Physics Informed Neural Networks for uncertainty quantification

- A simple continuum mechanics example -

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When solving physical problems governed by **partial differential equations**, the **finite element method (FEM),** or similar, has long proven its effectiveness.

Why then look for a new method to solve this same problem ?

First, FEM can be **too time consuming** to perform uncertainty quantification. Second, new sensors can change the game by providing **richer data**. On these two aspects **neural network** models have shown great potential, which motivates their use as PDE solvers in **a grey box** approach.

Grey-box approach

Goal : simulate observable phenomena, two approaches :

White box :	**Black box :**
numerical solution *of the problem* ***equated*** *according to* ***a physical theory***	***data driven solution = statistics****, then diversified* ***into machine learning***

combine the two ?

(not new : e.g., physical laws with empirical parameters)

➞ both methods have developed fast with **computing**

↳ **new possible hybrid models**

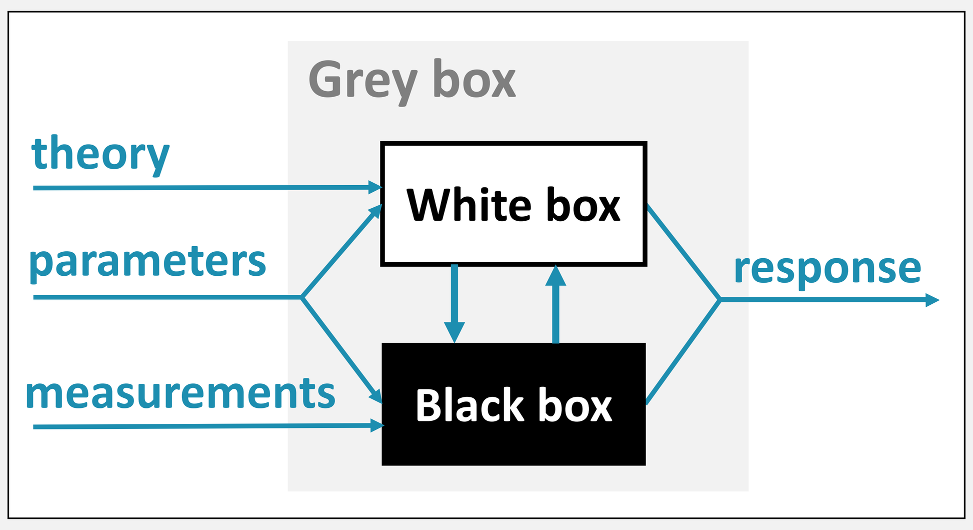

