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Enriching continuous Lagrange finite element approximation spaces using neural networks

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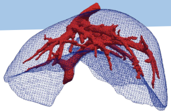
INSTITUT MONTPELLIERAIN ALEXANDER GROTHENDIECK

PhD student seminar

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

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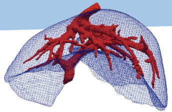

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accurate — quick + parameterized

Parametric Poisson problem (with homogeneous Dirichlet BC):
For one or several $\boldsymbol{\mu} \in \mathcal{M}$, find $u : \Omega \to \mathbb{R}$ such that

$$\begin{cases} -\Delta u(\boldsymbol{x};\boldsymbol{\mu}) = f(\boldsymbol{x};\boldsymbol{\mu}), & (\boldsymbol{x},\boldsymbol{\mu}) \in \Omega \times \mathcal{M}, \\ u(\boldsymbol{x};\boldsymbol{\mu}) = 0, & (\boldsymbol{x},\boldsymbol{\mu}) \in \partial\Omega \times \mathcal{M}, \end{cases} \qquad (\mathcal{P})$$

with $\Omega \subset \mathbb{R}^d$ a domain (d the spatial dimension).

Table of contents

Classical approaches

Physics-Informed Neural Networks

Standard PINNs: Find the optimal weights $\theta^\star$, such that

$$\theta^\star = \underset{\theta}{\operatorname{argmin}} \left(\omega_r J_r(\theta) + \omega_b J_b(\theta)\right), \qquad (\mathcal{P}_\theta)$$

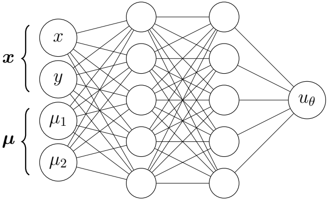
with

residual loss $$\boxed{J_r(\theta) = \int_{\mathcal{M}} \int_\Omega \left|\Delta u_\theta(\boldsymbol{x}, \boldsymbol{\mu}) + f(\boldsymbol{x}, \boldsymbol{\mu})\right|^2 d\boldsymbol{x} d\boldsymbol{\mu},}$$

boundary loss $$\boxed{J_b(\theta) = \int_{\mathcal{M}} \int_{\partial\Omega} \left|u_\theta(\boldsymbol{x}, \boldsymbol{\mu})\right|^2 d\boldsymbol{x} d\boldsymbol{\mu},}$$

with ω_r and ω_b are some weights.

u_θ is a neural network, e.g. fully-connected NN.
(see example in 2D with 2 parameters)



Monte-Carlo method: Discretize the cost functions by random process.

Finite Element Method[1]

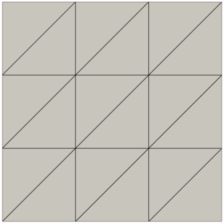
Variational Problem:

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

with h the characteristic mesh size, a and l the bilinear and linear forms given by

$$a(u_h, v_h) = \int_\Omega \nabla u_h \cdot \nabla v_h, \quad l(v_h) = \int_\Omega f v_h,$$

and V_h^0 a continuous, piecewise polynomial space of degree k.



Cartesian mesh

[1] [Ern and Guermond, 2004]

LECOURTIER Frédérique

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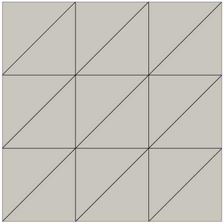
and V_h^0 a continuous, piecewise polynomial space of degree k.

Linear system: Let $(\phi_1, \dots, \phi_{N_{\text{dofs}}})$ a basis of V_h^0.
Find $U \in \mathbb{R}^{N_{\text{dofs}}}$ such that

$$AU = b,$$

$$A = \left(a(\phi_i, \phi_j)\right)_{1 \le i,j \le N_{\text{dofs}}} \in \mathbb{R}^{N_{\text{dofs}} \times N_{\text{dofs}}},$$

$$b = \left(l(\phi_j)\right)_{1 \le j \le N_{\text{dofs}}} \in \mathbb{R}^{N_{\text{dofs}}}.$$



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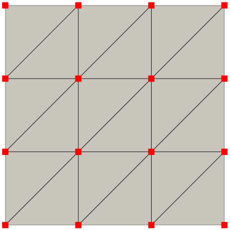

degrees of freedom

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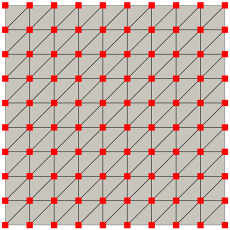

