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

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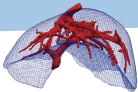
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Scientific context



- 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 linear elliptic PDE : For one or several $\mu \in \mathcal{M}$, find $u : \Omega \rightarrow \mathbb{R}$ such that

$$\mathcal{L}(u; \mathbf{x}, \mu) = f(\mathbf{x}, \mu), \tag{\mathcal{P}}$$

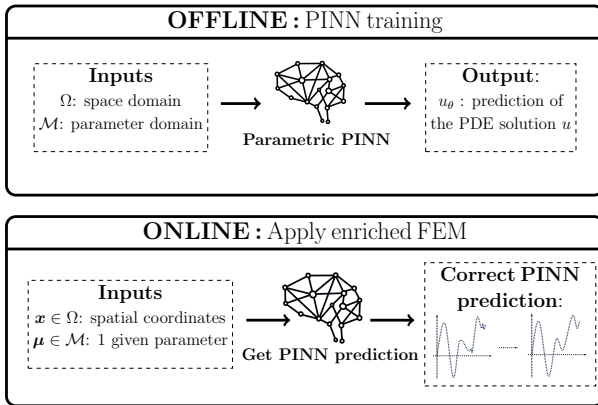
where \mathcal{L} is the parametric differential operator defined by

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

and some Dirichlet, Neumann or Robin BC (which can also depend on μ).

| | | | |
|----------------------------------|----------------------|-------------|------------------------|
| Ω | Spatial domain | f | Right-hand side |
| d | Spatial dimension | R | Reaction coefficient |
| $\mathbf{x} = (x_1, \dots, x_d)$ | Spatial coordinates | C | Convection coefficient |
| \mathcal{M} | Parameter space | D | Diffusion matrix |
| p | Number of parameters | Pe | Péclet number |
| $\mu = (\mu_1, \dots, \mu_p)$ | Parameter vector | | |

Pipeline of the Enriched FEM



Correction : Enriched continuous Lagrange finite element approximation spaces using the PINN prediction.

Physics-Informed Neural Networks

Standard PINNs¹ (Weak BC) : Find the optimal weights θ^* that satisfy

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

with the residual loss function and the boundary loss function defined by

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

$$J_b(\theta) = \int_{\mathcal{M}} \int_{\partial\Omega} |u_\theta(\mathbf{x}, \mu) - g(\mathbf{x}, \mu)|^2 d\mathbf{x} d\mu,$$

where u_θ is a neural network, $g = 0$ is the Dirichlet BC. In (\mathcal{P}_θ) , the weights ω_r and ω_b (hyperparameters) are used to balance the different terms of the loss function.

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

¹[Raissi et al., 2019]

Physics-Informed Neural Networks

Improved PINNs¹ (Strong BC) : Find the optimal weights θ^* that satisfy

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

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

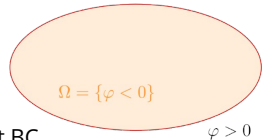
$$J_r(\theta) = \int_{\mathcal{M}} \int_{\Omega} |\mathcal{L}(u_{\theta}(\mathbf{x}, \mu); \mathbf{x}, \mu) - f(\mathbf{x}, \mu)|^2 d\mathbf{x} d\mu, \quad \partial\Omega = \{\varphi = 0\}$$

where u_{θ} is a neural network defined by

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

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 $\partial\Omega$.



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

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

Finite Element Method¹

Variational Problem :

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

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 the finite element space of dimension N_h defined by

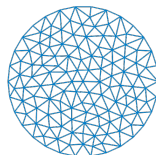
$$V_h = \{v_h \in C^0(\Omega), \forall K \in \mathcal{T}_h, v_h|_K \in \mathbb{P}_k, v_h|_{\partial\Omega} = 0\},$$

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

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

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

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



$$\mathcal{T}_h = \{K_1, \dots, K_{N_e}\}$$

(N_e : number of elements)

¹[Ern and Guermond, 2004]

How improve PINN prediction with FEM ?

Additive approach

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

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

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

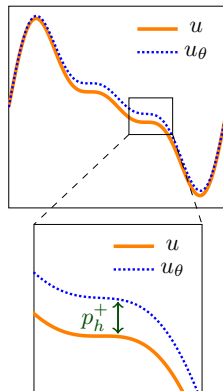
$$V_h^+ = \{u_h^+ = u_\theta + p_h^+, \quad p_h^+ \in V_h^0\}.$$

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 $1 \leq q \leq k$,

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

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 $1 \leq q \leq k$,

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

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

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

with $\mathbf{x} = (x, y) \in \Omega$ 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

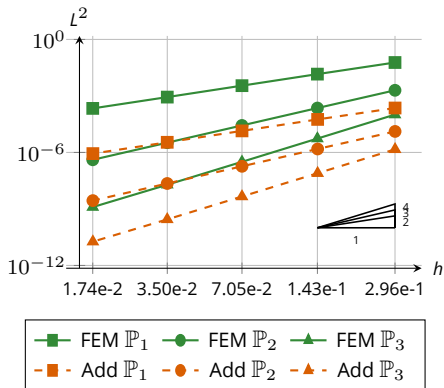
$$\varphi(\mathbf{x}) = (x + 0.5\pi)(x - 0.5\pi)(y + 0.5\pi)(y - 0.5\pi).$$

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

Numerical results

Error estimates : 1 given parameter.

