1st CSI

Development of hybrid finite element/neural network methods to help create digital surgical twins

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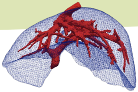
Introduction

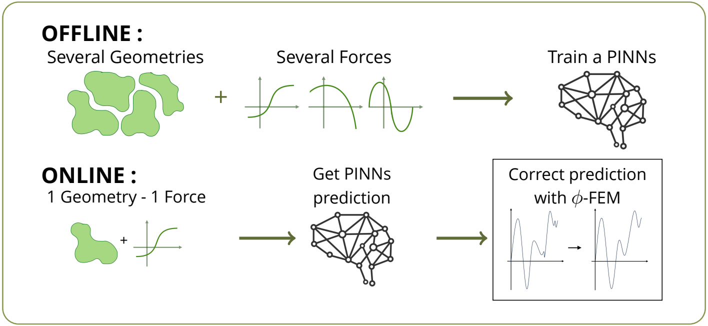
Scientific context



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

Current Objective : Develop hybrid finite element / neural network methods.

accurate quick + parameterized



ϕ-FEM : New fictitious domain finite element method. Appendix 2

$\Rightarrow$ domain given by a level-set function [Duprez and Lozinski, 2020]

Outline

Two lines of research :

1. How to deal with complex geometry in PINNs ?
2. Once we have the prediction, how can we improve it (using FEM-type methods) ?

Poisson problem with Dirichlet conditions :

Find $u : \Omega \to \mathbb{R}^d (d = 1, 2, 3)$ such that

$$\begin{cases} -\Delta u(x) = f(x) \quad \text{in } \Omega, \\ u(x) = g(x) \quad \text{on } \Gamma \end{cases} \qquad (\mathcal{P})$$

with Δ the Laplace operator, Ω a smooth bounded open set and Γ its boundary.

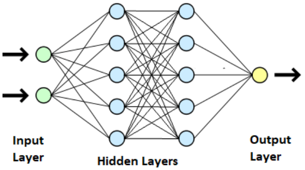
How to deal with complex geometry in PINNs ?

Standard PINNs

Implicit neural representation.

$$u_\theta(x) = u_{NN}(x)$$

with u_{NN} a neural network (e.g. a MLP).



DoFs Minimization Problem : [Raissi et al., 2019]
Considering the least-square form of ($\mathcal{P}$), our discrete problem is

$$\bar{\theta} = \underset{\theta \in \mathbb{R}^m}{\operatorname{argmin}} \, \alpha J_{in}(\theta) + \beta J_{bc}(\theta)$$

with m the number of parameters of the NN and

$$J_{in}(\theta) = \frac{1}{2} \int_\Omega (\Delta u_\theta + f)^2 \quad \text{and} \quad J_{bc}(\theta) = \frac{1}{2} \int_{\partial\Omega} (u_\theta - g)^2$$

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

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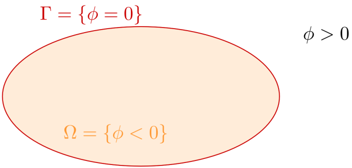
Limits

Claim on PINNs : No mesh, so easy to go on complex geometry !

⚠ *In practice :* Not so easy ! We need to find how to sample in the geometry.

Solution : Approach by levelset. [Sukumar and Srivastava, 2022]



Advantages :

➞ Sample is easy in this case.

➞ Allow to impose in hard the BC :

$$u_\theta(X) = \phi(X) w_\theta(X) + g(X)$$

(➞ Can be used for ϕ-FEM)

Natural LevelSet :

Signed Distance Function (SDF)

Problem : SDF is a $\mathcal{C}^0$ function

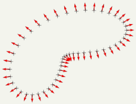
$\Rightarrow$ its derivatives explode

$\Rightarrow$ we need a regular levelset

Learn a regular levelset

If we have a boundary domain Γ, the SDF is solution to the Eikonal equation:

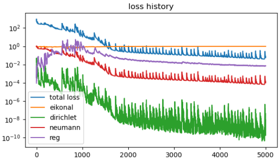
$$\begin{cases} ||\nabla\phi(X)|| = 1, \; X \in \mathcal{O} \\ \phi(X) = 0, \; X \in \Gamma \\ \nabla\phi(X) = n, \; X \in \Gamma \end{cases}$$

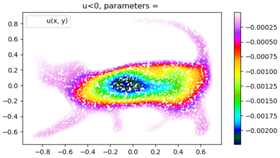


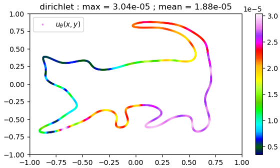
with $\mathcal{O}$ a box which contains Ω completely and n the exterior normal to Γ.