$h \searrow \Rightarrow N_{\text{dofs}} \nearrow$

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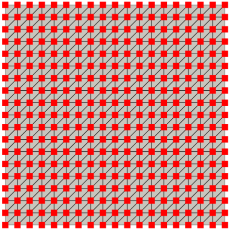

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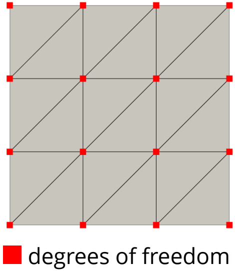

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and V_h^0 a continuous, piecewise polynomial space of degree k. $(k = 2)$

Linear system: Let $(\phi_1, \dots, \phi_{N_{\text{dofs}}})$ a basis of V_h^0.
Find $U \in \mathbb{R}^{N_{\text{dofs}}}$ such that

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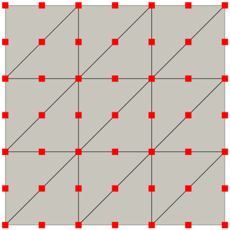

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Linear system: Let $(\phi_1, \dots, \phi_{N_\text{dofs}})$ a basis of V_h^0.
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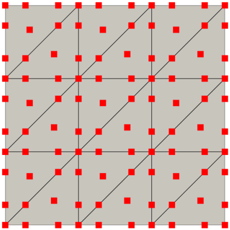

$k \nearrow \Rightarrow N_\text{dofs} \nearrow$

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Enriched finite element method using PINNs

Pipeline of the Enriched FEM

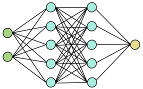
OFFLINE : PINN training

Inputs

$\boldsymbol{x} \in \Omega$: space coordinates

$\boldsymbol{\mu} \in \mathcal{M}$: parameter

$\longrightarrow$



Parametric PINN

$\longrightarrow$

Output

$u_\theta(\boldsymbol{x}, \boldsymbol{\mu})$: prediction of the PDE solution $u(\boldsymbol{x}, \boldsymbol{\mu})$

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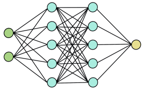


Parametric PINN

$\longrightarrow$

Output

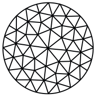
$u_\theta(\boldsymbol{x}, \boldsymbol{\mu})$: prediction of the PDE solution $u(\boldsymbol{x}, \boldsymbol{\mu})$

ONLINE (fixed $\boldsymbol{\mu}$) : PINN evaluation + Enriched FEM resolution

PINN evaluation

$u_\theta(\cdot, \boldsymbol{\mu})$: prediction for the given parameter μ

$\longrightarrow$



FEM solver enriched by u_θ

$\longrightarrow$

Output

enriched FEM solution (depending on the mesh size h)

Complete ONLINE process : quick + accurate

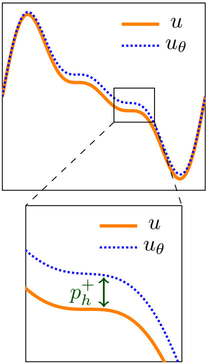
Additive approach

Variational Problem: Let $u_\theta \in H^{k+1}(\Omega) \cap H_0^1(\Omega)$ be a PINN prior.

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

with the enriched trial space V_h^+ defined by

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



General Dirichlet BC: If $u = g$ on $\partial\Omega$, then

$$C_h^+ = g - u_\theta \quad \text{on } \partial\Omega,$$

with u_θ the PINN prior.

We expect 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,

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

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

Theorem 2: Convergence analysis of the enriched FEM [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,

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

$$\boxed{\frac{|u-u_\theta|_{H^{k+1}}}{|u|_{H^{k+1}}}} < 1 \Rightarrow$$ Gains of the additive approach.

Numerical results

- 2D Poisson problem on Square - Dirichlet BC
- 3D Poisson problem on Cube - Dirichlet BC
- 2D Anisotropic Elliptic problem on Square - Dirichlet BC
- 2D Poisson problem on Annulus - Mixed BC

Numerical results

- 2D Poisson problem on Square - Dirichlet BC
- 3D Poisson problem on Cube - Dirichlet BC
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Problem considered

Problem statement: Consider the Poisson problem in 2D 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: $\boldsymbol{\mu} = (\mu_1, \mu_2) \in \mathcal{M}$

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

Parametric PINN training:

MLP 5 layers (sine - 40, 60, 60, 60, 40); LBFGs optimizer (5000 epochs - 6000 col. pts).

