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Combining Finite Element Methods and Neural Networks to Solve Elliptic Problems on 2D Geometries

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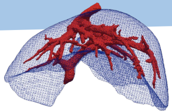
Scientific context



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

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

accurate quick + parameterized

Parametric elliptic convection/diffusion PDE : For one or several $\boldsymbol{\mu} \in \mathcal{M}$, find $u : \Omega \to \mathbb{R}$ such that

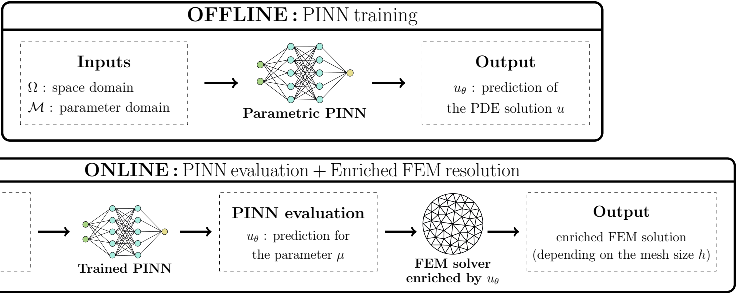
$$\mathcal{L}\big(u\,;\boldsymbol{x},\boldsymbol{\mu}\big) = f(\boldsymbol{x},\boldsymbol{\mu}), \qquad (\mathcal{P})$$

where $\mathcal{L}$ is the parametric differential operator defined by

$$\mathcal{L}(\cdot;\boldsymbol{x},\boldsymbol{\mu}) : u \mapsto R(\boldsymbol{x},\boldsymbol{\mu})u + C(\boldsymbol{\mu}) \cdot \nabla u - \frac{1}{\mathrm{Pe}} \nabla \cdot (D(\boldsymbol{x},\boldsymbol{\mu}) \nabla u),$$

and some Dirichlet, Neumann or Robin BC (which can also depend on $\boldsymbol{\mu}$).

Pipeline of the Enriched FEM



Remark : The PINN prediction enriched Finite element approximation spaces.

Physics-Informed Neural Networks

Standard PINNs[1] **(Weak BC) :** 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
$$\boxed{J_r(\theta) = \int_{\mathcal{M}} \int_{\Omega} \left| \mathcal{L}\big(u_\theta(\boldsymbol{x}, \boldsymbol{\mu}); \boldsymbol{x}, \boldsymbol{\mu}\big) - f(\boldsymbol{x}, \boldsymbol{\mu}) \right|^2 d\boldsymbol{x} d\boldsymbol{\mu},}$$

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

where u_θ is a neural network, $g = 0$ is the Dirichlet BC.

In ($\mathcal{P}_\theta$), ω_r and ω_b are some weights.

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

[1] [Raissi et al., 2019]

Physics-Informed Neural Networks

Improved PINNs[1] (Strong BC) : Find the optimal weights $\theta^\star$ that satisfy

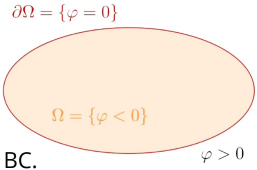
$$\theta^\star = \underset{\theta}{\operatorname{argmin}} \left(\omega_r J_r(\theta) + \cancel{\omega_b J_b(\theta)} \right),$$

with $\omega_r = 1$ and the residual loss function defined by

$$J_r(\theta) = \int_{\mathcal{M}} \int_{\Omega} \left| \mathcal{L}\big(u_\theta(\boldsymbol{x}, \boldsymbol{\mu}); \boldsymbol{x}, \boldsymbol{\mu}\big) - f(\boldsymbol{x}, \boldsymbol{\mu}) \right|^2 d\boldsymbol{x} d\boldsymbol{\mu},$$

where u_θ is a neural network defined by

$$u_\theta(\boldsymbol{x}, \boldsymbol{\mu}) = \varphi(\boldsymbol{x}) w_\theta(\boldsymbol{x}, \boldsymbol{\mu}) + g(\boldsymbol{x}, \boldsymbol{\mu}),$$



with φ a level-set function, w_θ a NN and $g = 0$ the Dirichlet BC.