How to do that ? with a PINNs [Clémot and Digne, 2023] by adding a regularization term,

$$J_{reg} = \int_{\mathcal{O}} |\Delta\phi|^2$$







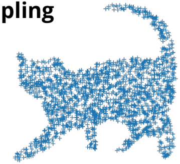
Remark : PINNs non parametric - 1 geometry

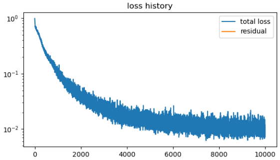
Poisson On Cat

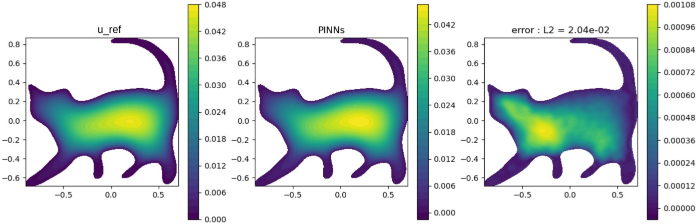
➞ Solving ($\mathcal{P}$) with $f = 1$ (non parametric) and homogeneous Dirichlet BC ($g = 0$).

➞ Looking for $u_\theta = \phi w_\theta$ with ϕ the levelset learned.

Sampling







Remark : Poisson on Bean Appendix 3

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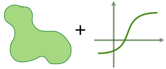
How improve PINNs prediction ?

⚠ Considering simple geometry (i.e analytic levelset ϕ).

Idea

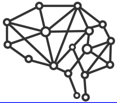
1 Geometry + 1 Force



ϕ and f

(and g)

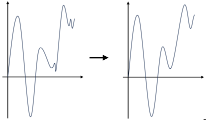
Get PINNs prediction



$$\boxed{u_{NN} = \phi w_{NN} + g}$$

$u_{NN} = g$ on Γ

Correct prediction with FEM



$u_{NN} \rightarrow \tilde{u} = u_{NN} + \tilde{C}$

Correct by adding : Considering u_{NN} as the prediction of our PINNs for ($\mathcal{P}$), the correction problem consists in writing the solution as

$$\tilde{u} = u_{NN} + \underbrace{\boxed{\tilde{C}}}_{\ll 1}$$

and searching $\tilde{C} : \Omega \rightarrow \mathbb{R}^d$ such that

$$\begin{cases} -\Delta \tilde{C} = \tilde{f}, & \text{in } \Omega, \\ \tilde{C} = 0, & \text{on } \Gamma, \end{cases} \qquad (\mathcal{P}^+)$$

with $\tilde{f} = f + \Delta u_{NN}$. Appendix 1 Appendix 5

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Poisson on Square

Solving ($\mathcal{P}$) with homogeneous Dirichlet BC ($g = 0$).

→ **Domain (fixed) :** $\Omega = [-0.5\pi, 0.5\pi]^2$

→ **Analytical levelset function :**

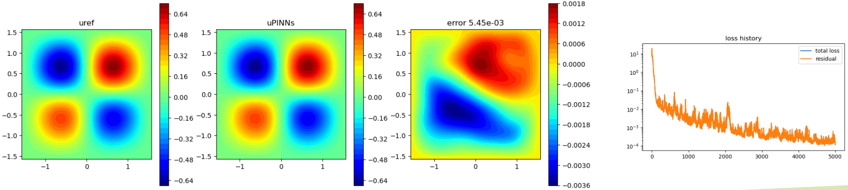
$$\phi(x, y) = (x - 0.5\pi)(x + 0.5\pi)(y - 0.5\pi)(y + 0.5\pi)$$

→ **Analytical solution :**

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

with $\mu_1, \mu_2 \in [-0.5, 0.5]$ (parametric).