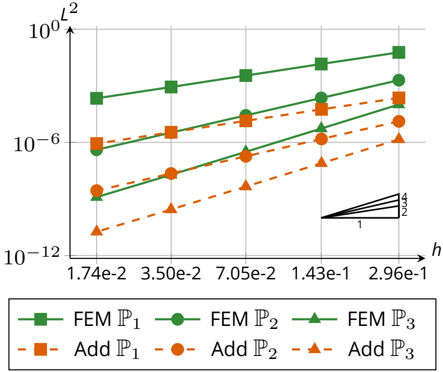
Imposing the Dirichlet BC exactly in the PINN with the levelset φ defined by

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

Online phase - 1 parameters instance

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

Error estimates in L^2 norm:



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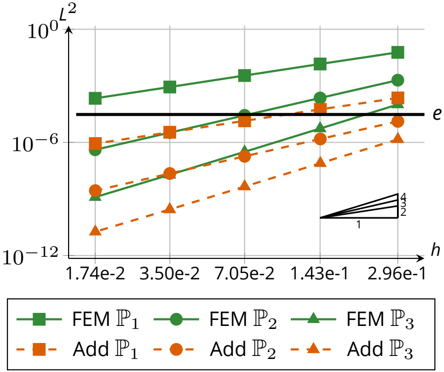


N_{dofs} required to reach the same error e:

k	e	N_{dofs} FEM	N_{dofs} 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

$$h \approx N_{\text{dofs}}^{-1/2}$$

Numerical results

2D Poisson problem on Square - Dirichlet BC

3D Poisson problem on Cube - Dirichlet BC

2D Anisotropic Elliptic problem on Square - Dirichlet BC

2D Poisson problem on Annulus - Mixed BC

Problem considered

Problem statement: Consider the Poisson problem in 3D 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 $\Omega = (-0.5\pi, 0.5\pi)^3$ and $\mathcal{M} = [-0.5, 0.5]^3$ ($p = 3$ parameters).

Analytical solution: $\boldsymbol{\mu} = (\mu_1, \mu_2, \mu_3) \in \mathcal{M}$

$$u(\boldsymbol{x}, \boldsymbol{\mu}) = \exp\left(-\frac{(x-\mu_1)^2 + (y-\mu_2)^2 + (z-\mu_3)^2}{2}\right) \sin(2x)\sin(2y)\sin(2z).$$

Parametric PINN training:

MLP 5 layers (tanh - 40, 60, 60, 60, 40); LBFGs optimizer (5000 epochs - 40000 col. pts).

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

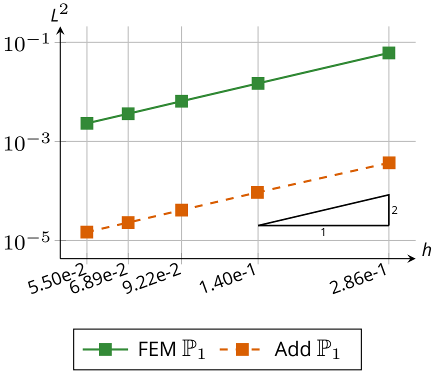
$$\varphi(\boldsymbol{x}) = (x+0.5\pi)(x-0.5\pi)(y+0.5\pi)(y-0.5\pi)(z+0.5\pi)(z-0.5\pi).$$

Training time: 12 minutes on NVIDIA RTX 2000 (8GB VRAM).

Online phase - 1 parameters instance I

$$\boldsymbol{\mu}^{(1)} = (0.05, 0.22, 0.1)$$

Error estimates in L^2 norm:



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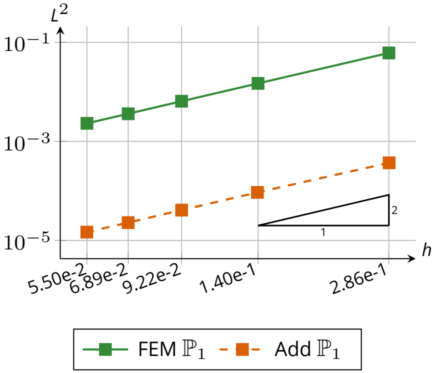
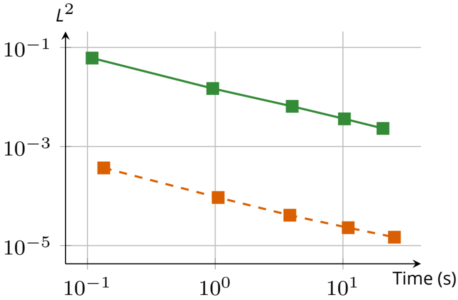