Fig.1 : The grey box methodology

A simple continuum mechanics example

Domain : clamped beam
Theory : linear elasticity

Fields :
- σ : stress tensor
- ε : strain tensor
- u : displacement

Equations :
1. momentum balance
2. small deformation
3. elastic relation

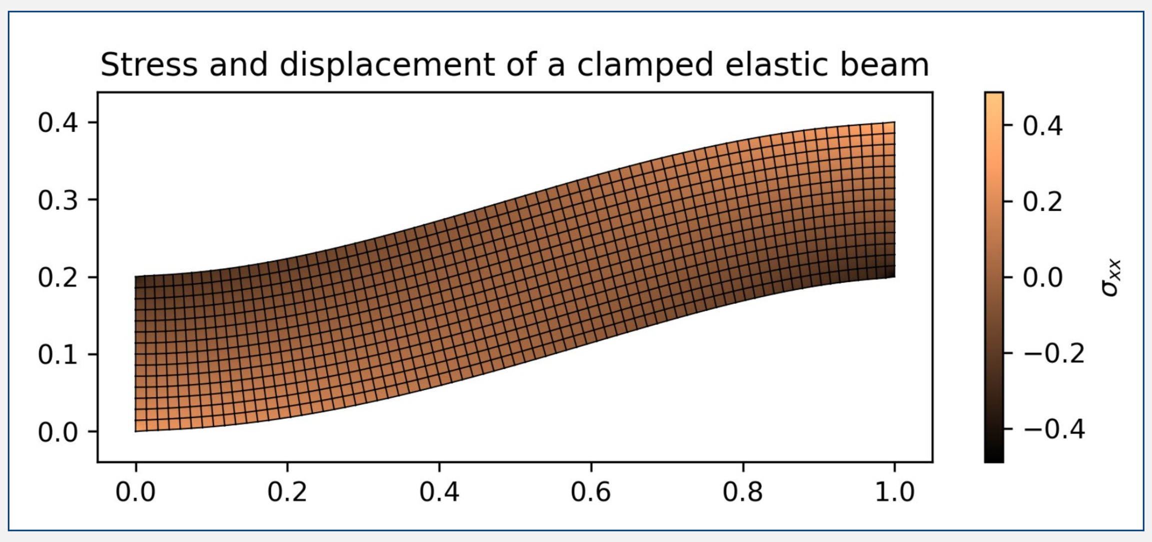

Fig.3 : Finite element ground truth solution

PINNs implementation : two networks (N_u; N_σ) / Boundary conditions enforced by shape functions

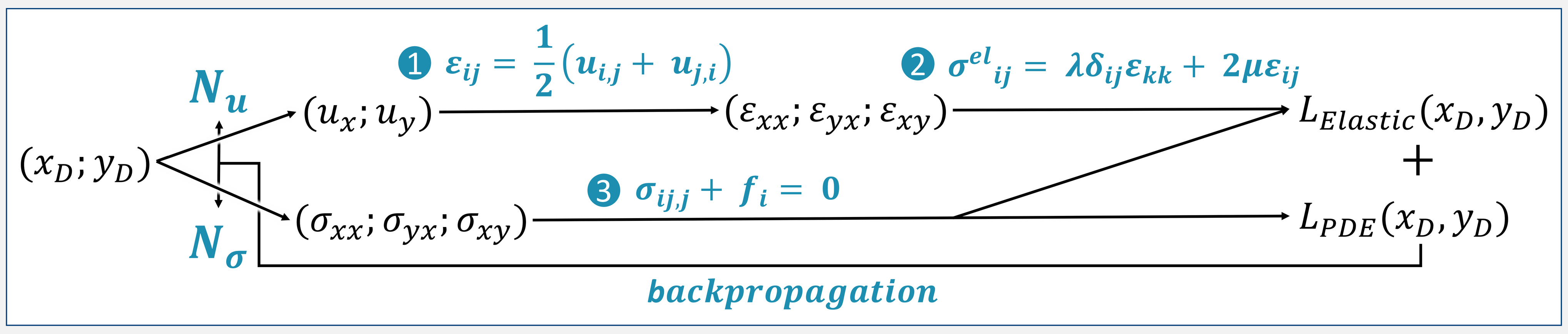

Fig.4 : Optimization for two distinct neural networks simulating stress and displacement

Physics Informed Neural Networks

Artificial neural networks : universal interpolator

↳ smart architecture based on prior knowledge gives better results

example : convolutional neural network (shift invariant) for image recognition

➞ **Physics Informed Neural Networks (PINNs):** impose physics prior

Introduced in 2019 by Raissi et Al. [1], very active research topic since

- **Hard constraint :** compliance forced by ad-hoc solution form
- **Soft constraint :** compliance reached by minimizing a loss

Common example : - calculate a PDE thanks automatic differentation
- add the residual to the loss function