Taking $\mu_1 = 0.05, \mu_2 = 0.22$, the solution is given by



Theoretical results

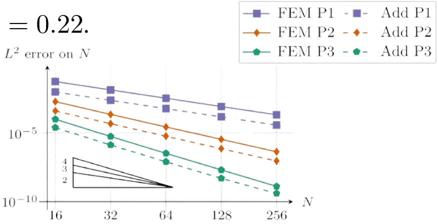
Theorem 1: [**Lecourtier** et al., in progress]

We denote u the solution of ($\mathcal{P}$) and u_h the discrete solution of the correction problem (10) with V_h a $\mathbb{P}_k$ Lagrange space. Thus

$$||u-u_h||_0 \leq \boxed{\frac{|u-u_\theta|_{H^{k+1}}}{|u|_{H^{k+1}}}} \left(\frac{\gamma}{\alpha} C h^{k+1} |u|_{H^{k+1}}\right)$$

with α and γ respectively the coercivity and continuity constant.

Taking $\mu_1 = 0.05, \mu_2 = 0.22$.



Remark : We note N the number of nodes in each direction of the square.

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Gains using our approach

Considering a set of $n_p = 50$ parameters : $\left\{(\mu_1^{(1)}, \mu_2^{(1)}), \ldots, (\mu_1^{(n_p)}, \mu_2^{(n_p)})\right\}$.

Solution $\mathbb{P}_1$

	Gains on PINNs				Gains on FEM			
N	min	max	mean	std	min	max	mean	std
20	15.7	48.35	33.64	5.57	134.31	377.36	269.4	43.67
40	61.47	195.75	135.41	23.21	131.18	362.09	262.12	41.67

Solution $\mathbb{P}_2$

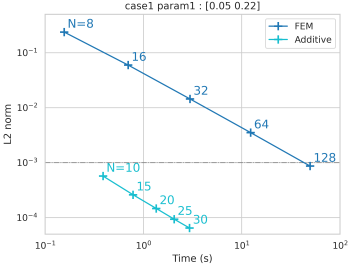
	Gains on PINNs				Gains on FEM			
N	min	max	mean	std	min	max	mean	std
20	244.81	996.23	655.08	153.63	67.12	165.13	135.21	21.37
40	2,056.2	8,345.4	5,504.89	1,287.16	66.52	159.73	132.05	20.38

Solution $\mathbb{P}_3$

	Gains on PINNs				Gains on FEM			
N	min	max	mean	std	min	max	mean	std
20	2,804.27	11,797.23	7,607.51	1,780.7	39.72	72.99	61.85	7.05
40	50,989.23	212,714.99	137,711.77	32,125.57	40.02	73	61.98	6.92

Time/Precision I

Taking $\mu_1 = 0.05, \mu_2 = 0.22.$



	N		time (s)	
Precision	FEM	Add	FEM	Add
$1e-3$	120	8	43	0.24
$1e-4$	373	25	423.89	1.93

t_{FEM} t_{Add}

Question : Where is the PINNs training time ? $t_{PINNs} \approx 240s$

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Time/Precision II

Taking a set of n_p parameters $\left\{(\mu_1^{(1)}, \mu_2^{(1)}), \dots, (\mu_1^{(n_p)}, \mu_2^{(n_p)})\right\}$.
The time of our approach (including the PINNs training) to solve n_p problems is

$$Tot_{Add} = t_{PINNs} + n_p t_{Add}$$

and the time of FEM is

$$Tot_{FEM} = n_p t_{FEM}.$$

Let's suppose we want to achieve an error of $1e-3$.
To solve n_p problems, our method is faster than FEM (when considering network training time) if

$$Tot_{Add} < Tot_{FEM} \quad \Rightarrow \quad n_p > \frac{t_{PINNs}}{t_{FEM} - t_{Add}} \approx 5.61 \quad \Rightarrow \quad \boxed{n_p = 6}$$

Remark: Considering that the times are of the same order for each parameter considered.

Conclusion

Conclusion

Current progress :

→ Levelset learning works on complex geometries
Advantage : enables "exact" imposition of BC in PINNs

→ Additive approach works on simple geometries
Advantage (compared with standard FEM) :

- More accurate solution (smaller error)
- Better execution time

Perspectives :

→ Working on parametric models for Levelset learning

→ Combine the 2 axis to improve NN predictions on complex geometries Appendix 4

→ Use ϕ-FEM (fictitious domain method) to improve NN predictions
Advantage : The levelset learned by PINNs can be used in ϕ-FEM

→ Start considering 3D cases

Supplementary work I

Teaching at the university

- 16h of Computer Science Practical Work (Python) - L2S3
- 34h of Computer Science Practical Work (C++) - L3S6

Formations (Total : $\approx 65h$)