Thus, the Dirichlet BC is imposed exactly in the PINN : $u_\theta = g$ on $\partial\Omega$.

[1] [Lagaris et al., 1998; Franck et al., 2024]

Finite Element Method[1]

Variational Problem :

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

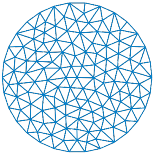
with h the characteristic mesh size, a and l the bilinear and linear forms given by

$$a(u_h, v_h) = \frac{1}{\text{Pe}} \int_\Omega D\nabla u_h \cdot \nabla v_h + \int_\Omega R\, u_h\, v_h + \int_\Omega v_h\, C \cdot \nabla u_h, \quad l(v_h) = \int_\Omega f\, v_h,$$

and V_h^0 the finite element space defined by

$$V_h^0 = \left\{ v_h \in C^0(\Omega),\ \forall K \in \mathcal{T}_h,\ v_h|_K \in \mathbb{P}_k, v_h|_{\partial\Omega} = 0 \right\},$$

where $\mathbb{P}_k$ is the space of polynomials of degree at most k.



$\mathcal{T}_h = \{K_1, \ldots, K_{N_e}\}$
(N_e : number of elements)

Linear system : Let $(\phi_1, \ldots, \phi_{N_h})$ a basis of V_h^0.

Find $U \in \mathbb{R}^{N_h}$ such that $\qquad AU = b$

with

$$A = \big(a(\phi_i, \phi_j)\big)_{1\le i,j\le N_h} \quad \text{and} \quad b = \big(l(\phi_j)\big)_{1\le j\le N_h}.$$

[1] [Ern and Guermond, 2004]

How improve PINN prediction with FEM ?

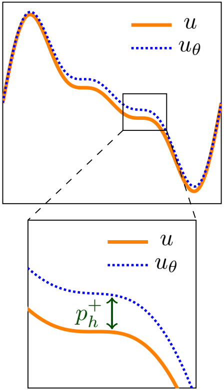
Additive approach

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

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

with the enriched trial space V_h^+ defined by

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



Impose BC : If our problem satisfies $u = g$ on $\partial\Omega$, then p_h^+ has to satisfy

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

with u_θ the PINN prior (weak BC).

Considering the strong BC, $p_h^+ = 0$ on $\partial\Omega$.

Convergence analysis

Let α and γ respectively the coercivity and continuity constants of a. Let u the solution of $(\mathcal{P})$.

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.
For all $1 \leqslant q \leqslant k$,

$$\|u - u_h\|_{L^2} \leqslant C \frac{\gamma^2}{\alpha} h^{q+1} |u|_{H^{q+1}}.$$

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

We denote $u_h^+ \in V_h^+$ the solution of $(\mathcal{P}_h^+)$ with V_h^+ the enriched trial space.
For all $1 \leqslant q \leqslant k$,

$$\|u - u_h^+\|_{L^2} \leqslant \boxed{\frac{|u-u_\theta|_{H^{q+1}}}{|u|_{H^{q+1}}}} \left(C \frac{\gamma^2}{\alpha} h^{q+1} |u|_{H^{q+1}} \right).$$

The same type of estimates holds for the H^1 norm.

Numerical results

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

Numerical results

2D Poisson problem on Square - Dirichlet BC

2D Anisotropic Elliptic problem on a Square - Dirichlet BC

2D Poisson problem on Annulus - Mixed BC

Problem considered

Problem statement: We consider the Poisson problem in 2D with homogeneous Dirichlet boundary conditions:

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

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

We define the right-hand side f such that the solution is given by

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

with $\boldsymbol{x} = (x, y) \in \Omega$ and some parameters $\boldsymbol{\mu} = (\mu_1, \mu_2) \in \mathcal{M}$.

