

Macaron/Tonus retreat presentation

Mesh-based methods and physically informed learning

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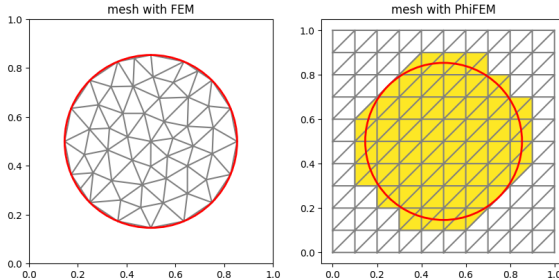
Introduction

Scientific context

Context : Create real-time digital twins of an organ (such as the liver).

ϕ -FEM Method : New fictitious domain finite element method.

- domain given by a level-set function \Rightarrow don't require a mesh fitting the boundary
- allow to work on complex geometries
- ensure geometric quality



Practical case: Real-time simulation, shape optimization...

Objective

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

OFFLINE :

Several Geometries



+

Several Functions

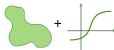


Train a PINNs



ONLINE :

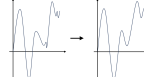
1 Geometry - 1 Function



Get PINNs prediction



Correct prediction with ϕ -FEM



Evolution :

- Geometry : 2D, simple, fixed (as circle, ellipse..) \rightarrow 3D / complex / variable
- PDE : simple, static (Poisson problem) \rightarrow complex / dynamic (elasticity, hyper-elasticity)
- Neural Network : simple and defined everywhere (PINNs) \rightarrow Neural Operator

Problem considered

Elliptic problem with Dirichlet conditions :

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

$$\begin{cases} L(u) = -\nabla \cdot (A(x)\nabla u(x)) + c(x)u(x) = f(x) & \text{in } \Omega, \\ u(x) = g(x) & \text{on } \partial\Omega \end{cases} \quad (1)$$

with A a definite positive coercivity condition and c a scalar. We consider Δ the Laplace operator, Ω a smooth bounded open set and Γ its boundary.

Remark : For simplicity, we will not consider 1st order terms.

Weak formulation :

Find $u \in V$ such that $a(u, v) = l(v) \forall v \in V$

with

$$a(u, v) = \int_{\Omega} (A(x)\nabla u(x)) \cdot \nabla v(x) + c(x)u(x)v(x) dx$$
$$l(v) = \int_{\Omega} f(x)v(x) dx$$

Numerical methods

Objective : Show that the philosophy behind most of the methods are the same.

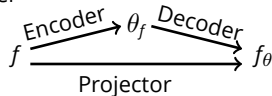
Mesh-based methods // Physically informed learning

Numerical methods : Discrete an infinite-dimensional problem (unknown = function) and solve it in a finite-dimensional space (unknown = vector).

- **Encoding :** we encode the problem in a finite-dimensional space
- **Approximation :** solve the problem in finite-dimensional space
- **Decoding :** bring the solution back into infinite dimensional space

Encoding	Approximation	Decoding
$f \rightarrow \theta_f$	$\theta_f \rightarrow \theta_u$	$\theta_u \rightarrow u_\theta$

Projector : Encoder + Decoder



Mesh-based methods

Encoding/Decoding
Approximation

Mesh-based methods

Encoding/Decoding

Approximation

Encoding/Decoding - FEMs

- **Decoding**: Linear combination of piecewise polynomial function φ_i .

$$u_\theta(x) = \mathcal{D}_{\theta_u}(x) = \sum_{i=1}^N (\theta_u)_i \varphi_i$$

⇒ linear decoding ⇒ approximation space $V_N = \text{vectorial space}$
⇒ existence and uniqueness of the orthogonal projector

- **Encoding**: Optimization process.

$$\theta_f = E(f) = \arg \min_{\theta \in \mathbb{R}^N} \int_{\Omega} \|f_\theta(x) - f(x)\|^2 dx$$

⇔ Orthogonal projection on vector space $V_N = \text{Vect}\{\varphi_1, \dots, \varphi_N\}$.