- "Charte de déontologie des métiers de la Recherche" (OBLIGATORY)
- MOOC Bordeaux - "Intégrité scientifique dans les métiers de la recherche" (OBLIGATORY)
- "Enseigner et apprendre (public : mission enseignement)"
- "Gérer ses ressources bibliographiques avec Zotero"
- 3 Workshops on EDP at IRMA
- 19 Remote Sessions ($\approx$ 40h) - "Formation Introduction au Deep Leraning" (FIDLE)

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Supplementary work II

Talks

- Team meeting (Mimesis) - December 12, 2023 - ”Development of hybrid finite element/neural network methods to help create digital surgical twins”
- Retreat (Macaron/Tonus) - February 6, 2024
  ”Mesh-based methods and physically informed learning”
- Exama project, WP2 reunion - March 26, 2024
  ”How to work with complex geometries in PINNs ?”

Publications

- **Lecourtier**, Victorion, Barucq, Duprez, Faucher, Franck, Lleras, and Michel-Dansac. Enhanced finite element methods using neural networks. in progress.

Coming soon...

- July 8 - 12, 2024 - Poster for a Workshop on Scientific Machine Learning (SciML 2024)

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Thank you !

Bibliography

Clémot and Digne. Neural skeleton: Implicit neural representation away from the surface. *Computers and Graphics*, 2023.

Cotin, Duprez, Lleras, Lozinski, and Vuillemot. ϕ-fem: an efficient simulation tool using simple meshes for problems in structure mechanics and heat transfer. 2021.

Duprez and Lozinski. ϕ-fem: A Finite Element Method on Domains Defined by Level-Sets. *SIAM Journal on Numerical Analysis*, 2020.

Duprez, Lleras, and Lozinski. A new ϕ-fem approach for problems with natural boundary conditions, 2020.

Duprez, Lleras, and Lozinski. ϕ-fem: an optimally convergent and easily implementable immersed boundary method for particulate flows and Stokes equations. *ESAIM: Mathematical Modelling and Numerical Analysis*, 2023.

Raissi, Perdikaris, and Karniadakis. Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations. *Journal of Computational Physics*, 2019.

Sukumar and Srivastava. Exact imposition of boundary conditions with distance functions in physics-informed deep neural networks. *Computer Methods in Applied Mechanics and Engineering*, 2022.

Lecourtier, Victorion, Barucq, Duprez, Faucher, Franck, Lleras, and Michel-Dansac. Enhanced finite element methods using neural networks. in progress.

Appendix

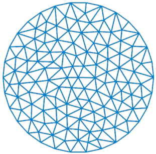
Appendix 1 : Standard FEM

Appendix 1 : General Idea

Variational Problem : Find $u \in V \mid a(u,v) = l(v), \ \forall v \in V$
with V - Hilbert space, a - bilinear form, l - linear form.

Approach Problem : Find $u_h \in V_h \mid a(u_h,v_h) = l(v_h), \ \forall v_h \in V_h$
with • $u_h \in V_h$ an approximate solution of u,
•$V_h \subset V, \ dimV_h = N_h < \infty, \ (\forall h > 0)$
$\Rightarrow$ Construct a piecewise continuous functions space

$$V_h := P_{C,h}^k = \{v_h \in C^0(\bar{\Omega}), \forall K \in \mathcal{T}_h, v_{h|K} \in \mathbb{P}_k\}$$



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

where $\mathbb{P}_k$ is the vector space of polynomials of total degree $\leq k$.

Finding an approximation of the PDE solution $\Rightarrow$ solving the following linear system:

$$AU = b$$

with

$$A = (a(\varphi_i,\varphi_j))_{1\leq i,j\leq N_h}, \quad U = (u_i)_{1\leq i\leq N_h} \quad \text{and} \quad b = (l(\varphi_j))_{1\leq j\leq N_h}$$

where $(\varphi_1, \ldots, \varphi_{N_h})$ is a basis of V_h.