loss minimized ➞ **compliance to the PDE**

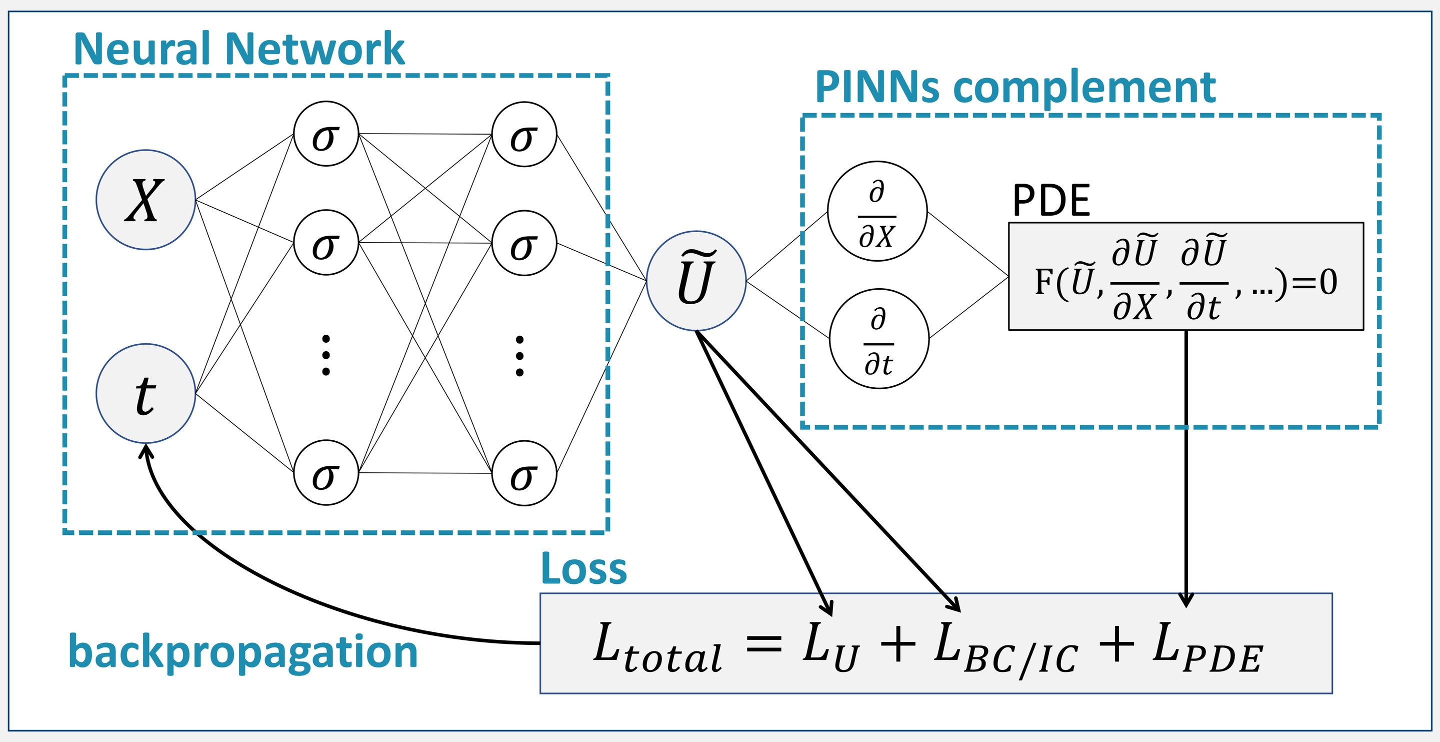

Fig.2 : The PINNs framework for a boundary value problem

Implementation using variational formulation

kinematically admissible displacement fields Σ ⟷ *find those that satisfy the* ***elastic equation*** ⟷ U **statically admissible stress fields**

➞ can be reformulated in the **complementary energy theorem :**

weak form

$$\sigma_{ij,j} + f_i = 0 \longrightarrow \iiint_\Omega \tilde{\sigma_{ij}}\tilde{\varepsilon_{ij}}\,dv - \iint_{S_u} \tilde{\sigma_{ij}} n_j u_i^d\,dS - \iint_{S_f} T_f^d\,\tilde{u_i}\,dS - \iiint_\Omega f_i\,\tilde{u_i}\,dv = 0$$

deformation energy

$$\frac{1}{2}\iiint_\Omega A_{ijkh}\,\tilde{\varepsilon_{ij}}\tilde{\varepsilon_{kh}}\,dv - \iint_{S_f} T_f^d\,\tilde{u_i}\,dS - \iiint_\Omega f_i\,\tilde{u_i}\,dv = \iint_{S_u} \tilde{\sigma_{ij}} n_j u_i^d\,dS - \frac{1}{2}\iiint_\Omega \Lambda_{ijkh}\,\tilde{\sigma_{ij}}\tilde{\sigma_{kh}}\,dv$$