L^2 error w.r.t. online time*:



* mesh + assembly + solve

+ prior derivatives evaluation

~~+ training time~~

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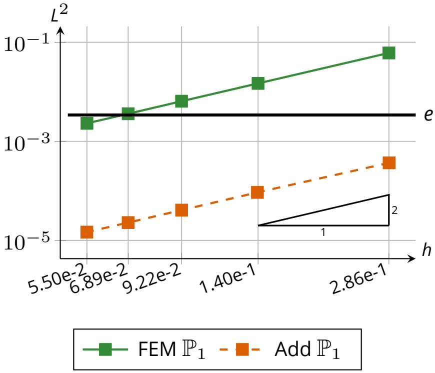

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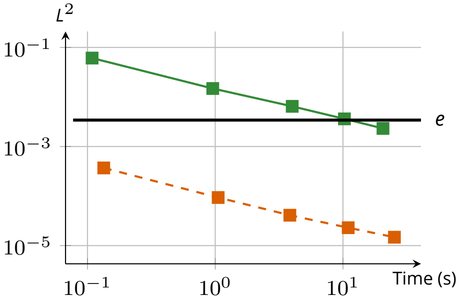


* mesh + assembly + solve

+ prior derivatives evaluation

~~+ training time~~

Online phase - 1 parameters instance II

$$\boldsymbol{\mu}^{(1)} = (0.05, 0.22, 0.1)$$

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

	N		N_{dofs}		Online time*	
e	**FEM**	**Add**	**FEM**	**Add**	**FEM**	**Add**
$1 \cdot 10^{-3}$	152	12	$3.51 \cdot 10^6$	$1.73 \cdot 10^3$	$(7.65 \cdot 10^1)$	$5.2 \cdot 10^{-2}$
$1 \cdot 10^{-4}$	484	39	$1.13 \cdot 10^8$	$5.93 \cdot 10^4$	$(2.8 \cdot 10^3)$	$9.26 \cdot 10^{-1}$
$1 \cdot 10^{-5}$	1 539	122	$3.65 \cdot 10^9$	$1.82 \cdot 10^6$	$(1.02 \cdot 10^5)$	$(5.26 \cdot 10^1)$

$\div 1471$

Cartesian mesh: $N_{\text{dofs}} = N^3$ nodes ($\mathbb{P}_1$ elements).

* The results in brackets are extrapolations.

Online phase - 1 parameters instance II

$$\boldsymbol{\mu}^{(1)} = (0.05, 0.22, 0.1)$$

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

	N		N_{dofs}		Online time*	
e	**FEM**	**Add**	**FEM**	**Add**	**FEM**	**Add**
$1 \cdot 10^{-3}$	152	12	$3.51 \cdot 10^{6}$	$1.73 \cdot 10^{3}$	$(7.65 \cdot 10^{1})$	$5.2 \cdot 10^{-2}$
$1 \cdot 10^{-4}$	484	39	$1.13 \cdot 10^{8}$	$5.93 \cdot 10^{4}$	$(2.8 \cdot 10^{3})$	$9.26 \cdot 10^{-1}$
$1 \cdot 10^{-5}$	1 539	122	$3.65 \cdot 10^{9}$	$1.82 \cdot 10^{6}$	$(1.02 \cdot 10^{5})$	$(5.26 \cdot 10^{1})$

$\div 1471$

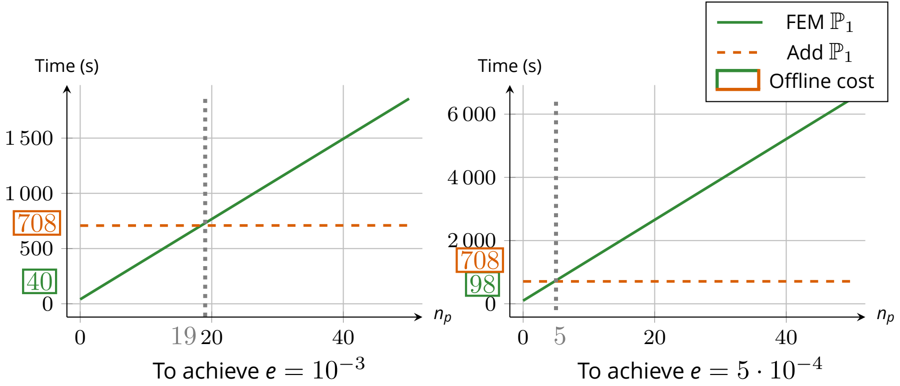
Cartesian mesh: $N_{\text{dofs}} = N^3$ nodes ($\mathbb{P}_1$ elements).