$$\theta_f = E(f) = M^{-1}b(f)$$

with $M_{ij} = \int_{\Omega} \varphi_i(x) \varphi_j(x)$ and $b_i(f) = \int_{\Omega} \varphi_i(x) f(x)$. Appendix 1

Mesh-based methods

Encoding/Decoding

Approximation

Approximation

Idea : Project a certain form of the equation onto the vector space V_N .
We introduce the residual of the equation defined by

$$R(v) = R_{in}(v)\mathbb{1}_{\Omega} + R_{bc}(v)\mathbb{1}_{\partial\Omega}$$

with

$$R_{in}(v) = L(v) - f \quad \text{and} \quad R_{bc}(v) = v - g$$

which respectively define the residues inside Ω and on the boundary $\partial\Omega$.

Discretization : Degrees of freedom problem (which also has a unique solution)

$$u = \arg \min_{v \in V_N} J(v) \quad \longrightarrow \quad \theta_u = \arg \min_{\theta \in \mathbb{R}^N} J(\theta)$$

with J a functional to minimize.

Variants : Depends on the problem form used for projection.

Spatial PDE	Any type of PDE
Problem - Energetic form	Problem - Least-square form
Galerkin projection	Galerkin Least-square projection

Energetic form

Minimization Problem :

$$u_\theta(x) = \arg \min_{v \in V_N} J(v), \quad J(v) = J_{in}(v) + J_{bc}(v) \quad (2)$$

with

$$J_{in}(v) = \frac{1}{2} \int_{\Omega} L(v)v - \int_{\Omega} f v \quad \text{and} \quad J_{bc}(v) = \frac{1}{2} \int_{\partial\Omega} R_{bc}(v)^2$$

Remark : This form of the problem is due to the Lax-Milgram theorem as a is symmetrical.

Minimization Problem (2) \Leftrightarrow PDE (1) :

$$\nabla_v J(v) = R(v)$$

Appendix 2

$$\begin{array}{ccc} u_\theta \text{ sol} & \Leftrightarrow \nabla_{u_\theta} J(u_\theta) = 0 \Leftrightarrow \begin{cases} R_{in}(u_\theta) = 0 \text{ in } \Omega \\ u_\theta = g \text{ on } \partial\Omega \end{cases} \Leftrightarrow & u_\theta \text{ sol} \\ \text{of (2)} & & \text{of (1)} \end{array}$$

Min pb

PDE

Galerkin Projection

Discrete minimization Problem :

$$\theta_u = \arg \min_{\theta \in \mathbb{R}^N} J(\theta), \quad J(\theta) = J_{in}(\theta) = \frac{1}{2} \int_{\Omega} L(v_{\theta}) v_{\theta} - \int_{\Omega} f v_{\theta} \quad (3)$$

Remark : In practice, boundary conditions can be imposed in different ways. We are therefore only interested in the minimization problem in Ω .

Galerkin projection : Consists in resolving

$$\langle R_{in}(u_{\theta}(x)), \varphi_i \rangle_{L^2} = 0, \quad \forall i \in \{1, \dots, N\} \quad (4)$$

Galerkin Projection (4) \Leftrightarrow PDE (1) :

$$\nabla_{\theta} J(\theta) = \left(\int_{\Omega} R_{in}(v_{\theta}) \varphi_i \right)_{i=1, \dots, N}$$

Appendix 3

u_{θ} sol of (1)	\Leftrightarrow	u_{θ} sol of (2)	\Leftrightarrow	u_{θ} sol of (3)	\Leftrightarrow	$\nabla_{\theta} J(\theta) = 0$	\Leftrightarrow	u_{θ} sol of (4)
PDE		Min pb		Discrete min pb				Galerkin projection

Least-Square form

Minimization Problem :

$$u_\theta(x) = \arg \min_{v \in V_N} J(v), \quad J(v) = J_{in}(v) + J_{bc}(v) \quad (5)$$

with

$$J_{in}(v) = \frac{1}{2} \int_{\Omega} R_{in}(v)^2 \quad \text{and} \quad J_{bc}(v) = \frac{1}{2} \int_{\partial\Omega} R_{bc}(v)^2$$

Remark : This form of the problem is due to the Lax-Milgram theorem as a is symmetrical.

