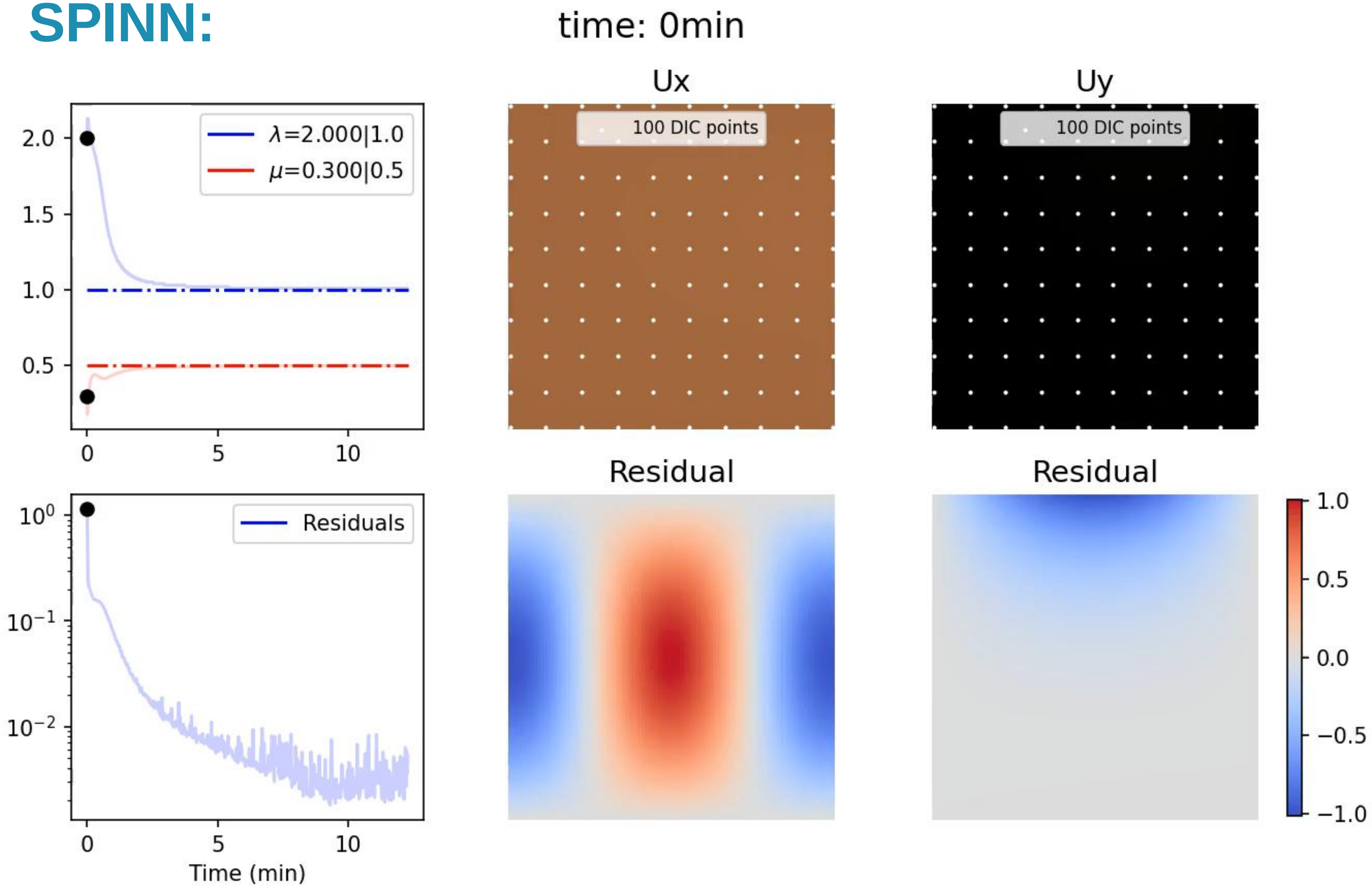


Fig. 2 : Exact displacement and stress solution of the problem

[1] Haghighat, Ehsan, Maziar Raissi, Adrian Moure, Hector Gomez, and Ruben Juanes. "A Deep Learning Framework for Solution and Discovery in Solid Mechanics." *ArXiv:2003.02751 [Cs, Stat]*, May 6, 2020.

