

Enriching continuous Lagrange finite element approximation spaces using neural networks

Michel Duprez¹, Emmanuel Franck², **Frédérique Lecourtier¹** and Vanessa Lleras³

¹Project-Team MIMESIS, Inria, Strasbourg, France

²Project-Team MACARON, Inria, Strasbourg, France

³IMAG, University of Montpellier, Montpellier, France

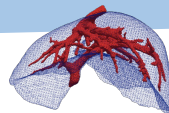
Joint work with:

H. Barucq, F. Faucher, N. Victorion and V. Michel-Dansac.



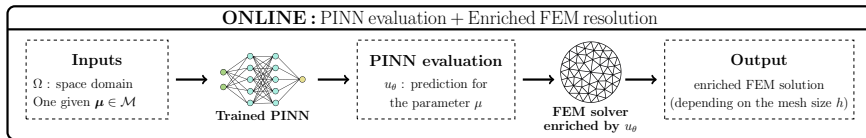
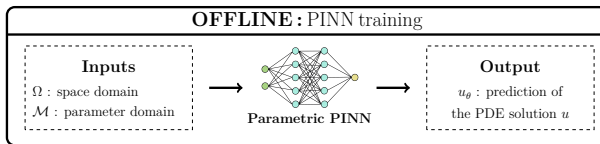
ICOSAHOM
MONTREAL 2025

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 $\mathbf{e}_y = (0, 1)$.

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

$$\left\{ \begin{array}{ll} (\mathbf{u} \cdot \nabla) \mathbf{u} + \nabla p - \nu \Delta \mathbf{u} - g(\beta T + 1) \mathbf{e}_y = 0 & \text{in } \Omega \quad (\text{momentum}) \\ \nabla \cdot \mathbf{u} = 0 & \text{in } \Omega \quad (\text{incompressibility}) \\ \mathbf{u} \cdot \nabla T - k_f \Delta T = 0 & \text{in } \Omega \quad (\text{energy}) \\ + \text{suitable BC} & \end{array} \right. \quad (\mathcal{P})$$

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]

¹The 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 $\mu = (\nu, k_f) \in \mathcal{M} = [0.01, 0.1]^2$.

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

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

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

$$\left\{ \begin{array}{ll} R_{mom}(\mathbf{U}; \mathbf{x}, \mu) = 0 & \text{in } \Omega \quad (\text{momentum}) \\ R_{inc}(\mathbf{U}; \mathbf{x}, \mu) = 0 & \text{in } \Omega \quad (\text{incompressibility}) \\ R_{ener}(\mathbf{U}; \mathbf{x}, \mu) = 0 & \text{in } \Omega \quad (\text{energy}) \\ + \text{suitable BC} & \end{array} \right. \quad (\mathcal{P})$$

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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]

Boundary Conditions:

No-slip BC : $\mathbf{u} = 0$ on $\partial\Omega$ **Isothermal BC :** $T = 1$ on the left wall ($x = -1$)
 $T = -1$ on the right wall ($x = 1$)

Adiabatic BC : $\frac{\partial T}{\partial n} = 0$ 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

¹Computed 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.

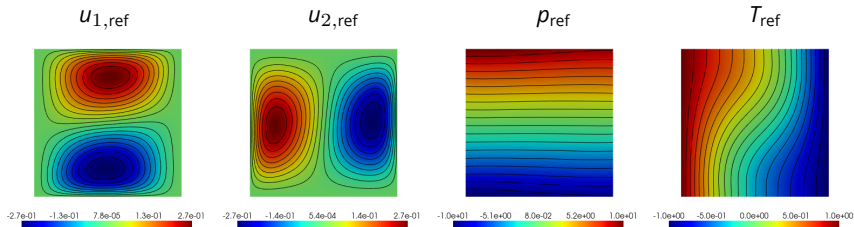
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Reference solution - Rayleigh number : $Ra = 1\,569.6$