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

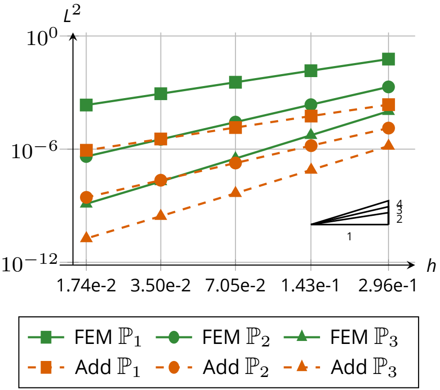
$$\varphi(\boldsymbol{x}) = (x + 0.5\pi)(x - 0.5\pi)(y + 0.5\pi)(y - 0.5\pi).$$

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

Numerical results

Error estimates : 1 given parameter.

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



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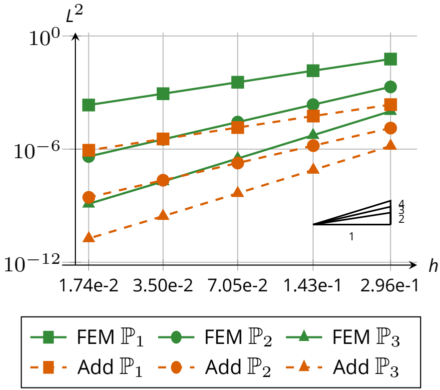


Gains achieved : $n_p = 50$ parameters.

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

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

$N = 20$

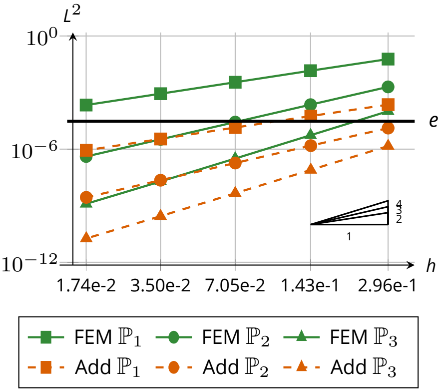
Gain : $\|u - u_h\|_{L^2} / \|u - u_h^+\|_{L^2}$

Cartesian mesh : N^2 nodes.

Numerical results

Error estimates : 1 given parameter.

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



Numerical costs of the two approaches :

N required to reach the same error *e*.

		N	
k	**e**	**FEM**	**Add**
1	$1 \cdot 10^{-3}$	119	8
	$1 \cdot 10^{-4}$	379	24
2	$1 \cdot 10^{-4}$	42	8
	$1 \cdot 10^{-5}$	89	17
3	$1 \cdot 10^{-5}$	28	10
	$1 \cdot 10^{-6}$	48	18

Numerical results

2D Poisson problem on Square - Dirichlet BC

2D Anisotropic Elliptic problem on a Square - Dirichlet BC

2D Poisson problem on Annulus - Mixed BC

Problem considered

Problem statement: We consider the Poisson problem in 2D with mixed BC:

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

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

We define the right-hand side f by

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

with $\boldsymbol{x} = (x, y) \in \Omega$ and some parameters $\boldsymbol{\mu} = (\mu_1, \mu_2, \epsilon, \sigma) \in \mathcal{M}$.
The diffusion matrix D (symmetric and positive definite) is given by

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

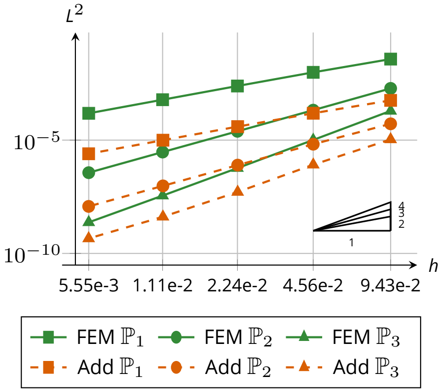
PINN training: MLP with Fourier Features[1] of 5 layers, trained with an Adam optimizer (15000 epochs). Imposing the Dirichlet BC exactly in the PINN with a levelset function.