Minimization Problem (5) \Leftrightarrow PDE (1) :

$$\nabla_v J(v) = L(R(v)) \mathbb{1}_{\Omega} + (v - g) \mathbb{1}_{\partial\Omega}$$

Appendix 4

$$\begin{array}{l} u_\theta \text{ sol} \\ \text{of (5)} \end{array} \Leftrightarrow \nabla_{u_\theta} J(u_\theta) = 0 \Leftrightarrow \begin{cases} L(R(u_\theta)) = 0 \text{ in } \Omega \\ R(u_\theta) = 0 \text{ on } \partial\Omega \end{cases} \Leftrightarrow R(u_\theta) = 0 \Leftrightarrow \begin{array}{l} u_\theta \text{ sol} \\ \text{of (1)} \end{array}$$

Min pb

PDE

Least-Square Galerkin Projection

Discrete minimization Problem :

$$\theta_u = \arg \min_{\theta \in \mathbb{R}^N} J(\theta), \quad J(\theta) = J_{in}(\theta) = \frac{1}{2} \int_{\Omega} (L(v_{\theta}) - f)^2 \quad (6)$$

Remark : In practice, boundary conditions can be imposed in different ways. We are therefore only interested in the minimization problem in Ω .

Galerkin projection : Consists in resolving

$$\langle R_{in}(u_{\theta}(x)), (\nabla_{\theta} R_{in}(u_{\theta}(x)))_i \rangle_{L^2} = 0, \quad \forall i \in \{1, \dots, N\} \quad (7)$$

Least-Square Galerkin Projection (7) \Leftrightarrow PDE (1) :

$$\nabla_{\theta} J(\theta) = \left(\int_{\Omega} L(R_{in}(v_{\theta})) \varphi_i \right)_{i=1, \dots, N}$$

Appendix 5

$$\begin{array}{ccccccc}
 u_{\theta} \text{ sol} & \Leftrightarrow & u_{\theta} \text{ sol} & \Leftrightarrow & u_{\theta} \text{ sol} & \Leftrightarrow & \nabla_{\theta} J(\theta) = 0 \Leftrightarrow u_{\theta} \text{ sol} \\
 \text{of (1)} & & \text{of (5)} & & \text{of (6)} & & \text{of (7)} \\
 \text{PDE} & & \text{Min pb} & & \text{Discrete} & & \text{LS Galerkin} \\
 & & & & \text{min pb} & & \text{projection}
 \end{array}$$

Steps Decomposition - FEMs

Encoding	Approximation		Decoding
$f \rightarrow \theta_f$	$\theta_f \rightarrow \theta_u$		$\theta_u \rightarrow u_\theta$
$\theta_f = \mathcal{E}(f)$ $= M^{-1}b(f)$	Galerkin	LS Galerkin	$u_\theta(x) = \mathcal{D}_\theta(x)$ $= \sum_{i=1}^N (\theta_u)_i \varphi_i$
	$\langle R(u_\theta), \varphi_i \rangle_{L^2} = 0$	$\langle R(u_\theta), (\nabla_\theta R(u_\theta))_i \rangle_{L^2} = 0$	
	$A\theta_u = B$		

Example : Galerkin projection.

For $i \in \{1, \dots, N\}$,

$$\langle R(u_\theta), \varphi_i \rangle_{L^2} = 0$$

$$\iff \int_{\Omega} L(u_\theta) \varphi_i = \int_{\Omega} f \varphi_i$$

$$\iff \sum_{j=1}^N (\theta_u)_j \int_{\Omega} \varphi_i L(\varphi_j) = \int_{\Omega} f \varphi_i$$

$$A\theta_u = B \text{ with}$$

$$A_{i,j} = \int_{\Omega} \varphi_i L(\varphi_j) \quad , \quad B_i = \int_{\Omega} f \varphi_i$$

Physically Informed Learning

Encoding/Decoding
Approximation

Physically Informed Learning

Encoding/Decoding

Approximation

Encoding/Decoding - NNs

- **Decoding**: Implicit neural representation.

$$u_{\theta}(x) = \mathcal{D}_{\theta_u}(x) = u_{NN}(x)$$

with u_{NN} a neural network (for example a MLP).

