July 15, 2025

Enriching continuous Lagrange finite element approximation spaces using neural networks

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Joint work with:
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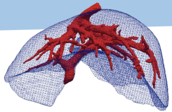
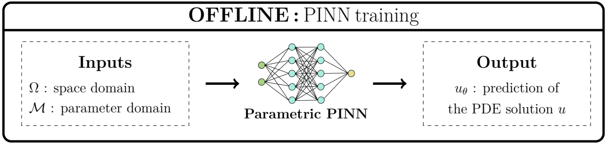
Scientific context

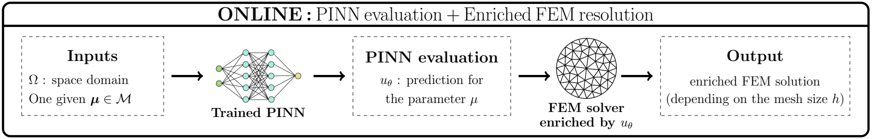


Context : Create real-time digital twins of an organ (e.g. liver).

Objective : Develop an hybrid finite element / neural network method.

accurate — quick + parameterized





Complete ONLINE process : quick + accurate

Heated cavity test case

Stationary incompressible Navier-Stokes equations (with buoyancy and gravity)[1] **:**

We consider $\Omega = [-1,1]^2$ a squared domain and $\boldsymbol{e}_y = (0,1)$.

Find the velocity $\boldsymbol{u} = (u_1, u_2)$, the pressure p and the temperature T such that

$$
\begin{cases}
(\boldsymbol{u}\cdot\nabla)\boldsymbol{u} + \nabla p - \nu\Delta\boldsymbol{u} - g(\beta T + 1)\boldsymbol{e}_y = 0 \text{ in } \Omega & \text{(momentum)} \\
\nabla\cdot\boldsymbol{u} = 0 \text{ in } \Omega & \text{(incompressibility)} \\
\boldsymbol{u}\cdot\nabla T - k_f\Delta T = 0 \text{ in } \Omega & \text{(energy)} \\
+ \text{ suitable BC} &
\end{cases}
\qquad (\mathcal{P})
$$

with $g = 9.81$ the gravity, $\beta = 0.1$ the expansion coefficient, ν the viscosity and k_f the thermal conductivity. [Coulaud et al., 2024]

[1] The approach will be shown on this example, but can be extended to other test cases.

Heated cavity test case

Objective: Simulation on a range of parameters $\boldsymbol{\mu} = (\nu, k_f) \in \mathcal{M} = [0.01, 0.1]^2$.

Stationary incompressible Navier-Stokes equations (with buoyancy and gravity) :

We consider $\boldsymbol{x} = (x, y) \in \Omega$ and $\boldsymbol{e}_y = (0, 1)$.

Find $\boldsymbol{U} = (\boldsymbol{u}, p, T) = (u_1, u_2, p, T)$ such that

$$\begin{cases} R_{mom}(U; \boldsymbol{x}, \boldsymbol{\mu}) = 0 \quad \text{in } \Omega & \text{(momentum)} \\ R_{inc}(U; \boldsymbol{x}, \boldsymbol{\mu}) = 0 \quad \text{in } \Omega & \text{(incompressibility)} \\ R_{ener}(U; \boldsymbol{x}, \boldsymbol{\mu}) = 0 \quad \text{in } \Omega & \text{(energy)} \\ + \text{ suitable BC} \end{cases} \qquad (\mathcal{P})$$

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Boundary Conditions:

No-slip BC : $\boldsymbol{u} = 0$ on $\partial\Omega$

Isothermal BC : $T = 1$ on the left wall ($x = -1$)
$T = -1$ on the right wall ($x = 1$)

Adiabatic BC : $\dfrac{\partial T}{\partial n} = 0$ on the top and bottom walls ($y = \pm 1$, denoted by Γ_{ad})

Evaluate quality of solutions

In the following, we are interested in three parameters (rising in complexity) :

$$\boldsymbol{\mu}^{(1)} = (0.1, 0.1),\ \boldsymbol{\mu}^{(2)} = (0.05, 0.05) \text{ and } \boldsymbol{\mu}^{(3)} = (0.01, 0.01)$$

We evaluate the quality of solutions by comparing them to a reference solution.[1]

[1] Computed on an over-refined mesh ($h = 7.10^{-3}$) on a $\mathbb{P}_3^2 \times \mathbb{P}_2 \times \mathbb{P}_3$ continuous Lagrange FE space.

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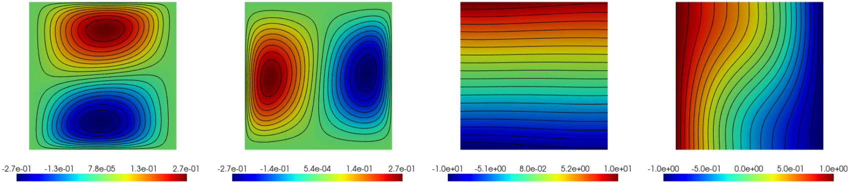
Reference solution - Rayleigh number : $Ra = 1\,569.6$

$u_{1,\mathrm{ref}}$ $u_{2,\mathrm{ref}}$ p_{ref} T_{ref}



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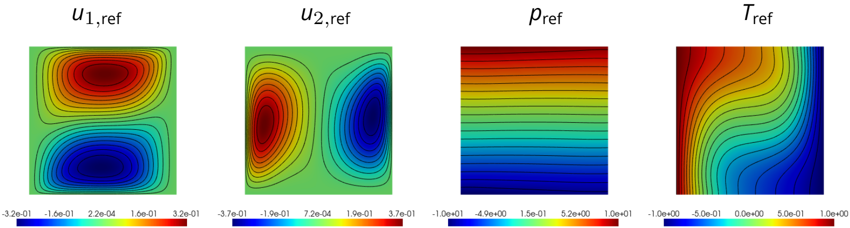
Reference solution - Rayleigh number : $Ra = 6\,278.4$



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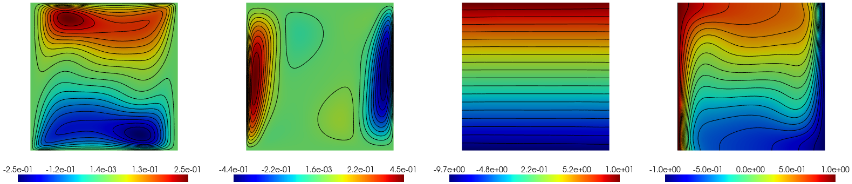
Reference solution - Rayleigh number : $Ra = 156\,960$

$u_{1,\mathrm{ref}}$ $u_{2,\mathrm{ref}}$ p_{ref} T_{ref}



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Parametric PINN

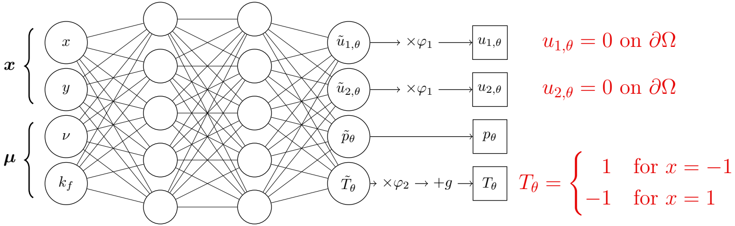
The PINN is parametrized by the $\boldsymbol{\mu}$ parameter.