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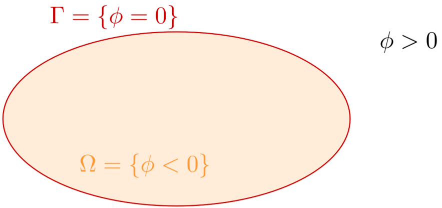
Appendix 2 : ϕ-FEM

Appendix 2 : Problem

Let $u = \phi w + g$ such that

$$\begin{cases} -\Delta u = f, & \text{in } \Omega, \\ u = g, & \text{on } \Gamma, \end{cases}$$

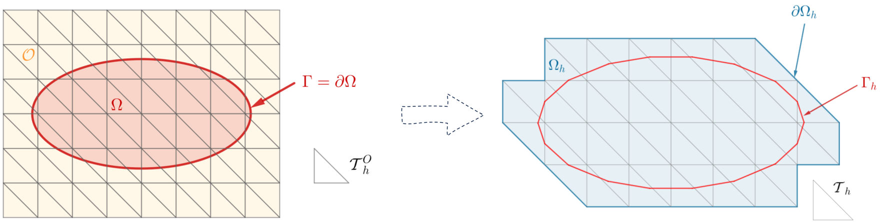
where ϕ is the level-set function and Ω and Γ are given by :



The level-set function ϕ is supposed to be known on $\mathbb{R}^d$ and sufficiently smooth. For instance, the signed distance to Γ is a good candidate.

Remark : Thanks to ϕ and g, the boundary conditions are respected.

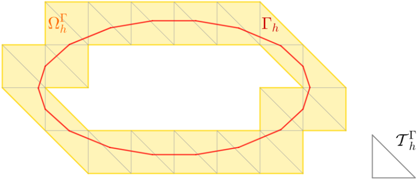
Appendix 2 : Fictitious domain

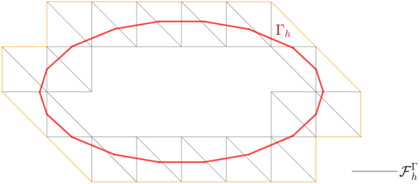


- ϕ_h : approximation of ϕ
- $\Gamma_h = \{\phi_h = 0\}$: approximate boundary of Γ
- Ω_h : computational mesh
- $\partial\Omega_h$: boundary of Ω_h ($\partial\Omega_h \neq \Gamma_h$)

Remark : n_{vert} will denote the number of vertices in each direction

Appendix 2 : Facets and Cells sets





- $\mathcal{T}_h^\Gamma$: mesh elements cut by Γ_h
- $\mathcal{F}_h^\Gamma$: collects the interior facets of $\mathcal{T}_h^\Gamma$
  (either cut by Γ_h or belonging to a cut mesh element)

Appendix 2 : Poisson problem

Approach Problem : Find $w_h \in V_h^{(k)}$ such that

$$a_h(w_h, v_h) = l_h(v_h) \quad \forall v_h \in V_h^{(k)}$$

where

$$a_h(w, v) = \int_{\Omega_h} \nabla(\phi_h w) \cdot \nabla(\phi_h v) - \int_{\partial\Omega_h} \frac{\partial}{\partial n}(\phi_h w)\phi_h v + \boxed{G_h(w, v)},$$

$$l_h(v) = \int_{\Omega_h} f\phi_h v + \boxed{G_h^{rhs}(v)}$$

Stabilization terms

and

$$V_h^{(k)} = \left\{v_h \in H^1(\Omega_h) : v_{h|_T} \in \mathbb{P}_k(T),\ \forall T \in \mathcal{T}_h\right\}.$$

For the non homogeneous case, we replace

$$u = \phi w \quad \rightarrow \quad u = \phi w + g$$

by supposing that g is currently given over the entire Ω_h.

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Appendix 2 : Stabilization terms

Independent parameter of h

Jump on the interface E

$$G_h(w,v) = \boxed{\sigma h \sum_{E\in\mathcal{F}_h^\Gamma} \int_E \left[\frac{\partial}{\partial n}(\phi_h w)\right]\left[\frac{\partial}{\partial n}(\phi_h v)\right]} + \boxed{\sigma h^2 \sum_{T\in\mathcal{T}_h^\Gamma} \int_T \Delta(\phi_h w)\Delta(\phi_h v)}$$

1st order term

$$G_h^{rhs}(v) = \boxed{-\sigma h^2 \sum_{T\in\mathcal{T}_h^\Gamma} \int_T f\Delta(\phi_h v)}$$

–

2nd order term

$$\sigma h^2 \sum_{T\in\mathcal{T}_h^\Gamma} \int_T \left(\Delta(\phi_h w) + f\right)\Delta(\phi_h v)$$

1st term : ensure continuity of the solution by penalizing gradient jumps.

$\rightarrow$ Ghost penalty [Burman, 2010]

2nd term : require the solution to verify the strong form on Ω_h^Γ.