⇒ non-linear decoding ⇒ approximation space V_N = finite-dimensional variety

⇒ there is no unique projector

- **Encoding**: Optimization process.

$$\theta_f = E(f) = \arg \min_{\theta \in \mathbb{R}^N} \int_{\Omega} \|f_{\theta}(x) - f(x)\|^2 dx$$

Non-Linear Decoder

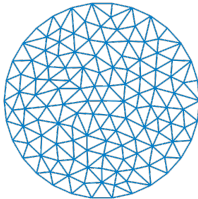
Advantages :

- We gain in the richness of the approximation
- We can hope to significantly reduce the number of degrees of freedom
- This avoids the need to use meshes.

polynomial models

⇒ local precision

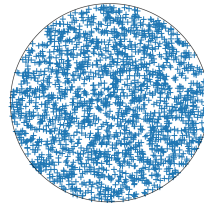
⇒ use meshes



NN models

⇒ global precision

⇒ no need to use meshes



Physically Informed Learning

Encoding/Decoding
Approximation

Approximation

Idea : Project a certain form of the equation onto the variety \mathcal{M}_N .

Discretization : Degrees of freedom problem (no mesh).

$$u = \arg \min_{v \in \mathcal{M}_N} J(v) \longrightarrow \theta_u = \arg \min_{\theta \in \mathbb{R}^N} J(\theta)$$

with J a functional to minimize.

Variants : Depends on the problem form used for projection.

Spatial PDE

Problem - Energetic form
Deep-Ritz
(Galerkin projection)

Any type of PDE

Problem - Least-square form
Standard PINNs
(Galerkin Least-square projection)

Deep-Ritz

Discrete minimization Problem : Considering the energetic form of our PDE, our discrete problem is

$$\theta_u = \arg \min_{\theta \in \mathbb{R}^N} J_{in}(\theta) + J_{bc}(\theta) \quad (8)$$

with

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

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

- (x_1, \dots, x_n) randomly drawn according to $\mu(x)$ defined on Ω

$$J_{in}(\theta) = \frac{1}{2n} \sum_{i=1}^n L(v_{\theta}(x_i)) v_{\theta}(x_i) - \frac{1}{n} \sum_{i=1}^n f(x_i) v_{\theta}(x_i)$$

- (y_1, \dots, y_{n_b}) randomly drawn according to $\mu_b(x)$ defined on $\partial\Omega$

$$J_{bc}(\theta) = \frac{1}{2n_b} \sum_{i=1}^{n_b} (v_{\theta}(y_i) - g(y_i))^2$$

Standard PINNs

Discrete minimization Problem : Considering the least-square form of our PDE, our discrete problem is

$$\theta_u = \arg \min_{\theta \in \mathbb{R}^N} J_{in}(\theta) + J_{bc}(\theta) \quad (9)$$

with

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

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

- (x_1, \dots, x_n) randomly drawn according to $\mu(x)$ defined on Ω

$$J_{in}(\theta) = \frac{1}{2n} \sum_{i=1}^n (L(v_{\theta}(x_i)) - f(x_i))^2$$

- (y_1, \dots, y_{n_b}) randomly drawn according to $\mu_b(x)$ defined on $\partial\Omega$

$$J_{bc}(\theta) = \frac{1}{2n_b} \sum_{i=1}^{n_b} (v_{\theta}(y_i) - g(y_i))^2$$

In practice...