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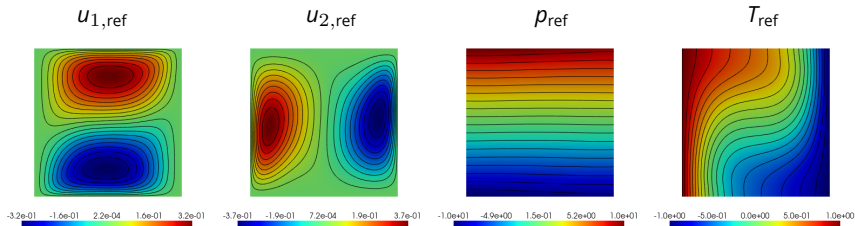
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Reference solution - Rayleigh number : $Ra = 6\,278.4$



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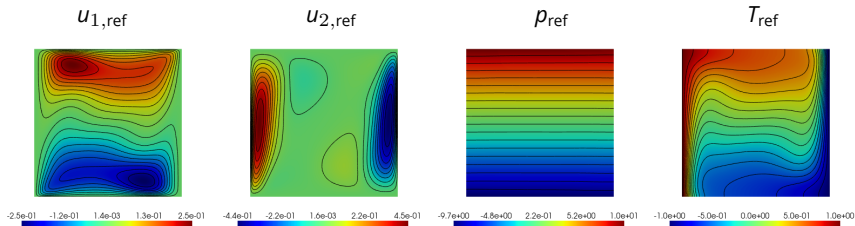
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We evaluate the quality of solutions by comparing them to a reference solution.¹

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



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Parametric PINN

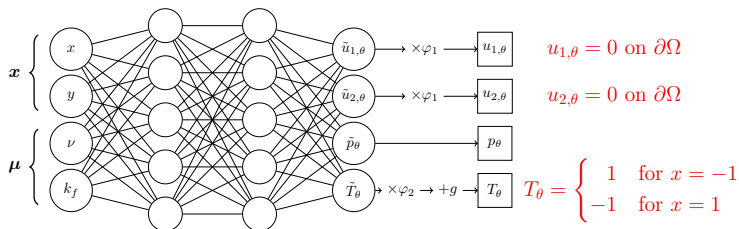
The PINN is parametrized by the μ parameter.

Neural Network considered

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

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

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 θ^* , such that

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

where the different cost functions¹ are defined by

adiabatic condition

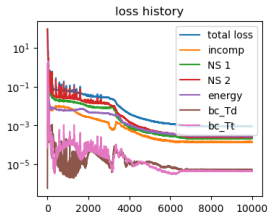
$$J_{ad}(\theta) = \int_{\mathcal{M}} \int_{\Gamma_{ad}} \left| \frac{\partial T_\theta(\mathbf{x}, \mu)}{\partial n} \right|^2 d\mathbf{x} d\mu,$$

3 residual losses

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

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

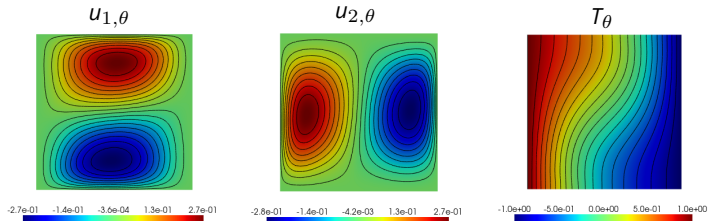
Network - MLP		Training (ADAM / LBFGS)			
<i>layers</i>	40, 60, 60, 60, 40	<i>lr</i>	7e-3	<i>N_{col}</i>	40000
<i>σ</i>	sine	<i>n_{epochs}</i>	10000	<i>N_{bc}</i>	30000



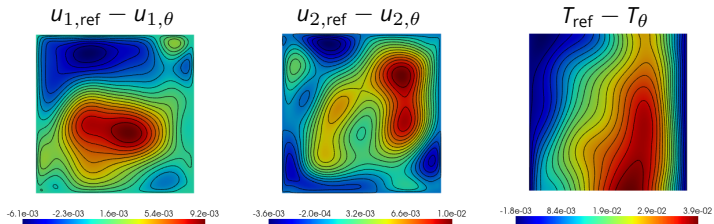
¹Discretized by a random process using Monte-Carlo method.