Inverse quantification of elasticity parameters : SPINN

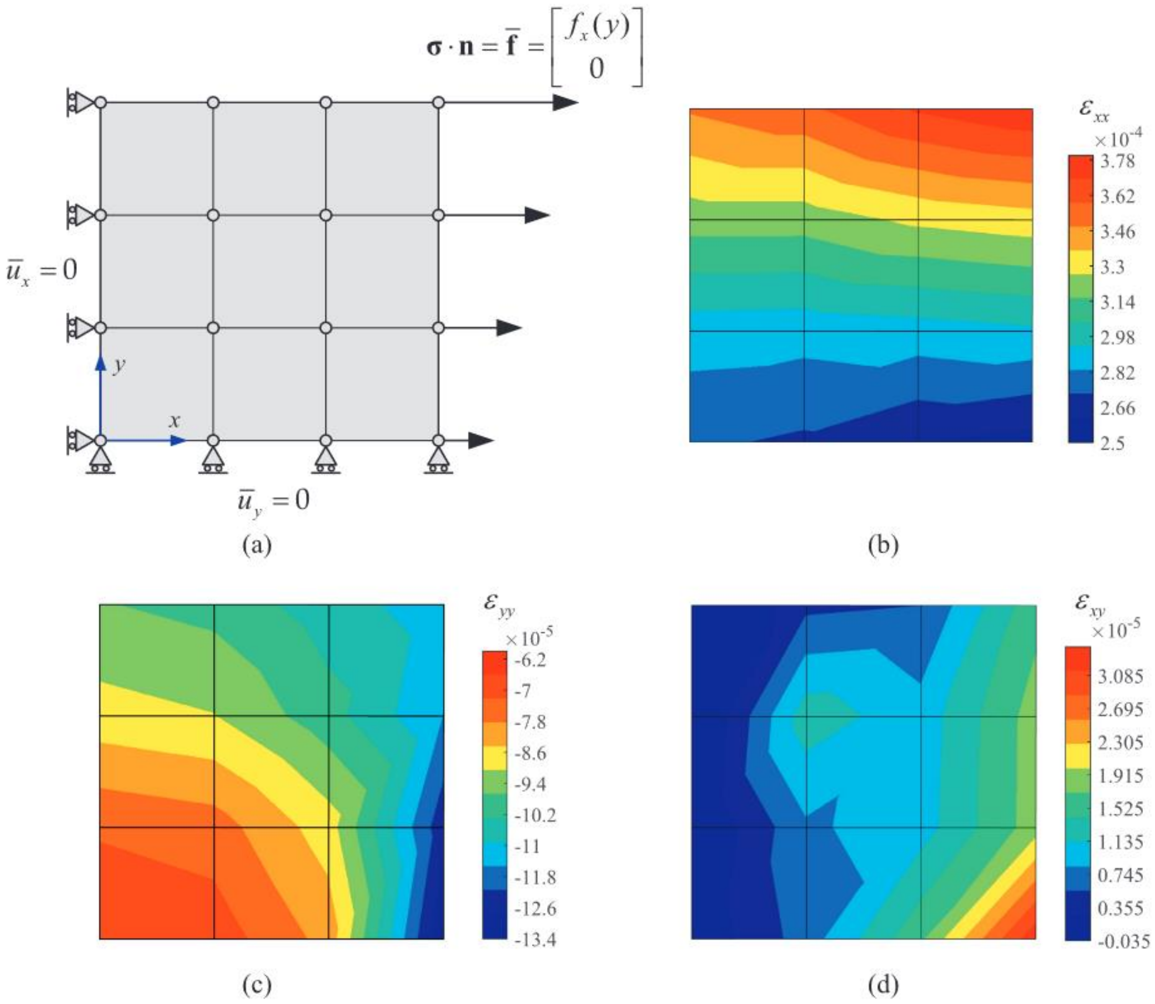
SPINN:



Converge directly in a few minutes

More realistic example ?