* The results in brackets are extrapolations.

⚠ Training time !

Parametric framework

How many parameters instance n_p are needed to balance training?



Online: assembly + solve + prior derivatives evaluation

Offline: mesh + training time

Numerical results

Problem considered

Problem statement: Considering an Anisotropic Elliptic problem with Dirichlet BC:

$$\begin{cases} -\mathrm{div}(D\nabla u) = f, & \text{in } \Omega \times \mathcal{M}, \\ u = 0, & \text{on } \partial\Omega \times \mathcal{M}, \end{cases}$$

with $\Omega = (0,1)^2$ and $\mathcal{M} = [0.4, 0.6]^2 \times [0.01, 1] \times [0.1, 0.8]$ ($p = 4$ parameters).

Right-hand side and diffusion matrix: $\boldsymbol{\mu} = (\mu_1, \mu_2, \sigma, \epsilon) \in \mathcal{M}$

$$f(\boldsymbol{x}, \boldsymbol{\mu}) = \exp\left(-\frac{(x-\mu_1)^2 + (y-\mu_2)^2}{0.025\sigma^2}\right).$$

$$D(\boldsymbol{x}, \boldsymbol{\mu}) = \begin{pmatrix} \epsilon x^2 + y^2 & (\epsilon - 1)xy \\ (\epsilon - 1)xy & x^2 + \epsilon y^2 \end{pmatrix}.$$

Parametric PINN training:

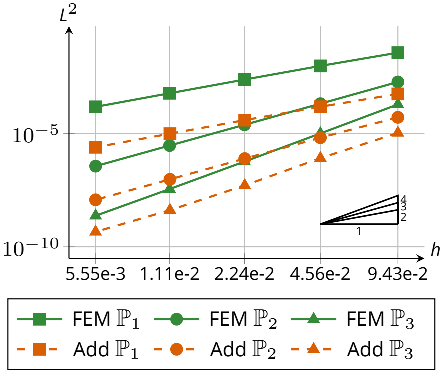
MLP[1] 5 layers (tanh - 40, 60, 60, 60, 40). Adam optimizer (15000 epochs - 8000 col. pts).
Imposing the Dirichlet BC exactly in the PINN with the a level-set function.

[1] with Fourier Features, Tancik et al. [2020]

Online phase

Error estimates: 1 parameter instance

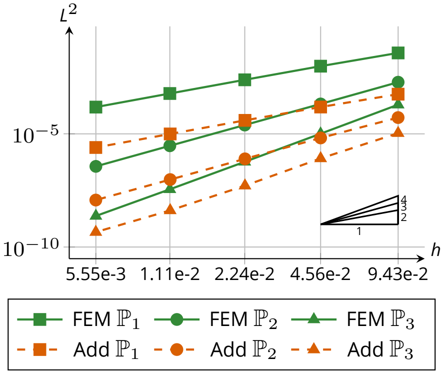
$$\boldsymbol{\mu}^{(1)} = (0.51, 0.54, 0.52, 0.55)$$



Online phase

Error estimates: 1 parameter instance

$$\boldsymbol{\mu}^{(1)} = (0.51, 0.54, 0.52, 0.55)$$



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

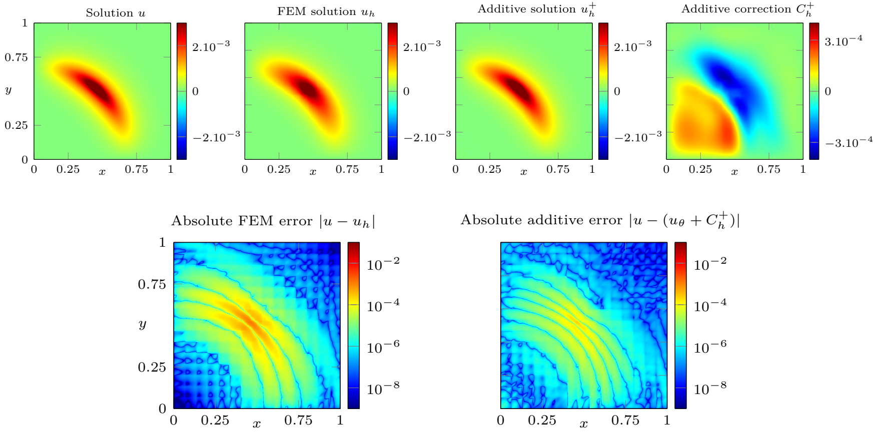
Considering $n_p = 50$ parameters instances