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

Prediction :



Error map :



L^2 error :
(relative)

$$2.98 \times 10^{-2}$$

$$3.17 \times 10^{-2}$$

$$3.90 \times 10^{-2}$$

Finite element method (FEM)

The μ parameter is fixed in the FE resolution.

Discrete weak formulation

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

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

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

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

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

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 $F : \mathbb{R}^{N_h} \rightarrow \mathbb{R}^{N_h}$ 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:

$$\vec{U}_{k,0} = (\vec{0}, \vec{0}, \vec{0}, \vec{\tau}_0)$$

where for $i = 1, \dots, \dim(W_h)$,

$$(\vec{\tau}_0)_i = g(\mathbf{x}^{(i)}) = 1 - (x^{(i)} + 1)$$

with $\mathbf{x}^{(i)} = (x^{(i)}, y^{(i)})$ the i -th dofs coordinates of W_h .

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

3 types of initialization

- **Natural** : Using constant or linear function.
- **PINN** : Using PINN prediction.

(UNet : [Odote 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 $i = 1, \dots, N_h$,

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

with $\mathbf{x}^{(i)} = (x^{(i)}, y^{(i)})$ 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.
- **PINN** : Using PINN prediction.
(UNet : [Odote 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 $\mu^{(k-1)}$.
 - We interpolate the coarse solution to the current mesh.
 - We use it as an initialization for the Newton method, i.e.

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

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 $\mu^{(k-1)}$.

Enriched finite element method using PINN

Very simple linear test case

The heated cavity test case considered

Enriched finite element method using PINN

Very simple linear test case

The heated cavity test case considered

What is the purpose of enrichment?

Poisson problem (with Dirichlet BC): Find $u : \Omega \rightarrow \mathbb{R}$ 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 ($k \geq 1$).

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

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

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Modified variational Problem : Let u_θ be a PINN prediction.

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

with the **enriched trial space** V_h^+ defined by

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

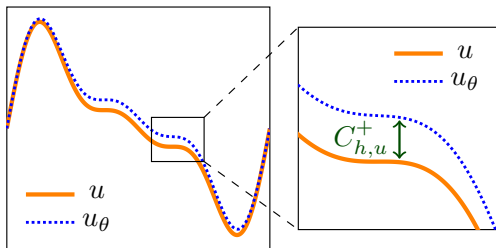
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with the enriched trial space V_h^+ defined by

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



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,

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

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

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,

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

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

Gains of the additive approach.

LECOURTIER Frédérique

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Enriched space using PINN

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

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

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

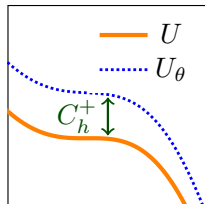
We can then define the three finite element subspaces of M_h^+ as follows:

$$V_h^+ = \{\mathbf{u}_h^+ = \mathbf{u}_\theta + \mathbf{c}_{h,\mathbf{u}}^+, \quad \mathbf{c}_{h,\mathbf{u}}^+ \in [V_h^0]^2\},$$

$$Q_h^+ = \{p_h^+ = p_\theta + c_{h,p}^+, \quad c_{h,p}^+ \in Q_h\},$$

$$W_h^+ = \{T_h^+ = T_\theta + c_{h,T}^+, \quad c_{h,T}^+ \in W_h^0\},$$

where $\mathbf{c}_{h,\mathbf{u}}^+$, $c_{h,p}^+$ and $c_{h,T}^+$ becomes the unknowns.