Inverse quantification benchmark from the literature[1]



16 simulated measurements

Using FEM as the reference

Strain corrupted with noise

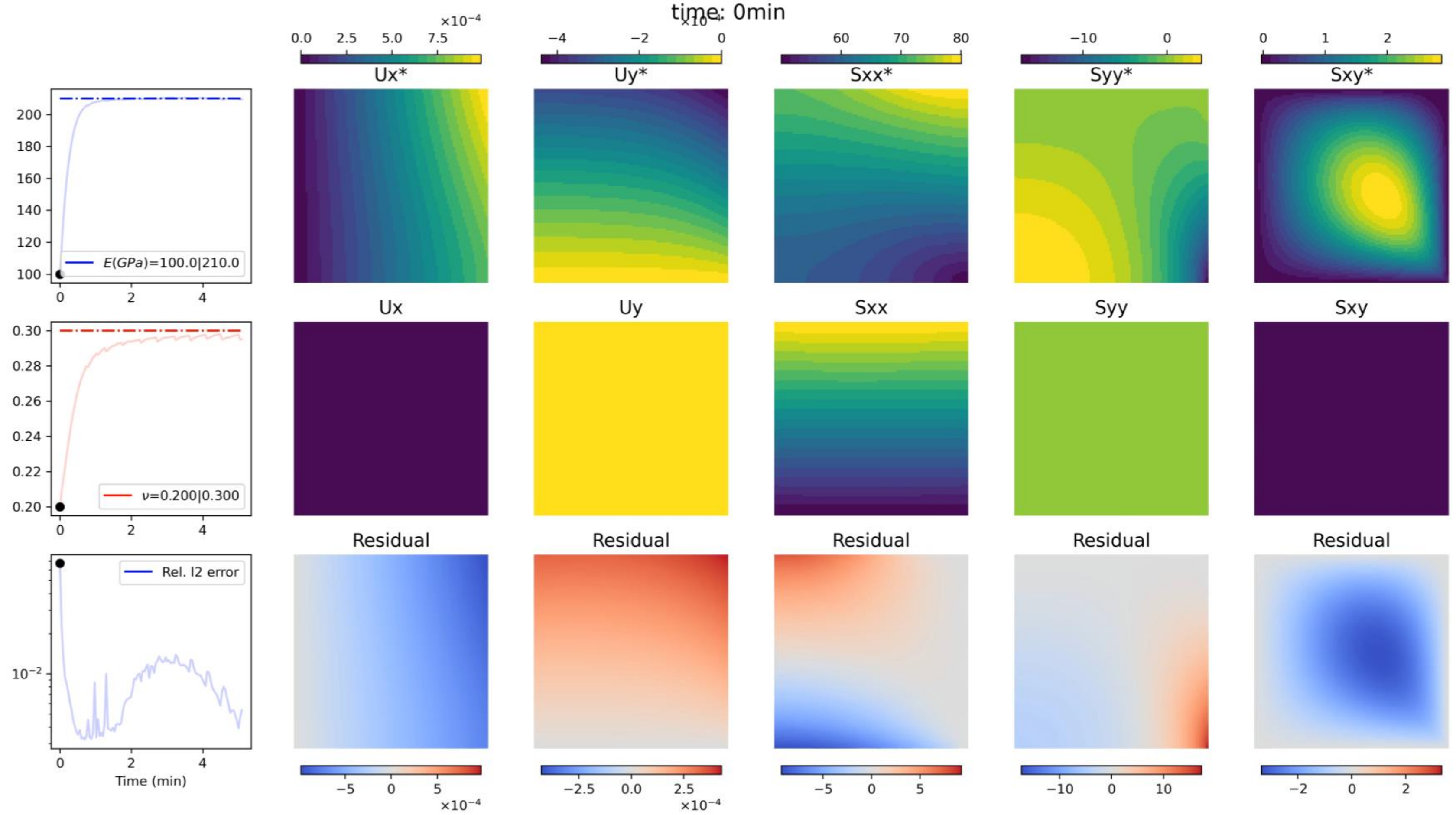
1$\mu\varepsilon$ gaussian noise (≈10% of std.)

	E (GPa)	ν	E - Error(%)	ν - Error(%)
Reference	210.00	0.3000		
FEMU	203.90	0.2706	2.90	9.789
CEGM	204.55	0.2728	2.59	9.058
EGM	195.10	0.2356	7.09	21.436
VFM	205.14	0.2753	2.31	8.207

→ **Compare with SPINN**

[1] Martins, J.M.P., António Andrade-Campos, et Sandrine Thuillier. 2018. « Comparison of inverse identification strategies for constitutive mechanical models using full-field measurements ». *International Journal of Mechanical Sciences* 145 (septembre): 330-45.