Neural Network considered

We consider a parametric NN with 4 inputs and 4 outputs, defined by

$$U_\theta(\boldsymbol{x}, \boldsymbol{\mu}) = \big(u_{1,\theta}, u_{2,\theta}, p_\theta, T_\theta\big)(\boldsymbol{x}, \boldsymbol{\mu}).$$

The Dirichlet boundary conditions are imposed on the outputs of the MLP by a **post-processing** step. [Sukumar and Srivastava, 2022]



We consider two levelsets functions φ_1 and φ_2, and the linear function g defined by

$$\varphi_1(x, y) = (x-1)(x+1)(y-1)(y+1),$$

$$\varphi_2(x, y) = (x-1)(x+1) \quad \text{and} \quad g(x, y) = 1 - (x+1).$$

PINN training

Approximate the solution of $(\mathcal{P})$ by a PINN : Find the optimal weights $\theta^\star$, such that

$$\theta^\star = \underset{\theta}{\operatorname{argmin}} \left(J_{inc}(\theta) + J_{mom}(\theta) + J_{ener}(\theta) + J_{ad}(\theta) \right), \qquad (\mathcal{P}_\theta)$$

where the different cost functions[1] are defined by

adiabatic condition

$$\boxed{J_{ad}(\theta) = \int_{\mathcal{M}} \int_{\Gamma_{\text{ad}}} \left| \frac{\partial T_\theta(\boldsymbol{x},\boldsymbol{\mu})}{\partial n} \right|^2 d\boldsymbol{x} d\boldsymbol{\mu},}$$

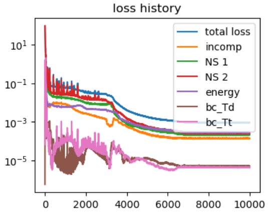
3 residual losses

$$\boxed{J_\bullet(\theta) = \int_{\mathcal{M}} \int_{\Omega} \left| R_\bullet(U_\theta(\boldsymbol{x},\boldsymbol{\mu}); \boldsymbol{x}, \boldsymbol{\mu}) \right|^2 d\boldsymbol{x} d\boldsymbol{\mu},}$$

with U_θ the parametric NN and $\bullet$ the PDE considered (i.e. *inc*, *mom* or *ener*).

Network - MLP	
layers	40, 60, 60, 60, 40
σ	sine

Training (ADAM / LBFGs)			
lr	7e-3	N_{col}	40000
n_{epochs}	10000	N_{bc}	30000

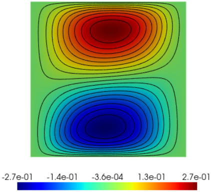


[1] Discretized by a random process using Monte-Carlo method.

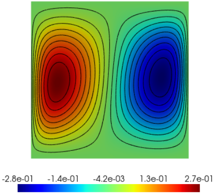
Prediction on $\mu^{(1)} = (0.1, 0.1)$

Prediction :

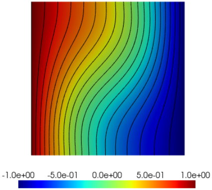
$u_{1,\theta}$



$u_{2,\theta}$

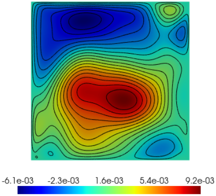


T_θ

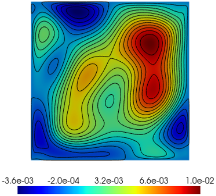


Error map :

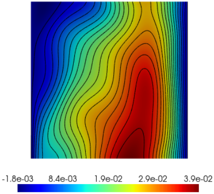
$u_{1,\mathrm{ref}} - u_{1,\theta}$



$u_{2,\mathrm{ref}} - u_{2,\theta}$



$T_{\mathrm{ref}} - T_\theta$



L^2 error : (relative) 2.98×10^{-2} 3.17×10^{-2} 3.90×10^{-2}

Finite element method (FEM)

The $\boldsymbol{\mu}$ parameter is fixed in the FE resolution.

Discrete weak formulation

We consider a mixed finite element space $\boxed{M_h = [V_h^0]^2 \times Q_h \times W_h}$ and

$$\left.\begin{array}{ccccccc} \boldsymbol{u}_h & \in & [V_h^0]^2 & \subset & [H_0^1(\Omega)]^2 & : & \mathbb{P}_2 \\ p_h & \in & Q_h & \subset & L_0^2(\Omega) & : & \mathbb{P}_1 \end{array}\right\} \text{(Taylor–Hood spaces)}$$

$$\begin{array}{ccccccc} T_h & \in & W_h & \subset & W & : & \mathbb{P}_2 \end{array}$$

with $W = \{w \in H^1(\Omega),\ w|_{x=-1} = 1,\ w|_{x=1} = -1\}$.