Weak formulation - Additive approach

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

$$\begin{aligned}
 & \int_{\Omega} [(\mathbf{u}_{\theta} \cdot \nabla) \mathbf{u}_{\theta} + (\mathbf{u}_{\theta} \cdot \nabla) \mathbf{c}_{h,u}^+ + (\mathbf{c}_{h,u}^+ \cdot \nabla) \mathbf{u}_{\theta} + (\mathbf{c}_{h,u}^+ \cdot \nabla) \mathbf{c}_{h,u}^+] \cdot \mathbf{v}_h \, d\mathbf{x} \\
 & + \mu \left(\int_{\Omega} \nabla \mathbf{u}_{\theta} : \nabla \mathbf{v}_h \, d\mathbf{x} + \int_{\Omega} \nabla \mathbf{c}_{h,u}^+ : \nabla \mathbf{v}_h \, d\mathbf{x} \right) + \left(\int_{\Omega} \nabla p_{\theta} \cdot \mathbf{v}_h \, d\mathbf{x} - \int_{\Omega} \mathbf{c}_{h,p}^+ \nabla \cdot \mathbf{v}_h \, d\mathbf{x} \right) \\
 & - g \int_{\Omega} (1 + \beta(\mathbf{T}_{\theta} + \mathbf{c}_{h,T}^+)) \mathbf{e}_y \cdot \mathbf{v}_h \, d\mathbf{x} = 0, \text{ (momentum)} \\
 & \int_{\Omega} q_h [\nabla \cdot \mathbf{u}_{\theta} + \nabla \cdot \mathbf{c}_{h,u}^+] \, d\mathbf{x} + 10^{-4} \int_{\Omega} q_h (p_{\theta} + \mathbf{c}_{h,p}^+) \, d\mathbf{x} = 0, \text{ (incompressibility + penal)} \\
 & \int_{\Omega} [\mathbf{u}_{\theta} \cdot \nabla T_{\theta} + \mathbf{u}_{\theta} \cdot \nabla \mathbf{c}_{h,T}^+ + \mathbf{c}_{h,u}^+ \cdot \nabla T_{\theta} + \mathbf{c}_{h,u}^+ \cdot \nabla \mathbf{c}_{h,T}^+] w_h \, d\mathbf{x} \\
 & + k_f \left(\int_{\Omega} \nabla T_{\theta} \cdot \nabla w_h \, d\mathbf{x} + \int_{\Omega} \nabla \mathbf{c}_{h,T}^+ \cdot \nabla w_h \, d\mathbf{x} \right) = 0, \text{ (energy)}
 \end{aligned} \tag{\mathcal{P}_h^+}$$

with $\mathbf{U}_{\theta} = (\mathbf{u}_{\theta}, p_{\theta}, T_{\theta})$ 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 $F_{\theta} : \mathbb{R}^{N_h} \rightarrow \mathbb{R}^{N_h}$ 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 initialization¹:

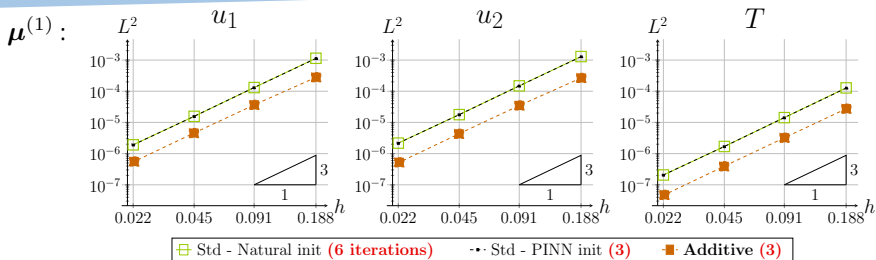
u_{θ} is not required to live in the same discrete space as C_h^+ .