- Two different random generation processes (to have enough boundary points)
- Weights in front of the cost functions still need to be determined
- Use regular model, derivable several times (and automatic differentiation)
- Activation functions regular enough to be derived 2 times (due to the Laplacian)
 - ⇒ Tangent Hyperbolic rather than ReLU
 - (or adaptive methods where we parameterize the activation functions)
- Stochastic gradient descent method (by mini-batch) - ADAM method

[Appendix 6](#)

To go further :

- Standard PINNs : possibility of adding a J_{data} cost function
 - to approximate already known solutions
- Impose boundary conditions using a LevelSet function

Steps Decomposition - NNs

Encoding	Approximation	Decoding
$f \rightarrow \theta_f$	$\theta_f \rightarrow \theta_u$	$\theta_u \rightarrow u_\theta$

Mesh-based Methods			
$\theta_f = \mathcal{E}(f)$ $= M^{-1}b(f)$	Galerkin	LS Galerkin	$u_\theta(x) = \mathcal{D}_\theta(x)$ $= \sum_{i=1}^N (\theta_u)_i \varphi_i$
	$\langle R(u_\theta), \varphi_i \rangle = 0$	$\langle R(u_\theta), (\nabla_\theta R(u_\theta))_i \rangle = 0$	
	$A\theta_u = B$		

Physically informed learning			
$\theta_f = \min_{\theta \in \mathbb{R}^N} \int_{\Omega} f_\theta - f ^2$	Deep-Ritz	Standard PINNs	$u_\theta(x) = u_{NN}(x)$
	Energetic Form	LS Form	
	$\theta_u = \arg \min_{\theta \in \mathbb{R}^N} J(\theta)$		

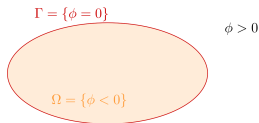
Our hybrid method

ϕ -FEM Method

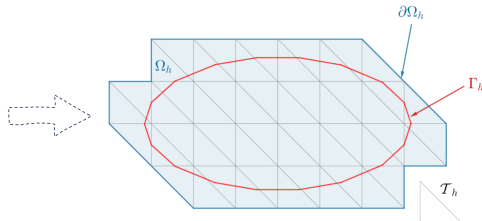
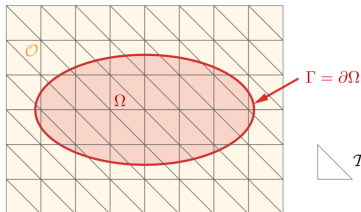
Main ideas :

Appendix 7

- Domain defined by a LevelSet Function ϕ .



- Mesh of a fictitious domain containing Ω .



- We are looking for w such that $u = \phi w + g$. Thus, the decoder is written as

$$u_\theta(x) = \mathcal{D}_{\theta_w}(x) = \phi(x) \sum_{i=1}^N (\theta_w)_i \varphi_i + g(x)$$

Impose exact BC in PINNs

Considering the least squares form of our PDE, we impose the exact boundary conditions by writing our solution as

$$u_\theta = \phi w_\theta + g$$

where w_θ is our decoder (defined by a neural network such as an MLP).

We then consider the same minimization problem by removing the cost function associated with the boundary

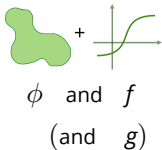
$$\theta_u = \arg \min_{\theta \in \mathbb{R}^N} J_{in}(\theta) + \cancel{J_{bc}(\theta)}$$

with

$$J_{in}(\theta) = \frac{1}{2} \int_{\Omega} (L(\phi w_\theta + g) - f)^2 \quad \text{and} \quad \cancel{J_{bc}(\theta) = \frac{1}{2} \int_{\partial\Omega} (v_\theta - g)^2}$$

Correct PINNs prediction with ϕ FEM

1 Geometry - 1 Function

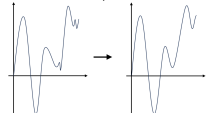


Get PINNs
prediction



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

Correct prediction
with ϕ -FEM



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

Correct by adding: Considering u_{NN} as the prediction of our PINNs (trained to learn the solution of the elliptic problem), the correction problem consists in writing the solution as

$$\tilde{u} = u_{NN} + \tilde{C} \approx 0$$

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

$$\begin{cases} L(\tilde{C}) = \tilde{f}, & \text{in } \Omega, \\ \tilde{C} = 0, & \text{on } \Gamma, \end{cases}$$

with $\tilde{f} = f - L(u_{NN})$ and $\tilde{C} = \phi C$ for the ϕ -FEM method.