Weak problem : Find $U_h = (\boldsymbol{u}_h, p_h, T_h) \in M_h$ s.t., $\forall(\boldsymbol{v}_h, q_h, w_h) \in M_h^0$,

$$\begin{aligned} &\int_\Omega (\boldsymbol{u}_h \cdot \nabla)\boldsymbol{u}_h \cdot \boldsymbol{v}_h \, d\boldsymbol{x} + \mu \int_\Omega \nabla \boldsymbol{u}_h : \nabla \boldsymbol{v}_h \, d\boldsymbol{x} \\ &\qquad - \int_\Omega p_h \nabla \cdot \boldsymbol{v}_h \, d\boldsymbol{x} - g \int_\Omega (1 + \beta T_h)\boldsymbol{e}_y \cdot \boldsymbol{v}_h \, d\boldsymbol{x} = 0, \qquad \text{(momentum)} \\ &\int_\Omega q_h \nabla \cdot \boldsymbol{u}_h \, d\boldsymbol{x} + 10^{-4} \int_\Omega q_h \, p_h \, d\boldsymbol{x} = 0, \qquad \text{(incompressibility + pressure penalization)} \\ &\int_\Omega (\boldsymbol{u}_h \cdot \nabla T_h) \, w_h \, d\boldsymbol{x} + \int_\Omega k_f \nabla T_h \cdot \nabla w_h \, d\boldsymbol{x} = 0, \qquad \text{(energy)} \end{aligned} \tag{$\mathcal{P}_h$}$$

where $M_h^0 = [V_h^0]^2 \times Q_h \times W_h^0$ with $W_h^0 \subset \{w \in H^1[\Omega],\ w|_{x=\pm 1} = 0\}$.

Newton method

We consider the following three parameters:

$$\boldsymbol{\mu}^{(1)} = (0.1, 0.1), \ \boldsymbol{\mu}^{(2)} = (0.05, 0.05) \text{ and } \boldsymbol{\mu}^{(3)} = (0.01, 0.01).$$

Denoting N_h the dimension of M_h, we want to solve the non linear system:

$$F(\vec{U}_k) = 0$$

with $F : \mathbb{R}^{N_h} \to \mathbb{R}^{N_h}$ a non linear operator and $\vec{U}_k \in \mathbb{R}^{N_h}$ the unknown vector associated to the k-th parameter $\boldsymbol{\mu}^{(k)}$ ($k = 1, 2, 3$). Appendix 1

Algorithm 1: Newton algorithm

Initialization step: set $\vec{U}_k^{(0)} = \vec{U}_{k,0}$;
for $n \geq 0$ **do**
  Solve the linear system $F(\vec{U}_k^{(n)}) + F'(\vec{U}_k^{(n)})\delta_k^{(n+1)} = 0$ for $\delta_k^{(n+1)}$;
  Update $\vec{U}_k^{(n+1)} = \vec{U}_k^{(n)} + \delta_k^{(n+1)}$;
end

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end

How to initialize the Newton solver?

3 types of initialization

- **Natural :**
- **PINN :**
- **Continuation method :**

3 types of initialization

- **Natural :** Using constant or linear function.
  Considering a fixed parameter with $k \in \{1,2,3\}$, we can use the following initialization:
  $$\vec{U}_{k,0} = \left(\vec{0}, \vec{0}, \vec{0}, \vec{T}_0\right)$$
  where for $i = 1, \dots, \mathrm{dim}(W_h)$,
  $$(\vec{T}_0)_i = g(\boldsymbol{x}^{(i)}) = 1 - (x^{(i)} + 1)$$
  with $\boldsymbol{x}^{(i)} = \left(x^{(i)}, y^{(i)}\right)$ the i-th dofs coordinates of W_h.
- **PINN :**
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3 types of initialization

- **Natural :** Using constant or linear function.
- **PINN :** Using PINN prediction.
  (UNet : [Odot et al., 2021] ; FNO : [Aghili et al., 2025])
  Considering a fixed parameter with $k \in \{1, 2, 3\}$, we can use the following initialization for $i = 1, \dots, N_h$,

$$\left(\vec{U}_{k,0}\right)_i = U_\theta\left(\boldsymbol{x}^{(i)}, \boldsymbol{\mu}^{(k)}\right)$$

  with $\boldsymbol{x}^{(i)} = \left(x^{(i)}, y^{(i)}\right)$ the i-th dofs coordinates of M_h and U_θ the PINN.
- **Continuation method :**

3 types of initialization

- **Natural :** Using constant or linear function.
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  (UNet : [Odot et al., 2021] ; FNO : [Aghili et al., 2025])
- **Continuation method :** Using a coarse FE solution of a simpler parameter.
  - We consider a fixed parameter with $k \in \{2,3\}$.
  - We consider a coarse grid (16×16 grid) and compute the FE solution of ($\mathcal{P}_h$) for the parameter $\boldsymbol{\mu}^{(k-1)}$.
  - We interpolate the coarse solution to the current mesh.
  - We use it as an initialization for the Newton method, i.e.

$$\vec{U}_{k,0} = \left(\vec{u}_{k-1}, \vec{v}_{k-1}, \vec{p}_{k-1}, \vec{T}_{k-1}\right)$$

where $\vec{u}_{k-1}$, $\vec{v}_{k-1}$, $\vec{p}_{k-1}$ and $\vec{T}_{k-1}$ are the FE solutions for the parameter $\boldsymbol{\mu}^{(k-1)}$.

Enriched finite element method using PINN

Very simple linear test case
The heated cavity test case considered

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What is the purpose of enrichment?

Poisson problem (with Dirichlet BC) **:** Find $u : \Omega \to \mathbb{R}$ such that

$$\begin{cases} -\Delta u = f, & \text{in } \Omega, \\ u = 0, & \text{on } \partial\Omega. \end{cases}$$

Variational Problem : We consider V_h^0 a $\mathbb{P}_k$ continuous Lagrange FE space ($k \geq 1$).

$$\text{Find } u_h \in V_h^0 \text{ such that}, \forall v_h \in V_h^0, a(u_h, v_h) = l(v_h), \qquad (\mathcal{P}_h)$$

with h the characteristic mesh size, a and l the associated bilinear and linear forms.

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with h the characteristic mesh size, a and l the associated bilinear and linear forms.

Modified variational Problem : Let u_θ be a PINN prediction.

$$\text{Find } C_{h,u}^+ \in V_h^0 \text{ such that, } \forall v_h \in V_h^0, a(C_{h,u}^+, v_h) = l(v_h) - a(u_\theta, v_h), \qquad (\mathcal{P}_h^+)$$

with the enriched trial space V_h^+ defined by

$$V_h^+ = \left\{ u_h^+ = u_\theta + C_{h,u}^+, \quad C_{h,u}^+ \in V_h^0 \right\}.$$

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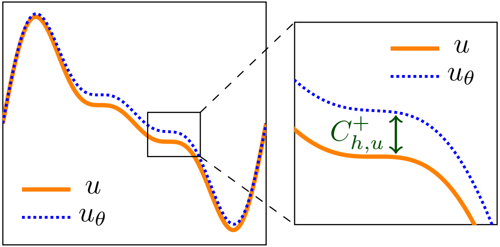


We hope that the modified problem will give the same results as the standard one on coarser meshes.