¹Taking U_{θ} and C_h^+ in the same space, additive approach is exactly the same as the PINN initialization.

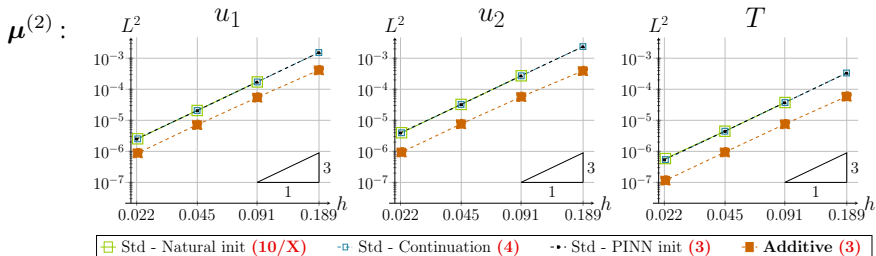
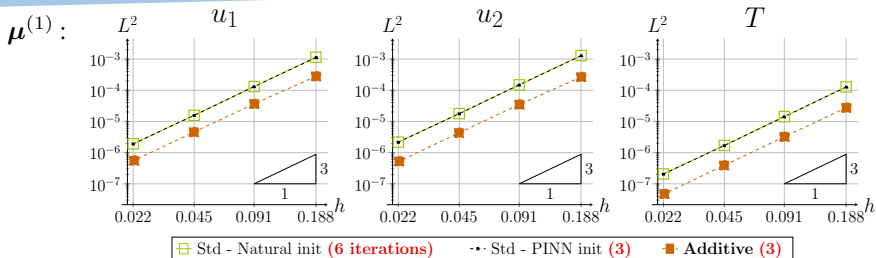
Numerical results

- Results obtained with a laptop GPU.
- The newton solver is the same for all methods ($\text{rtol} = 10^{-10}$, $\text{atol} = 10^{-10}$, $\text{max_it} = 30$).
- 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).

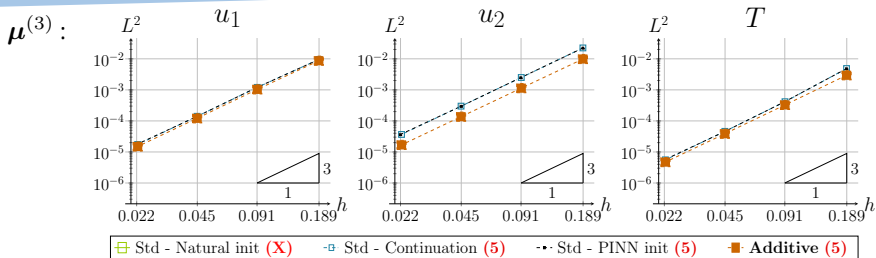
Error estimates I



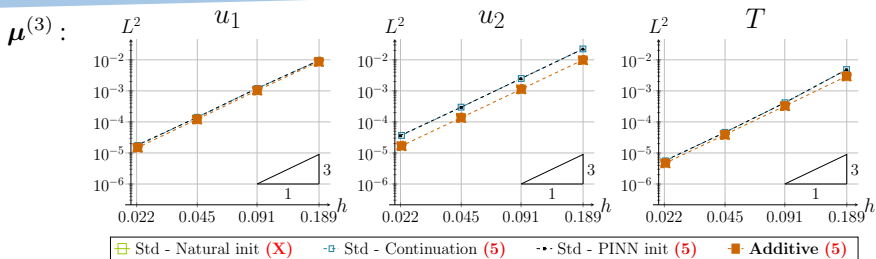
Error estimates I



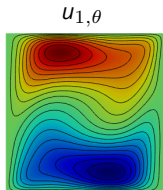
Error estimates II



Error estimates II

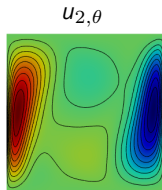


Prediction :