Purpose :

- reduce the errors created by the "fictitious" boundary
- ensure the correct condition number of the finite element matrix
- restore the coercivity of the bilinear scheme

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Other results

- Poisson on Bean
- Additive approach on Cat
- Multiplicative approach

Other results

Poisson on Bean

Additive approach on Cat

Multiplicative approach

Appendix 3 : Learn a levelset

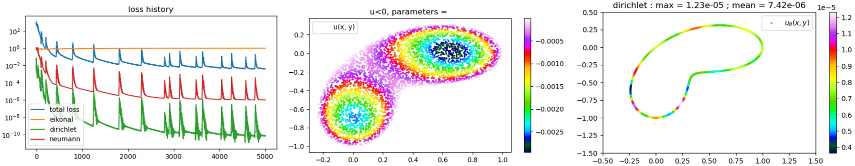
If we have a boundary domain Γ, the SDF is solution to the Eikonal equation:

$$\begin{cases} ||\nabla\phi(X)|| = 1, \ X \in \mathcal{O} \\ \phi(X) = 0, \ X \in \Gamma \\ \nabla\phi(X) = n, \ X \in \Gamma \end{cases}$$

with $\mathcal{O}$ a box which contains Ω completely and n the exterior normal to Γ.

How make that ? with a PINNs [Clémot and Digne, 2023]by adding a term to regularize.

$$J_{reg} = \int_{\mathcal{O}} |\Delta\phi|^2$$



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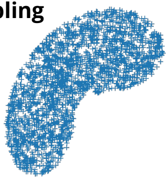
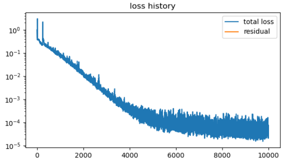
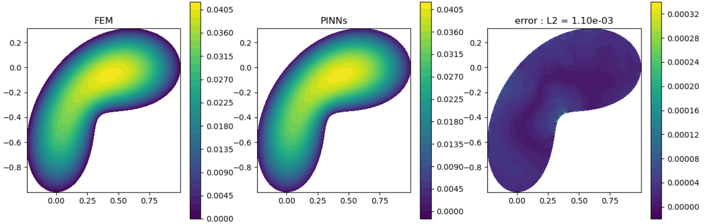
Appendix 3 : Poisson 2D

- ➞ Solving the Poisson problem with $f = 1$ and homogeneous Dirichlet BC.
- ➞ Looking for $u_\theta = \phi w_\theta$ with ϕ the levelset learned.

Sampling

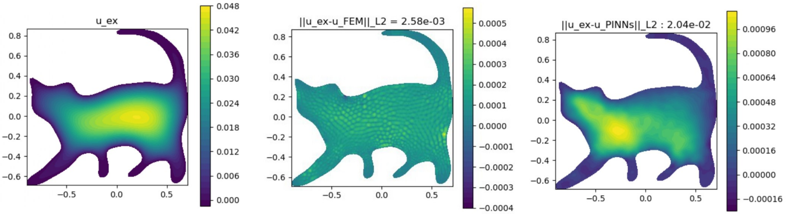






Other results

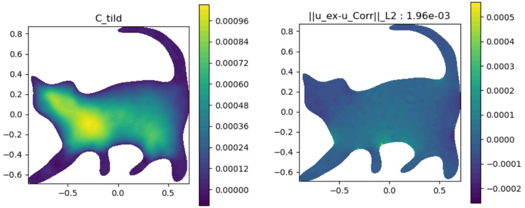
Appendix 4 : Add on Cat



FEM/PINNs = 0.13

FEM/Corr = 1.32

PINNs/Corr = 10.39



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Other results

Poisson on Bean

Additive approach on Cat

Multiplicative approach

Appendix 5 : Multiplicative approach

Correct by multiplying : Considering u_{NN} as the prediction of our PINNs for ($\mathcal{P}$), we define

$$u_M = u_{NN} + M$$

with M a constant chosen so that $u_M > 0$, called the enhancement constant. Thus, the correction problem consists in writing the solution as

$$\tilde{u} = u_M \times \underbrace{\boxed{\tilde{C}}}_{\approx 1}$$

and searching $\tilde{C} : \Omega \to \mathbb{R}^d$ such that

$$\begin{cases} -\Delta(u_M\tilde{C}) = f, & \text{in } \Omega, \\ \tilde{C} = 1, & \text{on } \Gamma. \end{cases}$$