Benchmark from the literature: SPINN results



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EGM	195.10	0.2356	7.09	21.436
VFM	205.14	0.2753	2.31	8.207
SPINN	**209.5**	**0.2952**	**0.24**	**1.667**

→ **SPINN 10x more accurate**

Expected: regression model dealing with an unbiased noise

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Resources

Physics-Informed Neural Networks to propagate random field properties of composite materials

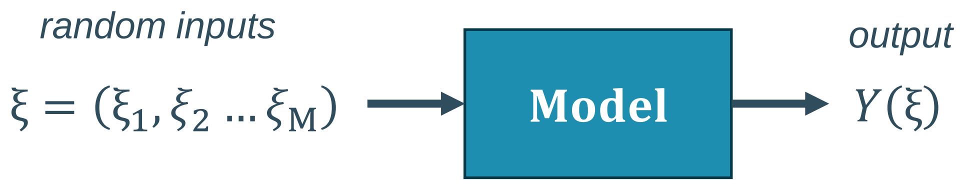
D. Bonnet-Eymard, A. Persoons, P. Gavallas, M. GR Faes, G. Stefanou, D. Moens

Presented at USD 2024 conference - Available on ResearchGate

Code and results are available online :

www.github.com/bonneted/USD2024

Polynomial Chaos Expansion (PC)



$$Y(\xi) \approx \sum_{\alpha \in \mathcal{A}} y_\alpha \Psi_\alpha(\xi)$$

multivariate polynomials of the random inputs

$\mathcal{A} \subset \mathbb{N}^M$, *multi-indices that define the truncation*

PCE coefficients to be found

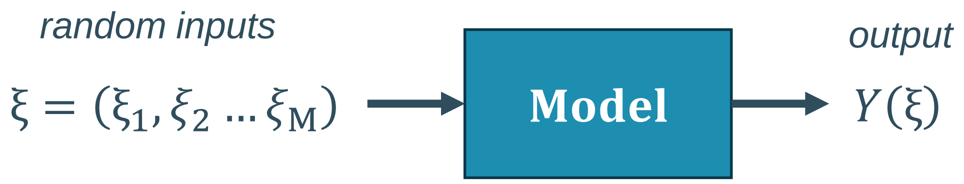
Resolution (determining y_α) :

- sampling
- y_α determined using least squares, least angle…

Space dependent output : $Y(\xi, x)$?

- discretization of the output (PCA…)
- Spatially dependant coefficients

Space dependent Polynomial Chaos Expansion



$$Y(\xi, x) \approx \sum_{\alpha \in \mathcal{A}} y_\alpha(x) \Psi_\alpha(\xi)$$

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Resolution (determining y_α) :

- sampling
- y_α determined using least squares, least angle…

Space dependent output : $Y(\xi, x)$?

- discretization of the output (PCA…)
- **Spatially dependant coefficients**

➢ Use a Neural Network as the approximator :

$$y_\alpha(x) = NN(x) \Rightarrow \textbf{PINN-PC}$$

PINN-PC[1]