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

	Gains in L^2 rel error of our method w.r.t. FEM		
k	**min**	**max**	**mean**
1	7.12	82.57	35.67
2	3.54	35.88	18.32
3	1.33	26.51	8.32

Cartesian mesh: N^2 nodes with $N = 20$.

Numerical solutions and errors



$$\boldsymbol{\mu}^{(2)} = (0.46, 0.52, 0.05, 0.12) \quad (k = 2, N = 16)$$

Numerical results

2D Poisson problem on Square - Dirichlet BC

3D Poisson problem on Cube - Dirichlet BC

2D Anisotropic Elliptic problem on Square - Dirichlet BC

2D Poisson problem on Annulus - Mixed BC

Problem considered

Problem statement: Considering the Poisson problem with mixed BC:

$$\begin{cases} -\Delta u = f, & \text{in } \Omega \times \mathcal{M}, \\ u = g, & \text{on } \Gamma_E \times \mathcal{M}, \\ \dfrac{\partial u}{\partial n} + u = g_R, & \text{on } \Gamma_I \times \mathcal{M}, \end{cases}$$

with $\Omega = \{(x,y) \in \mathbb{R}^2, 0.25 < x^2 + y^2 < 1\}$ and $\mathcal{M} = [2.4, 2.6]$ ($p = 1$ parameter).

Analytical solution and boundary conditions: $\boldsymbol{\mu} = \mu_1 \in \mathcal{M}$

$$u(\boldsymbol{x}; \boldsymbol{\mu}) = 1 - \frac{\ln\left(\mu_1 \sqrt{x^2 + y^2}\right)}{\ln(4)},$$

$$g(\boldsymbol{x}; \boldsymbol{\mu}) = 1 - \frac{\ln(\mu_1)}{\ln(4)} \quad \text{and} \quad g_R(\boldsymbol{x}; \boldsymbol{\mu}) = 2 + \frac{4 - \ln(\mu_1)}{\ln(4)}.$$

Parametric PINN training:

MLP 5 layers (tanh - 5×40); LBFGs optimizer (4000 epochs - 6000 col. pts).

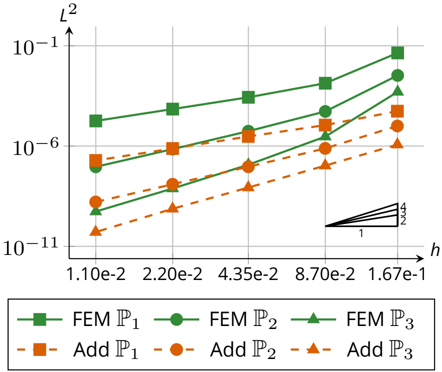
Imposing the mixed BC exactly in the PINN[1] (+ Sobolev training).

[1] [Sukumar and Srivastava, 2022]

Online phase

Error estimates: 1 parameters instance

$$\boldsymbol{\mu}^{(1)} = 2.51$$



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

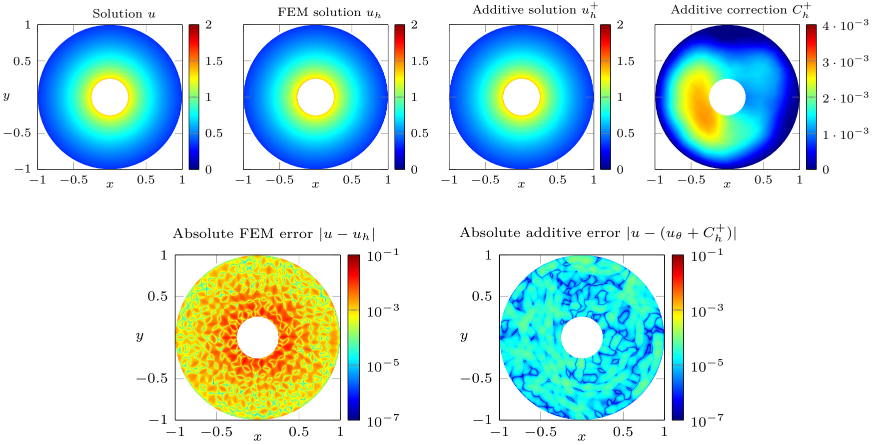
Considering $n_p = 50$ parameters instances