depends only on ***dipslacement*** — *depends only on* ***stress***

= potential energy to minimise — **= complementary energy** to maximise

↳ **decoupled** training or monitoring of N_u and N_σ

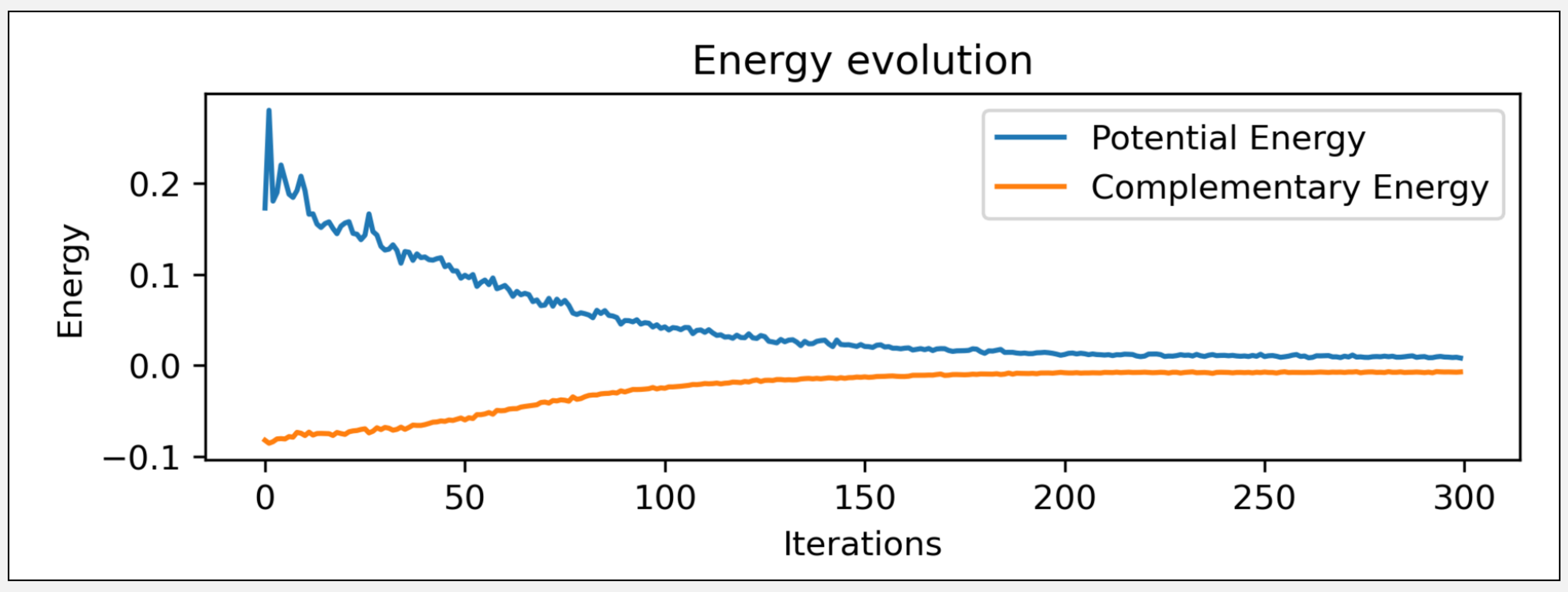

Fig.5 : Potential and complemantary energy during optimization

This work is still at early stage, the example is simple, and the use of linear elasticity brings limitation. Nevertheless, the use of two networks N_u and N_σ to simulate continuum mechanics response opens the path to further research. Two possible ways are to combine this idea with either :

- **Full field measurment** (e.g., obtained by Digital Image Correlation) that can be used as training data or for inverse quantification
- **Model free approach** that doesn't assume any empirical relation between stress and strain but directly infer them from data

References :

1. Raissi M, Perdikaris P, Karniadakis GE. Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations. J Comput Phys. 2019 Feb;
2. François Sidoroff. Mécanique des milieux continus. École d'ingénieur. École Centrale de Lyon, France. 1980

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