[1] [Tancik et al., 2020]

Numerical results

Error estimates : 1 given parameter.

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



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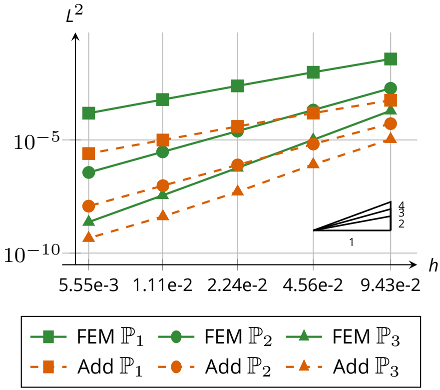


Gains achieved : $n_p = 50$ parameters.

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

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

$N = 20$

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

Cartesian mesh : N^2 nodes.

Numerical results

2D Poisson problem on Square - Dirichlet BC

2D Anisotropic Elliptic problem on a Square - Dirichlet BC

2D Poisson problem on Annulus - Mixed BC

Problem considered

Problem statement: We consider the Poisson problem in 2D 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 $\Omega = \{(x,y) \in \mathbb{R}^2,\ 0.25 \le x^2 + y^2 \le 1\}$ and $\mathcal{M} = [2.4, 2.6]$ ($p = 1$).

We define the right-hand side f such that the solution is given by

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

with $\boldsymbol{x} = (x,y) \in \Omega$ and some parameters $\boldsymbol{\mu} = \mu_1 \in \mathcal{M}$. The BC are given by

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

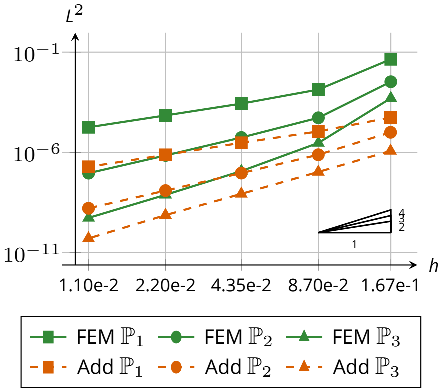
PINN training: MLP of 5 layers, trained with an LBFGs optimizer (4000 epochs). Imposing the mixed BC exactly in the PINN[1].

[1] [Sukumar and Srivastava, 2022]

Numerical results

Error estimates : 1 given parameter.

$$\boldsymbol{\mu}^{(1)} = \mu_1 = 2.51$$



Numerical results

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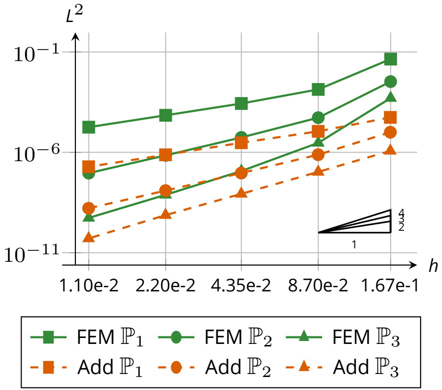

Gains achieved : $n_p = 50$ parameters.

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

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

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

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

LECOURTIER Frédérique

Conclusion

Conclusion and Perspectives

- PINNs are good candidates for the enriched approach.
- Numerical validation of the theoretical results.
- The enriched approach provides the same results as the standard FEM method, but with coarser meshes. $\Rightarrow$ Reduction of the computational cost.

Perspectives :

- Validate the additive approach on more complex geometry.
- Consider non-linear problems.
- Use the PINN prediction to build an optiaml mesh, wia a posteriori error estimates.

Add QR code with the paper + Image of the bean testcase

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