Convergence analysis

Theorem 1: Convergence analysis of the standard FEM [Ern and Guermond, 2004]

We denote $u_h \in V_h$ the solution of $(\mathcal{P}_h)$ with V_h the standard trial space. Then,

$$|u - u_h|_{H^1} \leqslant C_{H^1}\, h^k |u|_{H^{k+1}},$$

$$\|u - u_h\|_{L^2} \leqslant C_{L^2}\, h^{k+1} |u|_{H^{k+1}}.$$

Theorem 2: Convergence analysis of the enriched FEM [**F. Lecourtier** et al., 2025]

We denote $u_h^+ \in V_h^+$ the solution of $(\mathcal{P}_h^+)$ with V_h^+ the enriched trial space. Then,

$$|u - u_h^+|_{H^1} \leqslant \boxed{\frac{|u-u_\theta|_{H^{k+1}}}{|u|_{H^{k+1}}}} \left(C_{H^1}\, h^k |u|_{H^{k+1}} \right),$$

$$\|u - u_h^+\|_{L^2} \leqslant \boxed{\frac{|u-u_\theta|_{H^{k+1}}}{|u|_{H^{k+1}}}} \left(C_{L^2}\, h^{k+1} |u|_{H^{k+1}} \right).$$

Gains of the additive approach.

Enriched finite element method using PINN

Very simple linear test case

The heated cavity test case considered

Enriched space using PINN

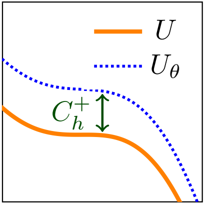
Considering the PINN prior $U_\theta = (\boldsymbol{u}_\theta, p_\theta, T_\theta)$, we define the mixed finite element space additively enriched by the PINN as follows:

$$\boxed{M_h^+ = \left\{U_h^+ = U_\theta + C_h^+, \quad C_h^+ \in M_h^0\right\}}$$

with $M_h^0 = [V_h^0]^2 \times Q_h \times W_h^0$, $U_h^+ = (\boldsymbol{u}_h^+, p_h^+, T_h^+) \in M_h^+$ and $C_h^+ = (\boldsymbol{C}_{h,\boldsymbol{u}}^+, C_{h,p}^+, C_{h,T}^+)$.

We can then define the three finite element subspaces of M_h^+ as follows:

$$\begin{aligned}
\boldsymbol{V}_h^+ &= \left\{\boldsymbol{u}_h^+ = \boldsymbol{u}_\theta + \boldsymbol{C}_{h,\boldsymbol{u}}^+, \ \boldsymbol{C}_{h,\boldsymbol{u}}^+ \in [V_h^0]^2\right\}, \\
Q_h^+ &= \left\{p_h^+ = p_\theta + C_{h,p}^+, \ C_{h,p}^+ \in Q_h\right\}, \\
W_h^+ &= \left\{T_h^+ = T_\theta + C_{h,T}^+, \ C_{h,T}^+ \in W_h^0\right\},
\end{aligned}$$



where $\boldsymbol{C}_{h,\boldsymbol{u}}^+$, $C_{h,p}^+$ and $C_{h,T}^+$ becomes the unknowns.

Weak formulation - Additive approach

Weak problem : Find $C_h^+ = (C_{h,\boldsymbol{u}}^+, C_{h,p}^+, C_{h,T}^+) \in M_h^0$ s.t., $\forall(\boldsymbol{v}_h, q_h, w_h) \in M_h^0$,

$$\int_\Omega \left[(\boldsymbol{u}_\theta \cdot \nabla)\boldsymbol{u}_\theta + (\boldsymbol{u}_\theta \cdot \nabla)\boldsymbol{C}_{h,\boldsymbol{u}}^+ + (\boldsymbol{C}_{h,\boldsymbol{u}}^+ \cdot \nabla)\boldsymbol{u}_\theta + (\boldsymbol{C}_{h,\boldsymbol{u}}^+ \cdot \nabla)\boldsymbol{C}_{h,\boldsymbol{u}}^+\right] \cdot \boldsymbol{v_h}\, d\boldsymbol{x}$$
$$+ \mu \left(\int_\Omega \nabla \boldsymbol{u}_\theta : \nabla \boldsymbol{v}_h \, d\boldsymbol{x} + \int_\Omega \nabla \boldsymbol{C}_{h,\boldsymbol{u}}^+ : \nabla \boldsymbol{v}_h \, d\boldsymbol{x}\right) + \left(\int_\Omega \nabla p_\theta \cdot \boldsymbol{v}_h \, d\boldsymbol{x} - \int_\Omega C_{h,p}^+ \nabla \cdot \boldsymbol{v}_h \, d\boldsymbol{x}\right)$$
$$- g \int_\Omega (1 + \beta(T_\theta + C_{h,T}^+))\boldsymbol{e}_y \cdot \boldsymbol{v}_h \, d\boldsymbol{x} = 0, \text{ (momentum)}$$
$$\int_\Omega q_h \left[\nabla \cdot \boldsymbol{u}_\theta + \nabla \cdot \boldsymbol{C}_{h,\boldsymbol{u}}^+\right] d\boldsymbol{x} + 10^{-4} \int_\Omega q_h \left(p_\theta + C_{h,p}^+\right) d\boldsymbol{x} = 0, \text{ (incompressibility + penal)} \qquad (\mathcal{P}_h^+)$$
$$\int_\Omega \left[\boldsymbol{u}_\theta \cdot \nabla T_\theta + \boldsymbol{u}_\theta \cdot \nabla C_{h,T}^+ + \boldsymbol{C}_{h,\boldsymbol{u}}^+ \cdot \nabla T_\theta + \boldsymbol{C}_{h,\boldsymbol{u}}^+ \cdot \nabla C_{h,T}^+\right] w_h \, d\boldsymbol{x}$$
$$+ k_f \left(\int_\Omega \nabla T_\theta \cdot \nabla w_h \, d\boldsymbol{x} + \int_\Omega \nabla C_{h,T}^+ \cdot \nabla w_h \, d\boldsymbol{x}\, w_h \, d\boldsymbol{s}\right) = 0, \text{ (energy)}$$

with $U_\theta = (\boldsymbol{u}_\theta, p_\theta, T_\theta)$ the PINN prior and some modified boundary conditions.