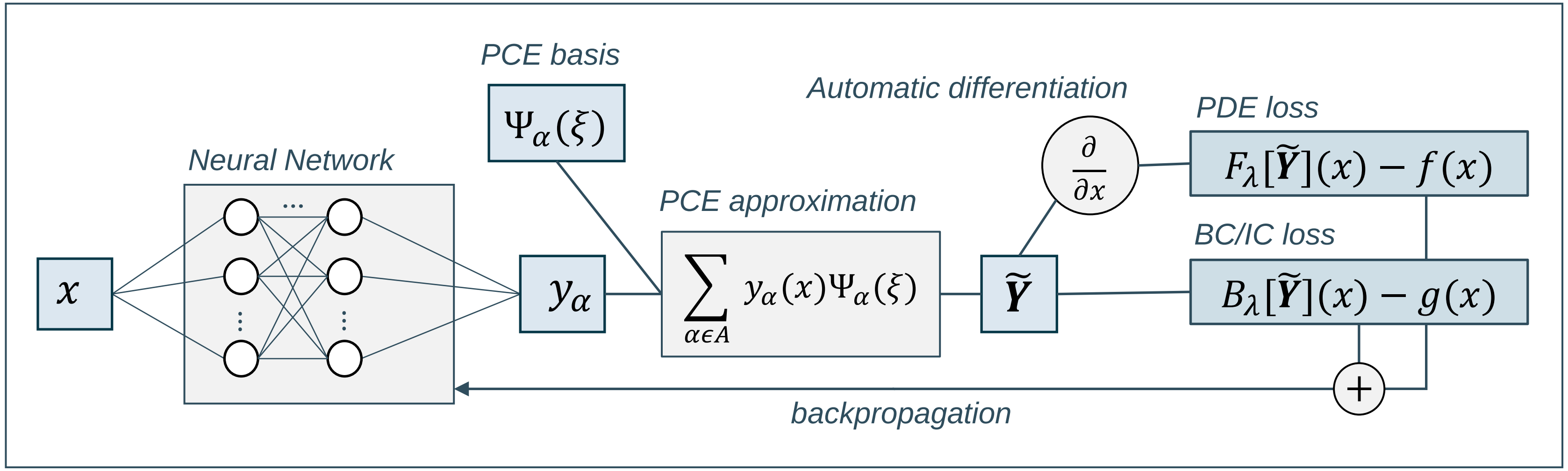

Fig. 1 : Schematic representation of the PINN-PC framework.

Several coefficients to predict :

- grouping them by their polynomial degree
- using a separate neural network for each group

⚠ **Increase the computational cost**

by a factor N = the number of samples

[1] Zhang, Dongkun, Lu Lu, Ling Guo, et George Em Karniadakis. « Quantifying Total Uncertainty in Physics-Informed Neural Networks for Solving Forward and Inverse Stochastic Problems ». *Journal of Computational Physics* 397 (15 novembre 2019): 108850. https://doi.org/10.1016/j.jcp.2019.07.048.

Poisson equation : reference solution

Problem setup :

Poisson equation

$$-\frac{d^2}{dx^2}u = f(x;\omega), \quad x \in [-1,1] \text{ and } \omega \in \Omega,$$
$$u(-1) = u(1) = 0.$$

Forcing term

$$f(x;\omega) \sim \mathcal{GP}(f_0(x), \mathrm{Cov}(x,x'))$$

$$f_0(x) = 10\sin(\pi x)$$

$$\mathrm{Cov}(x,x') = \sigma^2 \exp\left(-\frac{(x-x')^2}{l_c^2}\right),$$

Finite difference solution :

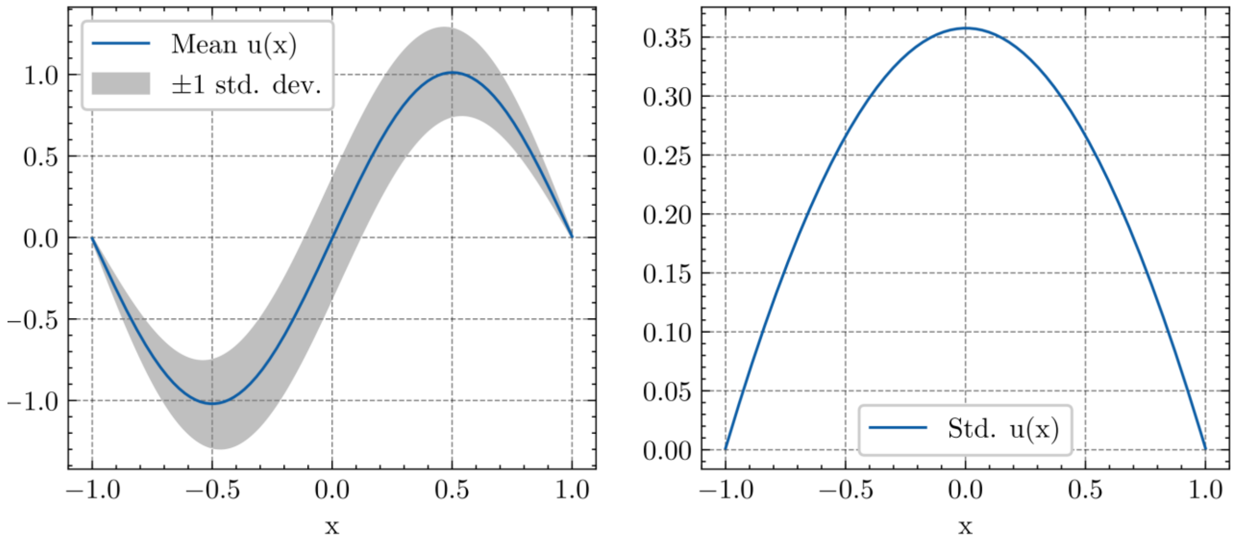

Fig. 2: Mean and standard deviation of the solution computed using 10^6 Monte Carlo simulations.