Conclusion

Conclusion - What has been seen

- "Physical Informed Learning" methods are simply an extension of classic numerical methods such as FEM, where the decoder belongs to a variety (whose properties are different from those of vector spaces).
- These approaches have real advantages in high dimensions, particularly in the context of parametric PDEs.
- Moreover, as they are mesh-free methods, they have a major advantage in the context of complex geometries.

Conclusion - Our hybrid approach

Interest of our approach:

- It combines
 - ➔ Speed of neural networks in predicting a solution
 - ➔ Precision of FEM methods to correct and certify the prediction of the neural network (which can be completely wrong, on an unknown dataset for example)
- In the context of complex geometry (or in application domains such as real-time or shape optimisation), like NNs, ϕ -FEM makes it possible to avoid mesh (re-)generation.

Current results:

- Encouraging results on simple geometries [Appendix 8](#)
- Difficulties on complex geometries - Importance of the regularity of the LevelSet function
 - ➔ Next step: learning levelset functions (Eikonal equation)

Thank you !

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Mesh-based methods

Appendix 1 : Encoding - FEMs

We want to project f onto the vector subspace V_N so that $f_\theta = p_{V_N}(f)$
 then $\forall i \in \{1, \dots, N\}$, we have

$$\begin{aligned} \langle f_\theta - f, \varphi_i \rangle &= 0 \\ \iff \langle f_\theta, \varphi_i \rangle &= \langle f, \varphi_i \rangle \\ \iff \sum_{j=1}^N (\theta_f)_j \langle \varphi_j, \varphi_i \rangle &= \langle f, \varphi_i \rangle \\ \iff M \theta_f &= b(f) \\ \iff \theta_f &= M^{-1} b(f) \end{aligned}$$

with

$$\begin{aligned} M_{ij} &= \langle \varphi_i, \varphi_j \rangle = \int_{\Omega} \varphi_i(x) \varphi_j(x) dx \\ b_i(f) &= \langle f, \varphi_i \rangle = \int_{\Omega} f(x) \varphi_i(x) dx \end{aligned}$$

Appendix 2 : Energetic form I

Let's compute the gradient of J with respect to v with

$$J(v) = J_{in}(v) + J_{bc}(v) = \left(\frac{1}{2} \int_{\Omega} L(v)v - \int_{\Omega} f v \right) + \left(\frac{1}{2} \int_{\partial\Omega} R_{bc}(v)^2 \right)$$

- First, let's calculate the differential of J_{in} with respect to v .

$$J_{in}(v + \epsilon h) = \frac{1}{2} \int_{\Omega} (A \nabla(v + \epsilon h)) \cdot \nabla(v + \epsilon h) + c(v + \epsilon h)^2 - \int_{\Omega} f(v + \epsilon h)$$

By bilinearity of the scalar product and by symmetry of A , we finally obtain

$$\mathcal{D}J_{in}(v) \cdot h = \lim_{\epsilon \rightarrow 0} \frac{J_{in}(v + \epsilon h) - J_{in}(v)}{\epsilon} = \int_{\Omega} (-\nabla \cdot (A \nabla v) + cv - f)h$$

And thus

$$\nabla_v J_{in}(v) = L(v) - f = R_{in}(v)$$

Appendix 2 : Energetic form II

- In the same way, we can compute the differential of J_{bc} with respect to v .

$$J_{bc}(v + \epsilon h) = \frac{1}{2} \int_{\partial\Omega} v^2 + 2\epsilon v h + \epsilon^2 h^2 - 2v g - 2\epsilon h g + g^2$$

Then

$$\mathcal{D}J_{bc}(v) \cdot h = \lim_{\epsilon \rightarrow 0} \frac{J_{bc}(v + \epsilon h) - J_{bc}(v)}{\epsilon} = \int_{\partial\Omega} (v - g)h$$

And thus

$$\nabla_v J_{bc}(v) = (v - g) = R_{bc}(v)$$

Finally

$$\nabla_v J(v) = \nabla_v J_i(v) + \nabla_v J_{bc}(v) = R(v)$$

Appendix 3 : Galerkin Projection

Let's compute the gradient of J with respect to θ with

$$J(\theta) = J_{in}(\theta) = \frac{1}{2} \int_{\Omega} L(u_{\theta}) v_{\theta} - \int_{\Omega} f v_{\theta}$$