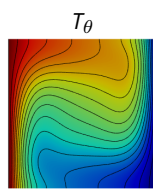
-3.8e-01 -1.9e-01 7.7e-04 1.9e-01 3.8e-01

5.75×10^{-1}



-5.8e-01 -2.9e-01 -4.7e-03 2.8e-01 5.7e-01

4.89×10^{-1}



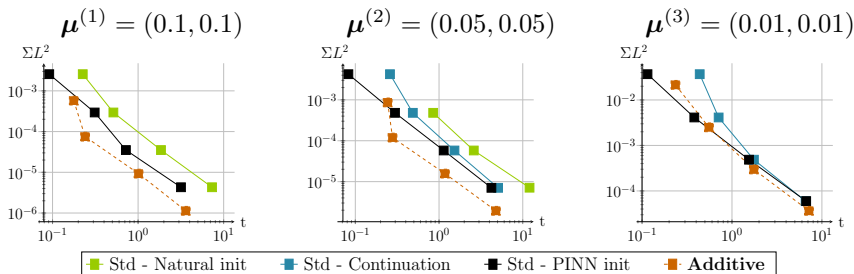
-1.0e+00 -5.0e-01 0.0e+00 5.0e-01 1.0e+00

2.57×10^{-1}

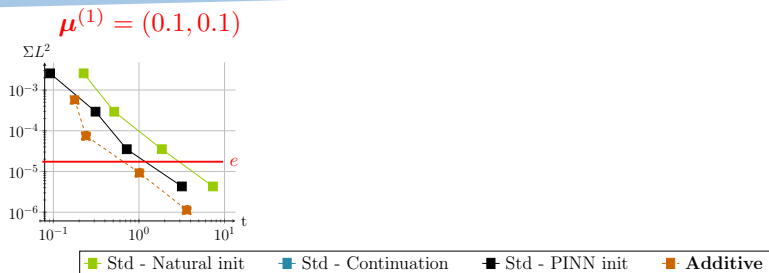
L^2 error :
(relative)

Numerical costs

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



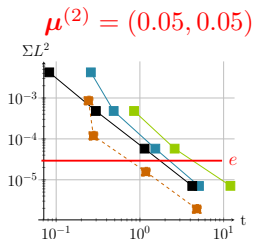
Numerical costs



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)	(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

Numerical costs



■ Std - Natural init
 ■ Std - Continuation
 ■ Std - PINN init
 ■ Additive

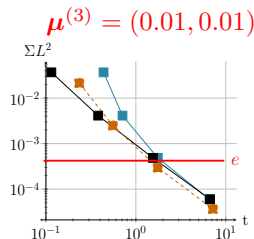
N_{dofs} and execution time required to reach the same global L^2 relative error e :

Std vs Add e	Number of DoFs		Execution times			
	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

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

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Numerical costs



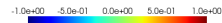
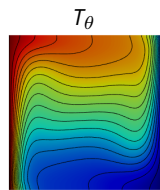
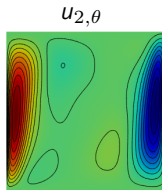
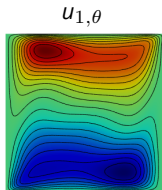
■ Std - Natural init
 ■ Std - Continuation
 ■ Std - PINN init
 ■ Additive

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

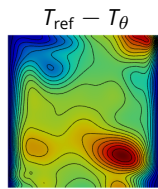
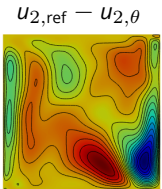
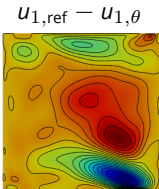
Std vs Add e	Number of DoFs		Execution times			
	Std	Add	(nat)	(cont)	(PINN)	Add
$1 \cdot 10^{-3}$	33,204	23,524	X	1.29	0.96	0.91
$1 \cdot 10^{-4}$	150,339	108,931	X	4.76	4.67	3.65
$1 \cdot 10^{-5}$	690,924	502,156	X	20.34	23.3	17.23