Newton method - Additive approach

We want to solve the non linear system:

$$F_\theta(\vec{C}) = 0$$

with $F_\theta : \mathbb{R}^{N_h} \to \mathbb{R}^{N_h}$ the non linear operator associated to the weak problem $(\mathcal{P}_h^+)$ and $\vec{C} \in \mathbb{R}^{N_h}$ the correction vector (unknown).

Algorithm 2: Newton algorithm [Aghili et al., 2025]

Initialization step: set $\vec{C}^{(0)} = 0$;
for $n \geq 0$ **do**
  Solve the linear system $F_\theta(\vec{C}^{(n)}) + F'_\theta(\vec{C}^{(n)})\delta^{(n+1)} = 0$ for $\delta^{(n+1)}$;
  Update $\vec{C}^{(n+1)} = \vec{C}^{(n)} + \delta^{(n+1)}$;
end

Advantage compared to PINN initialization[1]**:**

u_θ is not required to live in the same discrete space as C_h^+.

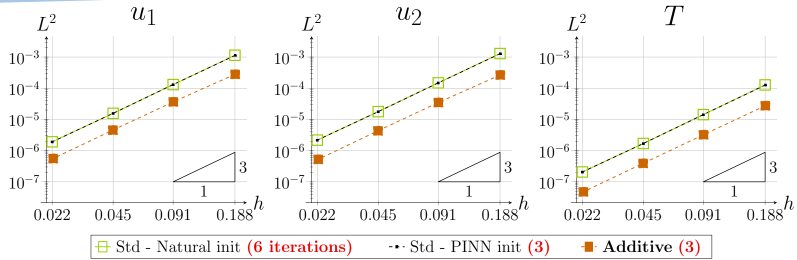
[1] Taking U_θ and C_h^+ in the same space, additive approach is exactly the same as the PINN initialization.

Numerical results

- Results obtained with a laptop GPU.
- The newton solver is the same for all methods (rtol$= 10^{-10}$, atol$= 10^{-10}$, max_it$= 30$).
- Additive approach : we consider u_θ in a $\mathbb{P}_3^2 \times \mathbb{P}_2 \times \mathbb{P}_3$ continuous Lagrange FE space (defined on the current mesh).

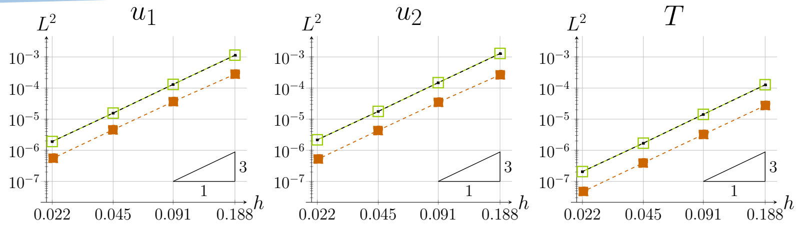
Error estimates I

$\boldsymbol{\mu}^{(1)}$:



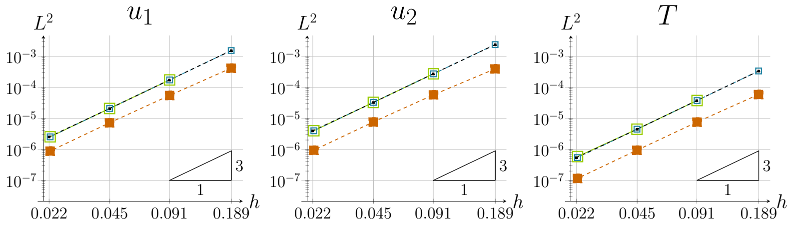
Error estimates I

$\boldsymbol{\mu}^{(1)}$:



□ Std - Natural init **(6 iterations)** ·▪· Std - PINN init **(3)** ■ **Additive (3)**

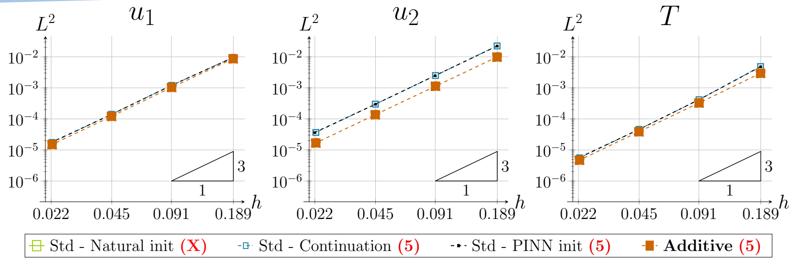
$\boldsymbol{\mu}^{(2)}$:



□ Std - Natural init **(10/X)** ·□· Std - Continuation **(4)** ·▪· Std - PINN init **(3)** ■ **Additive (3)**

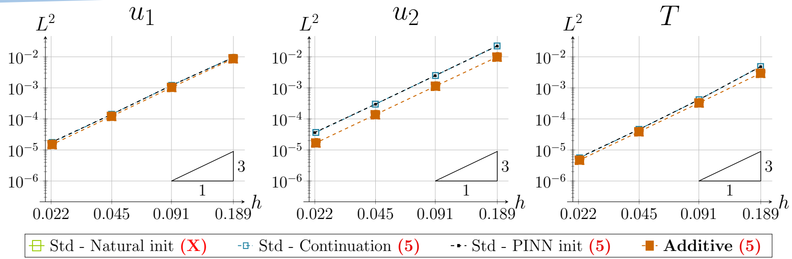
Error estimates II

$\boldsymbol{\mu}^{(3)}$:

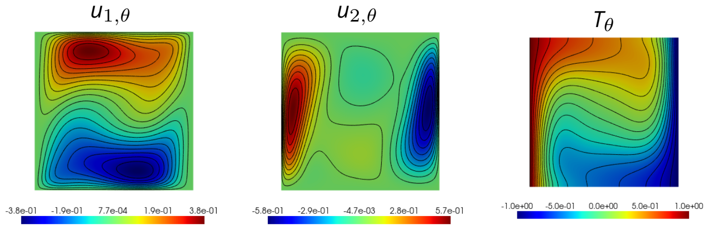


Error estimates II

$\boldsymbol{\mu}^{(3)}$:



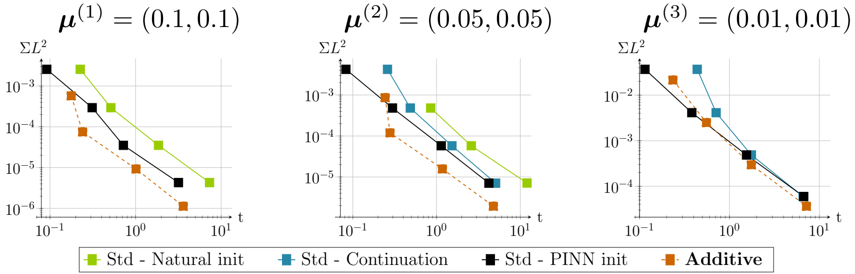
Prediction :



L^2 error : (relative) 5.75×10^{-1} 4.89×10^{-1} 2.57×10^{-1}

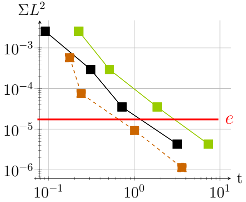
Numerical costs

Defining the global error as the sum of the L^2 relatives errors on $\boldsymbol{u}$ and T.