Poisson equation : random field discretization

Discretization of $f(x, \omega)$:

Forcing term

$$f(x;\omega) \sim \mathcal{GP}(f_0(x), \mathrm{Cov}(x,x'))$$

$$f_0(x) = 10\sin(\pi x)$$

$$\mathrm{Cov}(x,x') = \sigma^2 \exp\left(-\frac{(x-x')^2}{l_c^2}\right),$$

Karhunen–Loève expansion

$$f(x) = f_0(x) + \sum_{n=1}^{\infty} \sqrt{\lambda_n}\, \phi_n(x)\, \xi_n$$

On a discrete space :

$Cov(x,x') = Mcov$

K-L $\leftrightarrow$ Spectral decomposition **of** $\boldsymbol{Mcov}$

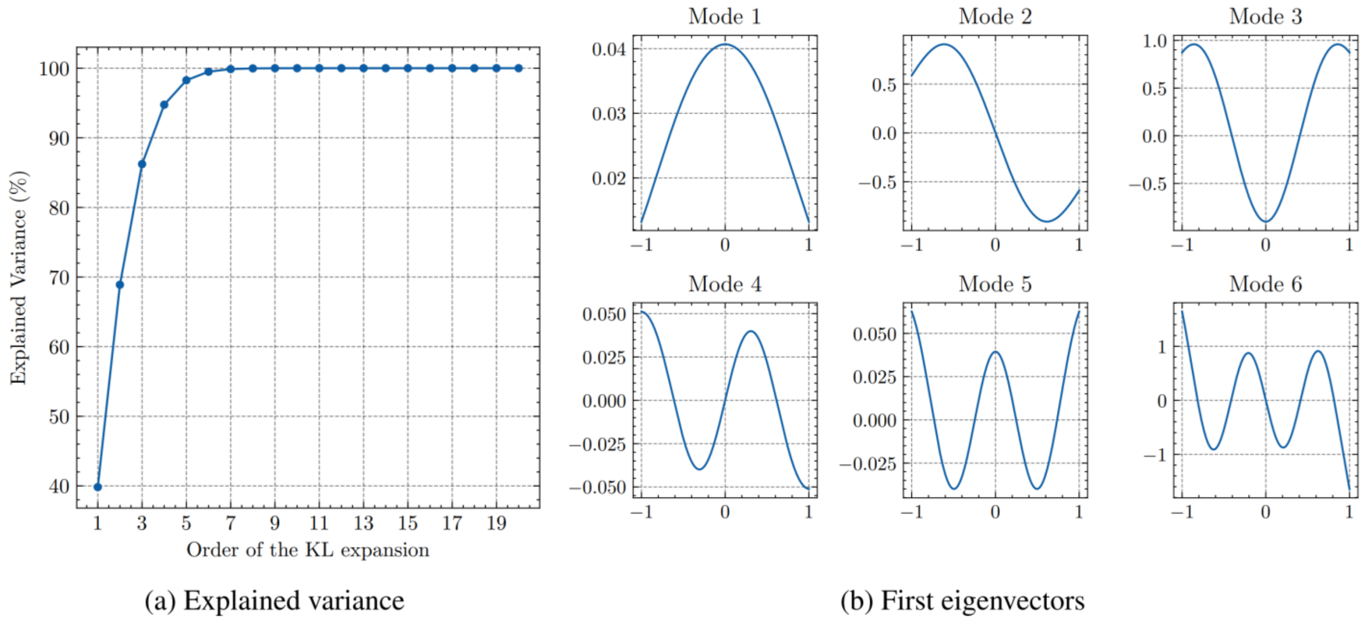

Fig. 3: Eigendecomposition of the covariance matrix to construct the K-L expansion.