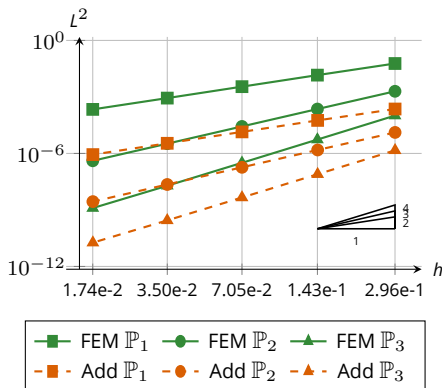
$$\mu^{(1)} = (0.05, 0.22)$$



Numerical results

Error estimates : 1 given parameter.

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



Gains achieved : $n_p = 50$ 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 |

$N = 20$

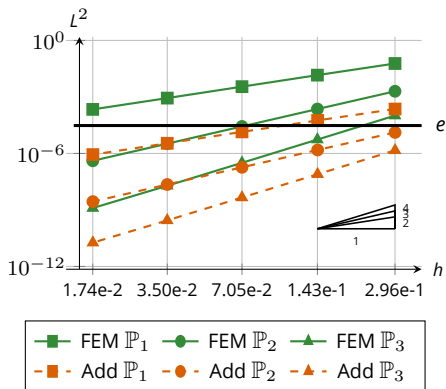
$$\text{Gain} : \|u - u_h\|_{L^2} / \|u - u_h^+\|_{L^2}$$

Cartesian mesh : N^2 nodes.

Numerical results

Error estimates : 1 given parameter.

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



Numerical costs of the two approaches :

N required to reach the same error e .

| k | e | N | |
|---|-------------------|-----|-----|
| | | 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:

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

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

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

with $\mathbf{x} = (x, y) \in \Omega$ 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

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

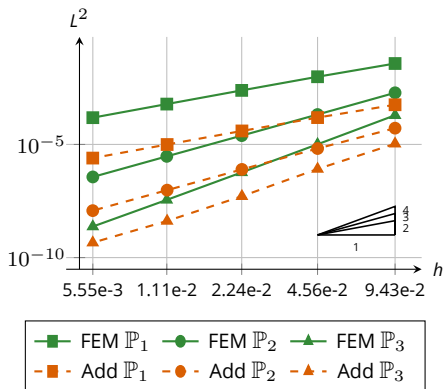
PINN training: MLP with Fourier Features¹ of 5 layers, trained with an Adam optimizer (15000 epochs). Imposing the Dirichlet BC exactly in the PINN with a levelset function.

¹[Tancik et al., 2020]

Numerical results

Error estimates : 1 given parameter.

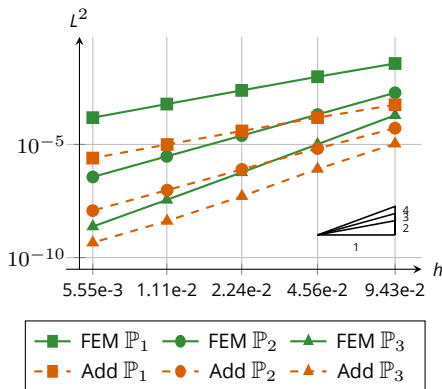
$$\mu^{(1)} = (0.51, 0.54, 0.52, 0.55)$$



Numerical results

Error estimates : 1 given parameter.

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



Gains achieved : $n_p = 50$ 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 | 7.12 | 82.57 | 35.67 |
| 2 | 3.54 | 35.88 | 18.32 |
| 3 | 1.33 | 26.51 | 8.32 |

$N = 20$

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

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:

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

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

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

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

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

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

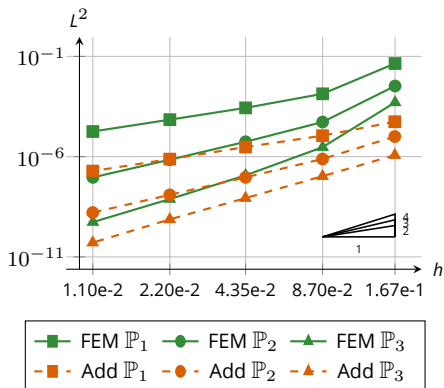
PINN training: MLP of 5 layers, trained with an LBFGs optimizer (4000 epochs).
Imposing the mixed BC exactly in the PINN¹.

¹[Sukumar and Srivastava, 2022]

Numerical results

Error estimates : 1 given parameter.

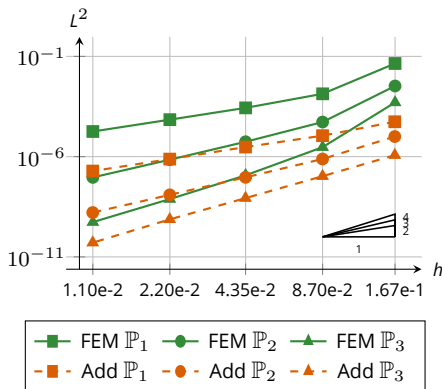
$$\mu^{(1)} = \mu_1 = 2.51$$



Numerical results

Error estimates : 1 given parameter.

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



Gains achieved : $n_p = 50$ 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 | 15.12 | 137.72 | 55.5 |
| 2 | 31 | 77.46 | 58.41 |
| 3 | 18.72 | 21.49 | 20.6 |

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

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

Conclusion

Conclusion

TODO

References

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Appendix

Appendix 1 : Standard FEM

Appendix 1 : General Idea

TODO