Non parametric PINN¹ for $\mu^{(3)}$

Prediction :



Error map :



L^2 error :
(relative)

$$7.60 \times 10^{-2}$$

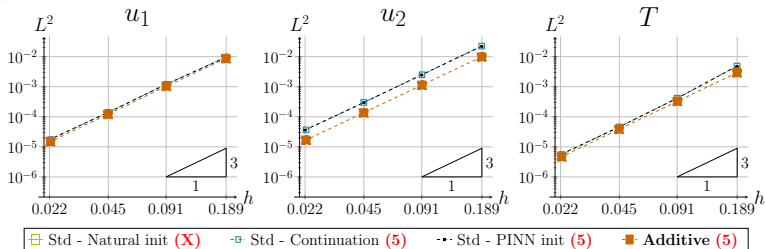
$$5.38 \times 10^{-2}$$

$$9.63 \times 10^{-2}$$

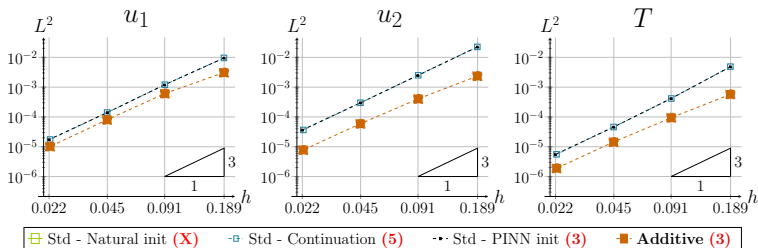
¹We consider exactly the same architecture, but this time we train the PINN non-parametrically.

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

Parametric

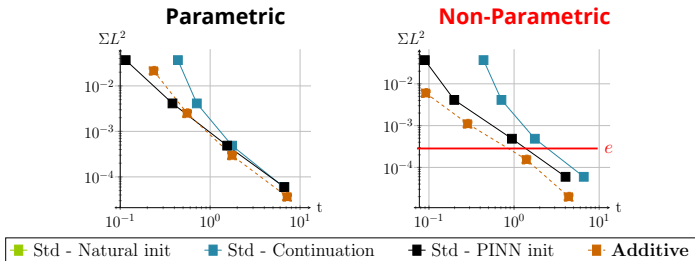


Non-Parametric



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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**.
⇒ 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](#)
⇒ PINNs are good candidates for the enriched approach.
- The gains obtained on linear problems were much higher. [Appendix 3](#)
⇒ **Improved training** of parametric PINN (or Neural Operators).

Preprint (linear)



References

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- Guillaume Coulaud, Maxime Le, and Régis Duvigneau. Investigations on Physics-Informed Neural Networks for Aerodynamics, 2024.
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- N. Sukumar and A. Srivastava. Exact imposition of boundary conditions with distance functions in physics-informed deep neural networks. 2022.
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Preprint (linear)



Appendix 1 : 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:

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

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

$$\vec{u} = (u_i)_{i=1}^{N_u} \in \mathbb{R}^{N_u}, \quad \vec{v} = (v_i)_{i=1}^{N_u} \in \mathbb{R}^{N_u},$$

$$\vec{p} = (p_j)_{j=1}^{N_p} \in \mathbb{R}^{N_p} \quad \text{and} \quad \vec{T} = (T_k)_{k=1}^{N_T} \in \mathbb{R}^{N_T}.$$

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 $F : \mathbb{R}^{N_h} \rightarrow \mathbb{R}^{N_h}$ 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 :

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

PINN training: MLP of 5 layers; LBFGs optimizer (5000 epochs).