Keep **6 order** to have **99%** explained variance

- *GP represented by 6 variables :* $(\xi_1, \xi_2 \dots \xi_6)$
- *1 order PCE : only 6 polynomials* $\Psi_i(\xi) = \xi_i$

Poisson equation : implementation

Neural Network

- MeanNN: [1, 4, 4, 1], to approximate $u_0(x)$
- CoeffNN: [1, 36, 36, 36, 36, 6], to approximate $y_\alpha(x)$
- Tanh activation function

Training :

- 1000 samples of f
- 13 training points in [-1, 1]
- Adam (20000 epochs, lr = 1e-3)

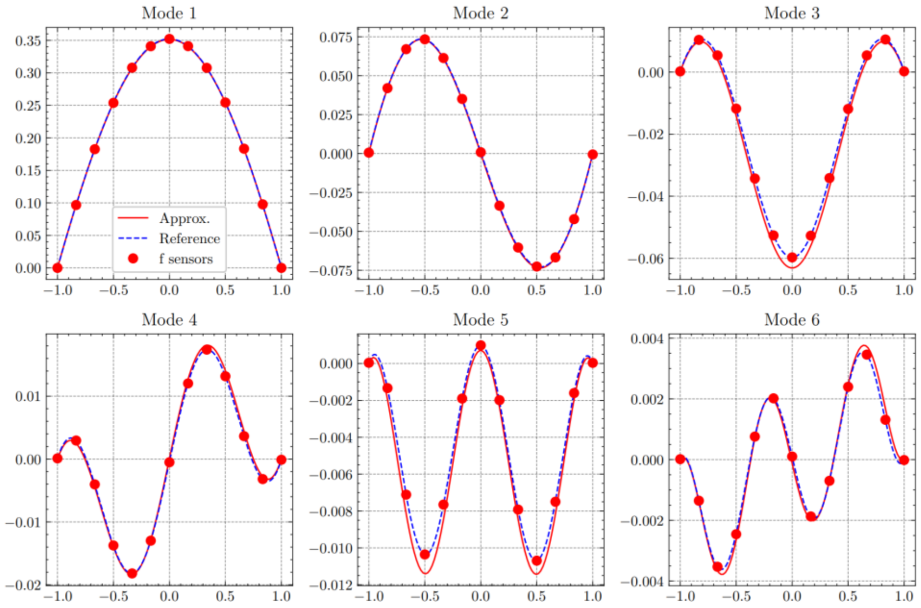

Fig. 4: approximated PCE coefficients

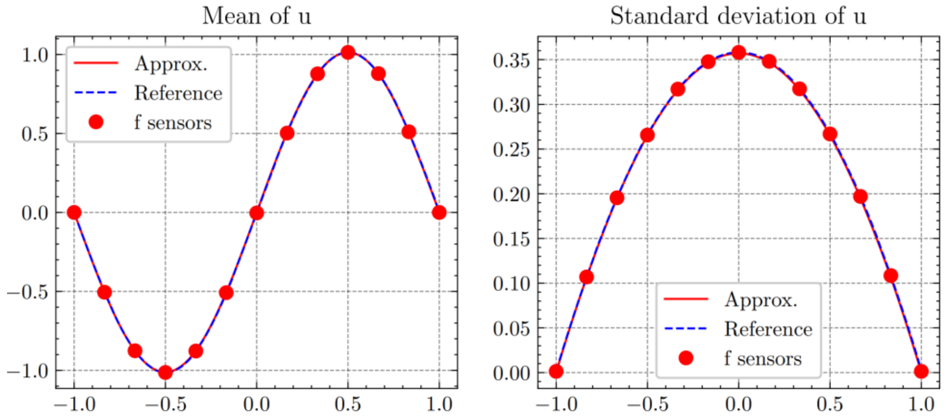

Fig. 5: Mean and standard deviation of the solution

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Conclusion

PINN: a powerful tool that is becoming increasingly mature

Idea : use an **artificial neural network** to approximate the solution of a **boundary value problem** defined by a partial differential equation (**PDE**) and boundary conditions (**BCs**)

Physics-Informed loss function : $L_{total} = L_U + L_{BC/IC} + L_{PDE}$

- L_{PDE} **:** PDE calculated through automatic differentiation
- $L_{BC/IC}$ **:** Residual between PINN approximation and BCs values
- L_U **:** Residual between PINN approximation and measurements

loss minimized → **compliance to the PDE, BCs and data**

⚠ The training (i.e., finding the network parameters that minimize the loss) rely on stochastic optimization and can struggle to converge

Techniques to improve convergence

- Hard constraints
- Mixed formulation
- Separable-PINN
- Adaptative sampling

Possible applications

- Inverse quantification
- Uncertainty propagation

Damien Bonnet-Eymard
PhD student at KU Leuven

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The project leading to this application has received funding from the European Union's Horizon 2020 research and innovation program under the Marie Skłodowska-Curie grant agreement No 955393.

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