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

	Gains in L^2 rel error of our method w.r.t. FEM		
k	**min**	**max**	**mean**
1	15.12	137.72	55.5
2	31	77.46	58.41
3	18.72	21.49	20.6

Mesh size: $h = 1.33 \cdot 10^{-1}$

Numerical solutions and errors



$$\mu^{(1)} = 2.51 \quad (k = 1, h = 1.67 \cdot 10^{-1})$$

Extension to non-linear problems

Physics-Informed Neural Network (PINN)
Finite Element Method (FEM)
Enriched finite element method using PINNs

Heated cavity test case[1]

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

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, $\nu = 0.01$ the viscosity and $k_f = 0.01$ the thermal conductivity. (Rayleigh number: $156\,960$)

[1] Non-parametric study.

Heated cavity test case[1]

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

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

with $g = 9.81$ the gravity, $\beta = 0.1$ the expansion coefficient, $\nu = 0.01$ the viscosity and $k_f = 0.01$ the thermal conductivity. (Rayleigh number: $156\,960$)

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})

[1] Non-parametric study.

Extension to non-linear problems

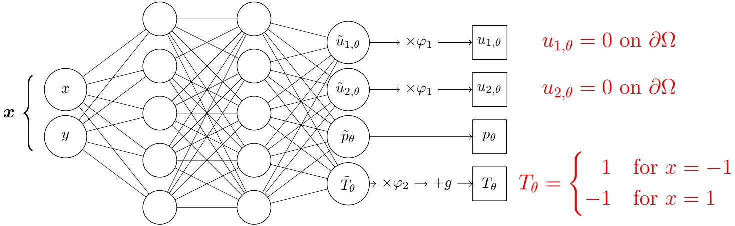
Physics-Informed Neural Network (PINN)
Finite Element Method (FEM)
Enriched finite element method using PINNs

Neural Network considered

We consider a non-parametric NN with 2 inputs and 4 outputs, defined by

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

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

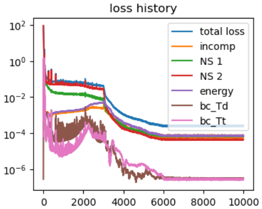
$$\boxed{J_\bullet(\theta) = \int_{\mathcal{M}} \int_{\Omega} \left| R_\bullet(U_\theta(\boldsymbol{x},\boldsymbol{\mu}); \boldsymbol{x}, \boldsymbol{\mu}) \right|^2 d\boldsymbol{x} d\boldsymbol{\mu},}$$

with U_θ the non-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

+ some weights to balance the different losses.

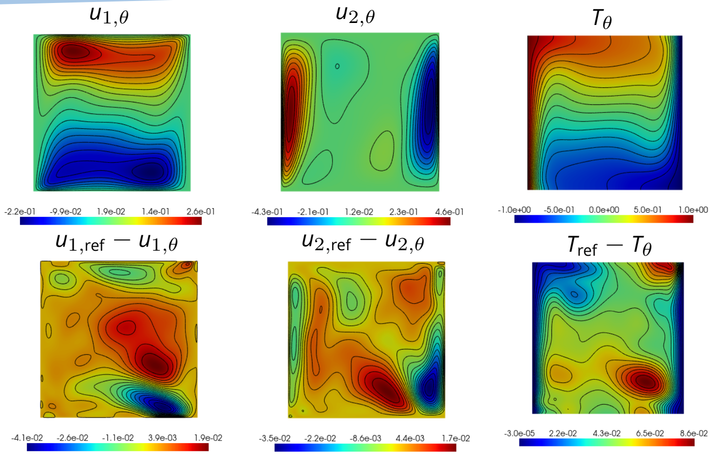


[1] Discretized by a random process using Monte-Carlo method.

Non parametric PINN prediction

Prediction:

Error map[1]:



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

[1] Reference solution computed by FEM on an over-refined mesh.

Extension to non-linear problems

Physics-Informed Neural Network (PINN)

Finite Element Method (FEM)

Enriched finite element method using PINNs

Discrete variational formulation

We consider a mixed finite element space $M_h = [V_h^0]^2 \times Q_h \times W_h$ (4 unknowns).