Numerical costs

$\boldsymbol{\mu}^{(1)} = (0.1, 0.1)$



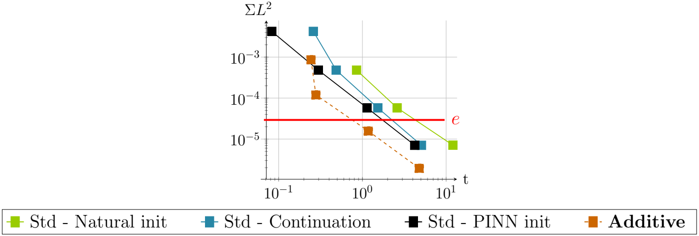
N_{dofs} and execution time required to reach the same global L^2 relative error e :

Std vs Add	Number of DoFs		Execution times		
e	**Std**	**Add**	**(nat)**	**(PINN)**	**Add**
$1 \cdot 10^{-3}$	6,031	2,044	0.32	0.16	0.16
$1 \cdot 10^{-4}$	26,959	10,588	0.99	0.48	0.23
$1 \cdot 10^{-5}$	121,156	49,231	4.21	1.75	0.96

$\div 2.5$ $\div 2$ $\div 4$

Numerical costs

$\boldsymbol{\mu}^{(2)} = (0.05, 0.05)$

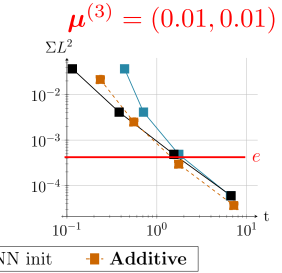


N_{dofs} and execution time required to reach the same global L^2 relative error e :

Std vs Add	Number of DoFs		Execution times			
e	Std	Add	(nat)	(cont)	(PINN)	Add
$1 \cdot 10^{-3}$	7,828	2,748	0.58	0.39	0.19	0.24
$1 \cdot 10^{-4}$	35,884	14,623	1.95	1.14	0.8	0.32
$1 \cdot 10^{-5}$	167,583	70,303	9.39	4.16	3.4	1.59

$\div 2.4$ $\div 2$ $\div 2.5$ $\div 6$

Numerical costs



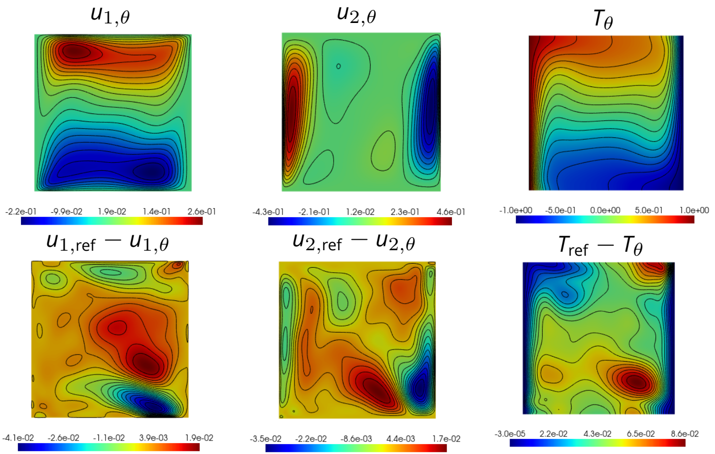
N_{dofs} and execution time required to reach the same global L^2 relative error e :

Std vs Add	Number of DoFs		Execution times			
e	Std	Add	(nat)	(cont)	(PINN)	Add
$1 \cdot 10^{-3}$	33,204	23,524	X	1.29	0.96	0.91
$1 \cdot 10^{-4}$	150,339	108,931	X	4.76	4.67	3.65
$1 \cdot 10^{-5}$	690,924	502,156	X	20.34	23.3	17.23

Non parametric PINN[1] for $\mu^{(3)}$

Prediction :

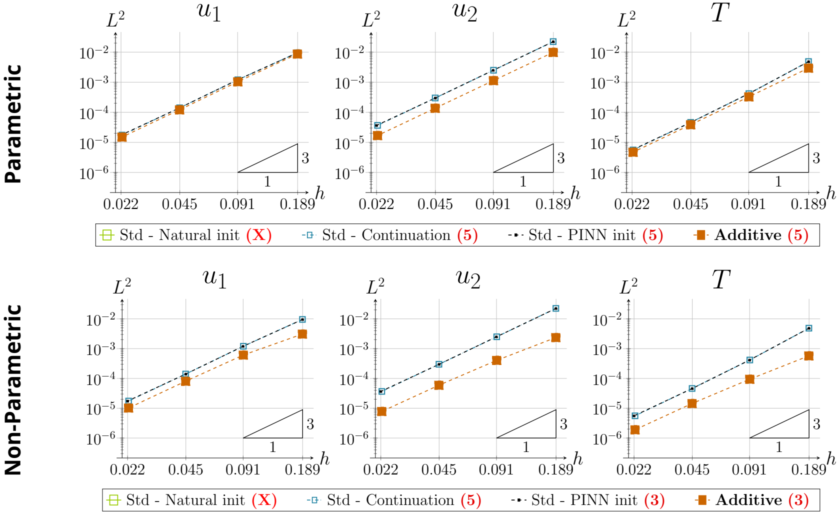
Error map :



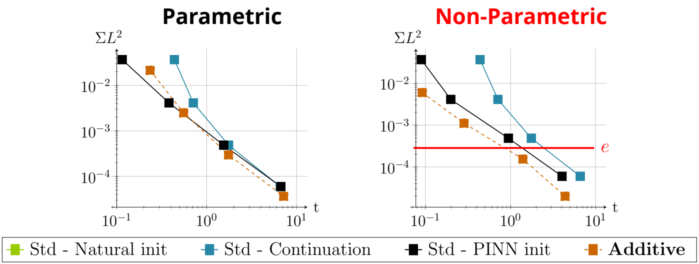
L^2 error : (relative) 7.60×10^{-2} 5.38×10^{-2} 9.63×10^{-2}

[1] We consider exactly the same architecture, but this time we train the PINN non-parametrically.