Imposing the Dirichlet BC exactly in the PINN with the levelset φ defined by

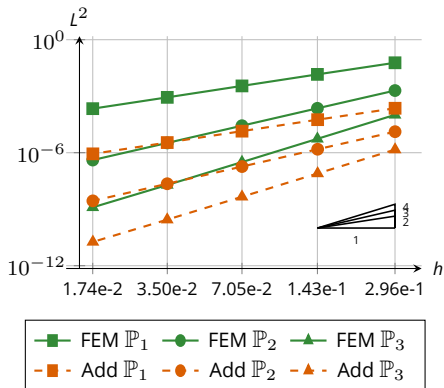
$$\varphi(\mathbf{x}) = (x + 0.5\pi)(x - 0.5\pi)(y + 0.5\pi)(y - 0.5\pi).$$

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

A3 – Numerical results

Error estimates : 1 set of parameters.

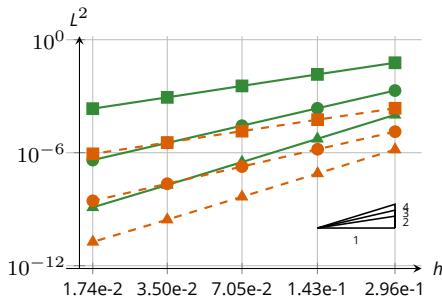
$$\mu^{(1)} = (0.05, 0.22)$$



A3 – Numerical results

Error estimates : 1 set of parameters.

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



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

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

**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

$$N = 20$$

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

Cartesian mesh : N^2 nodes.

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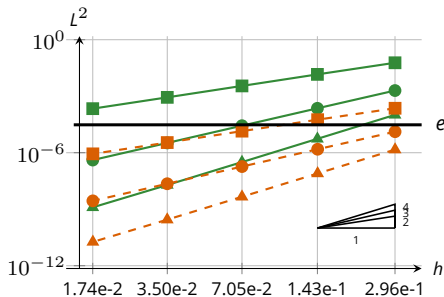
Enriching continuous Lagrange FE approximation spaces using NN

A3 – Numerical results

Error estimates : 1 set of parameters.

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

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



k	e	N_{dofs}	
		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

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

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.

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

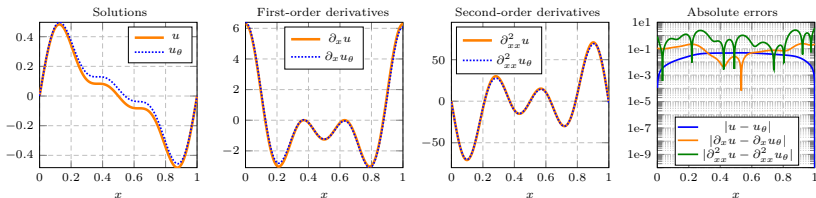
- **Data-driven training:** $N_{\text{data}} = 5000$ data.

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

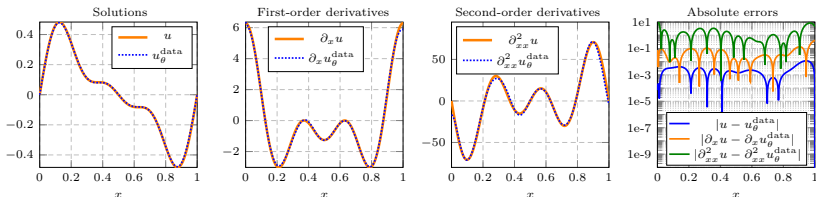
A4 – Priors derivatives

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

PINN



Data



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

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

FEM		PINN prior u_θ			Data prior u_θ^{data}	
N	error	N	error	gain	error	gain
16	$5.18 \cdot 10^{-2}$	16	$1.29 \cdot 10^{-3}$	40.34	$3.51 \cdot 10^{-3}$	14.78
32	$1.24 \cdot 10^{-2}$	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						
N	PINN prior u_θ			Data prior u_θ^{data}		
	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^2 nodes.