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

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

Discrete variational formulation

We consider a mixed finite element space $M_h = [V_h^0]^2 \times Q_h \times W_h$ (4 unknowns).

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

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

Non-linear terms $\Rightarrow$ Non-linear system to solve.

Newton method

Denoting N_{dofs} the dimension of M_h, we want to solve the-non linear system:

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

with $F : \mathbb{R}^{N_{\text{dofs}}} \to \mathbb{R}^{N_{\text{dofs}}}$ the non-linear operator associated to $(\mathcal{P}_h)$ and $\vec{U} \in \mathbb{R}^{N_{\text{dofs}}}$ the unknown vector.

Algorithm 1: Newton algorithm

Initialization step: set $\vec{U}^{(0)} = \vec{U}_0$;
for $\underline{n \geq 0}$ **do**
  Solve the linear system $F(\vec{U}^{(n)}) + F'(\vec{U}^{(n)})\delta^{(n+1)} = 0$ for $\delta^{(n+1)}$;
  Update $\vec{U}^{(n+1)} = \vec{U}^{(n)} + \delta^{(n+1)}$;
end

Newton method

Denoting N_{dofs} the dimension of M_h, we want to solve the-non linear system:

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

with $F : \mathbb{R}^{N_{\text{dofs}}} \to \mathbb{R}^{N_{\text{dofs}}}$ the non-linear operator associated to $(\mathcal{P}_h)$ and $\vec{U} \in \mathbb{R}^{N_{\text{dofs}}}$ the unknown vector.

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  Update $\vec{U}^{(n+1)} = \vec{U}^{(n)} + \delta^{(n+1)}$;
end

⚠ The choice of the $\vec{U}_0$ is crucial for the convergence of the Newton method.

Solution: Continuation method where we progressively increase the non-linearity of the problem.

Extension to non-linear problems

Physics-Informed Neural Network (PINN)
Finite Element Method (FEM)
Enriched finite element method using PINNs

Additive approach

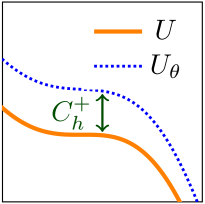
Considering the PINN prior $U_\theta = (\boldsymbol{u}_\theta, p_\theta, T_\theta)$, we define the mixed finite element space additively enriched by the PINN as follows:

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

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.

Modified variational formulation

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

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

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

Newton method - Additive approach

Denoting N_{dofs} the dimension of M_h^+, we want to solve the non-linear system:

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

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

Algorithm 2: Newton algorithm

Initialization step: set $\vec{C}^{(0)} = 0$;

for $\underline{n \geq 0}$ **do**

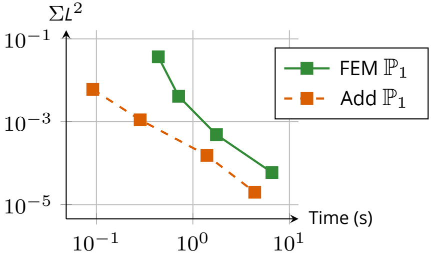
  Solve the linear system $F_\theta(\vec{C}^{(n)}) + F'_\theta(\vec{C}^{(n)})\delta^{(n+1)} = 0$ for $\delta^{(n+1)}$;

  Update $\vec{C}^{(n+1)} = \vec{C}^{(n)} + \delta^{(n+1)}$;

end

Numerical results

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



	N_{dofs}		Online time	
e	**FEM**	**Add**	**FEM**	**Add**
$1 \cdot 10^{-3}$	33 204	13 764	1.29	0.31
$1 \cdot 10^{-4}$	150 339	70 303	4.76	1.78
$1 \cdot 10^{-5}$	690 924	339 231	20.34	6.42

Conclusion

- **Offline/online framework:**
  - **Offline phase:** Training a PINN over a parametric space.
  - **Online phase:** (fixed parameter instance)
    Quick and accurate resolution of the FEM correction problem using the PINN prior.
- **Numerical results:** Several parametrics PDEs.
- **Extension to non-linear problems** :
  First promising results for the incompressible Navier-Stokes equations.

Perspectives:

- Improve Navier-Stokes results:
  - Improved parametric PINN training.
  - Different meshes by unknowns (+ parameter dependency).
- Extend the approach to more complex geometries.

Preprint (linear)

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Preprint (linear)