Error estimates on $\mu^{(3)}$



Numerical costs on $\mu^{(3)}$



N_{dofs} and execution time required to reach the same global L^2 relative error e :

e	Number of DoFs			Execution times			
	(PINN)	Add	Add+	(PINN)	(PINN)+	Add	Add+
$1 \cdot 10^{-3}$	33,204	23,524	13,764	0.96	0.56	0.91	0.31
$1 \cdot 10^{-4}$	150,339	108,931	70,303	4.67	2.82	3.65	1.78
$1 \cdot 10^{-5}$	690,924	502,156	339,231	23.3	13.84	17.23	6.42

$\div 2$ $\div 3$

Conclusion

- The enriched approach provides the same results as the standard FEM method, but with **coarser meshes**.
  $\Rightarrow$ Reduction of the computational cost : DoFs, iterations, execution times.
- Theory on linear problems shows that it's the **derivatives** of the prior that are the most crucial. Appendix 4
  $\Rightarrow$ PINNs are good candidates for the enriched approach.
- The gains obtained on linear problems were much higher. Appendix 3
  $\Rightarrow$ **Improved training** of parametric PINN (or Neural Operators).

Preprint (linear)

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Preprint (linear)

Appendix 1 : Finite element method (FEM)

A1 – Construction of the unknown vector

Considering $(\phi_i)_{i=1}^{N_u}$, $(\psi_j)_{j=1}^{N_p}$ and $(\eta_k)_{k=1}^{N_T}$ the basis functions of the finite element spaces V_h^0, Q_h and W_h respectively, we can write the discrete solutions as:

$$\boldsymbol{u}_h(\boldsymbol{x}) = \sum_{i=1}^{N_u} \begin{pmatrix} u_i \\ v_i \end{pmatrix} \phi_i(\boldsymbol{x}), \quad p_h(\boldsymbol{x}) = \sum_{j=1}^{N_p} p_j \psi_j(\boldsymbol{x}) \quad \text{and} \quad T_h(\boldsymbol{x}) = \sum_{k=1}^{N_T} T_k \eta_k(\boldsymbol{x}),$$

with the unknown vectors for velocity, pressure and temperature defined by

$$\vec{u} = (u_i)_{i=1}^{N_u} \in \mathbb{R}^{N_u}, \quad \vec{v} = (v_i)_{i=1}^{N_u} \in \mathbb{R}^{N_u},$$
$$\vec{p} = (p_j)_{j=1}^{N_p} \in \mathbb{R}^{N_p} \text{ and } \vec{T} = (T_k)_{k=1}^{N_T} \in \mathbb{R}^{N_T}.$$

Considering $N_h = 2N_u + N_p + N_T$, we can define the global vector of unknowns as:

$$\vec{U} = (\vec{u}, \vec{v}, \vec{p}, \vec{T}) \in \mathbb{R}^{N_h}.$$

and $F : \mathbb{R}^{N_h} \to \mathbb{R}^{N_h}$ the nonlinear operator associated to the weak formulation $(\mathcal{P}_h)$.

Appendix 2 : PINN Initialization / Additive approach

A2 – Comparison of the 2 approaches

Taking U_θ and C_h^+ in the same space, we have :

$$F_\theta(\vec{C}) = F(\vec{U}_\theta + \vec{C}),$$

with $\vec{C}$ the correction vector and $\vec{U}_\theta$ the PINN vector (PINN evaluation at the dofs), both of size N_h.
The first iteration of the additive approach :

$$F_\theta(\vec{C}^{(0)}) + F'_\theta(\vec{C}^{(0)})\delta^{(1)} = 0$$

becomes (as $C^{(0)} = 0$) :

$$F(\vec{U}_\theta) + F'(\vec{U}_\theta)\delta^{(1)} = 0,$$

which is equivalent as the standard method with the PINN initialization.

Appendix 3 : Results - Linear problem

A3 – Problem considered

Problem statement: Consider the Poisson problem with Dirichlet BC:

$$\begin{cases} -\Delta u = f, & \text{in } \Omega \times \mathcal{M}, \\ u = 0, & \text{on } \partial\Omega \times \mathcal{M}, \end{cases}$$

with $\Omega = [-0.5\pi, 0.5\pi]^2$ and $\mathcal{M} = [-0.5, 0.5]^2$ ($p = 2$ parameters).

Analytical solution :

$$u(\boldsymbol{x}, \boldsymbol{\mu}) = \exp\left(-\frac{(x-\mu_1)^2 + (y-\mu_2)^2}{2}\right) \sin(2x)\sin(2y).$$

PINN training: MLP of 5 layers; LBFGs optimizer (5000 epochs).
Imposing the Dirichlet BC exactly in the PINN with the levelset φ defined by

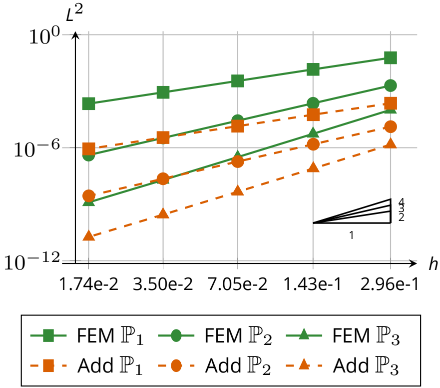
$$\varphi(\boldsymbol{x}) = (x + 0.5\pi)(x - 0.5\pi)(y + 0.5\pi)(y - 0.5\pi).$$

Training time : less than 1 hour on a laptop GPU.

A3 – Numerical results

Error estimates : 1 set of parameters.

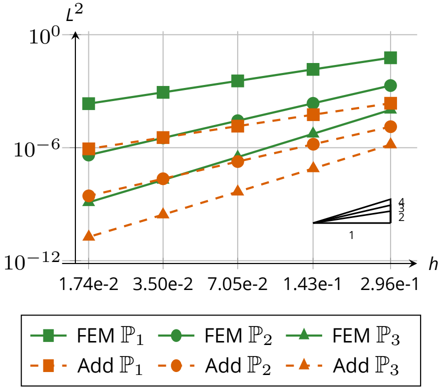
$$\boldsymbol{\mu}^{(1)} = (0.05, 0.22)$$



A3 – Numerical results

Error estimates : 1 set of parameters.

$$\boldsymbol{\mu}^{(1)} = (0.05, 0.22)$$



Gains achieved : $n_p = 50$ sets of parameters.

$$\mathcal{S} = \left\{ \boldsymbol{\mu}^{(1)}, \ldots, \boldsymbol{\mu}^{(n_p)} \right\}$$

Gains in L^2 rel error of our method w.r.t. FEM

k	min	max	mean
1	134.32	377.36	269.39
2	67.02	164.65	134.85
3	39.52	72.65	61.55

$N = 20$

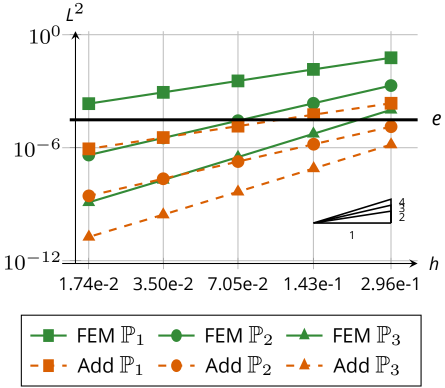
Gain : $\|u - u_h\|_{L^2} / \|u - u_h^+\|_{L^2}$

Cartesian mesh : N^2 nodes.

A3 – Numerical results

Error estimates : 1 set of parameters.

$$\boldsymbol{\mu}^{(1)} = (0.05, 0.22)$$



N_{dofs} **required to reach the same error** e **:**

		N_{dofs}	
k	**e**	**FEM**	**Add**
1	$1 \cdot 10^{-3}$	14,161	64
	$1 \cdot 10^{-4}$	143,641	576
2	$1 \cdot 10^{-4}$	6,889	225
	$1 \cdot 10^{-5}$	31,329	1,089
3	$1 \cdot 10^{-5}$	6,724	784
	$1 \cdot 10^{-6}$	20,164	2,704

Appendix 4 : Data-driven vs Physics-Informed training

A4 – Problem considered

Problem statement: Consider the Poisson problem in 1D with Dirichlet BC:

$$\begin{cases} -\partial_{xx} u = f, & \text{in } \Omega \times \mathcal{M}, \\ u = 0, & \text{on } \partial\Omega \times \mathcal{M}, \end{cases}$$

with $\Omega = [0,1]^2$ and $\mathcal{M} = [0,1]^3$ ($p = 3$ parameters).

Analytical solution : $u(x;\boldsymbol{\mu}) = \mu_1 \sin(2\pi x) + \mu_2 \sin(4\pi x) + \mu_3 \sin(6\pi x)$.

Construction of two priors: MLP of 6 layers; Adam optimizer (10000 epochs).
Imposing the Dirichlet BC exactly in the PINN with $\varphi(x) = x(x-1)$.

- **Physics-informed training:** $N_{\text{col}} = 5000$ collocation points.

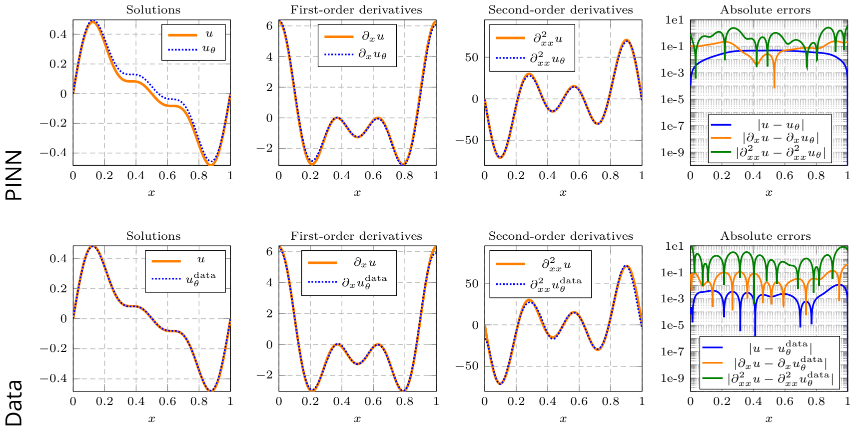
$$J_r(\theta) \simeq \frac{1}{N_{\text{col}}} \sum_{i=1}^{N_{\text{col}}} \left| \partial_{xx} u_\theta\left(\boldsymbol{x}_{\text{col}}^{(i)}; \boldsymbol{\mu}_{\text{col}}^{(i)}\right) + f\left(\boldsymbol{x}_{\text{col}}^{(i)}; \boldsymbol{\mu}_{\text{col}}^{(i)}\right) \right|^2.$$

- **Data-driven training:** $N_{\text{data}} = 5000$ data.

$$J_{\text{data}}(\theta) = \frac{1}{N_{\text{data}}} \sum_{i=1}^{N_{\text{data}}} \left| u_\theta^{\text{data}}\left(\boldsymbol{x}_{\text{data}}^{(i)}; \boldsymbol{\mu}_{\text{data}}^{(i)}\right) - u\left(\boldsymbol{x}_{\text{data}}^{(i)}; \boldsymbol{\mu}_{\text{data}}^{(i)}\right) \right|^2.$$

A4 – Priors derivatives

$$\boldsymbol{\mu}^{(1)} = (0.3, 0.2, 0.1)$$



A4 – Additive approach in $\mathbb{P}_1$

1 set of parameters: $\boldsymbol{\mu}^{(1)} = (0.3, 0.2, 0.1)$

	FEM
N	**error**
16	$5.18 \cdot 10^{-2}$
32	$1.24 \cdot 10^{-2}$

	PINN prior u_θ		Data prior u_θ^{data}	
N	**error**	**gain**	**error**	**gain**
16	$1.29 \cdot 10^{-3}$	40.34	$3.51 \cdot 10^{-3}$	14.78
32	$3.49 \cdot 10^{-4}$	35.41	$8.8 \cdot 10^{-4}$	14.06

50 set of parameters:

	Gains in L^2 rel error of our method w.r.t. FEM					
	PINN prior u_θ			Data prior u_θ^{data}		
N	**min**	**max**	**mean**	**min**	**max**	**mean**
20	26.49	271.92	140.74	6.91	60.85	26.12
40	23.4	258.37	134.11	7.13	39.34	20.55

N : Nodes.