First, we define

$$v_{\theta} = \sum_{i=1}^N \theta_i \varphi_i = \theta \cdot \varphi \quad \text{and} \quad v_{\theta+\epsilon h} = (\theta + \epsilon h) \cdot \varphi = v_{\theta} + \epsilon v_h$$

Then since A is symmetric

$$\mathcal{D}J(\theta) \cdot h = \int_{\Omega} R(v_{\theta}) v_h = \sum_{i=1}^N h_i \int_{\Omega} R(v_{\theta}) \varphi_i$$

Finally

$$\nabla_{\theta} J(\theta) = \left(\int_{\Omega} R(v_{\theta}) \varphi_i \right)_{i=1, \dots, N}$$

Appendix 4 : Least-Square form I

Let's compute the gradient of J with respect to v with

$$J(v) = J_{in}(v) + J_{bc}(v) = \left(\frac{1}{2} \int_{\Omega} R_{in}(v)^2 \right) + \left(\frac{1}{2} \int_{\partial\Omega} R_{bc}(v)^2 \right)$$

- First, let's calculate the differential of J_{in} with respect to v .

$$\begin{aligned} \mathcal{D}J_{in}(v) \cdot h &= \langle \nabla \cdot (A \nabla h), \nabla \cdot (A \nabla v) - cv + f \rangle + \langle ch, -\nabla \cdot (A \nabla v) + cv - f \rangle \\ &= -\langle \nabla \cdot (A \nabla h), R_{in}(v) \rangle + \langle ch, R_{in}(v) \rangle \\ &= \langle -\nabla \cdot (A \nabla R_{in}(v)) + c R_{in}(v), h \rangle \\ &= \langle L(R_{in}(v)), h \rangle \end{aligned}$$

And thus

$$\nabla_v J_{in}(v) = L(R_{in}(v))$$

Appendix 4 : Least-Square form II

- In the same way, we can compute the differential of J_{bc} with respect to v .

$$J_{bc}(v + \epsilon h) = \frac{1}{2} \int_{\partial\Omega} v^2 + 2\epsilon v h + \epsilon^2 h^2 - 2vg - 2\epsilon h g + g^2$$

Then

$$\mathcal{D}J_{bc}(v) \cdot h = \lim_{\epsilon \rightarrow 0} \frac{J_{bc}(v + \epsilon h) - J_{bc}(v)}{\epsilon} = \int_{\partial\Omega} (v - g)h$$

And thus

$$\nabla_v J_{bc}(v) = (v - g) = R_{bc}(v)$$

Finally

$$\nabla_v J(v) = L(R(v))\mathbb{1}_\Omega + (v - g)\mathbb{1}_{\partial\Omega}$$

Appendix 5 : LS Galerkin Projection

Let's compute the gradient of J with respect to θ with

$$J(\theta) = J_{in}(\theta) = \frac{1}{2} \int_{\Omega} (L(u_{\theta}) - f)^2$$

First, we define

$$v_{\theta} = \sum_{i=1}^N \theta_i \varphi_i = \theta \cdot \varphi \quad \text{and} \quad v_{\theta+\epsilon h} = (\theta + \epsilon h) \cdot \varphi = v_{\theta} + \epsilon v_h$$

Then since A is symmetric

$$\mathcal{D}J(\theta) \cdot h = \int_{\Omega} L(R(v_{\theta})) v_h = \sum_{i=1}^N h_i \int_{\Omega} L(R(v_{\theta})) \varphi_i$$

Finally

$$\nabla_{\theta} J(\theta) = \left(\int_{\Omega} L(R(v_{\theta})) \varphi_i \right)_{i=1, \dots, N}$$

Physically Informed Learning

Appendix 6 : ADAM Method

Adam = Adaptive Moment Estimation" - combine les idées du moment et de RMSProp.

$$\begin{aligned}
 1 : \quad m &\leftarrow \frac{\beta_1 m + (1 - \beta_1) \nabla f_x}{1 - \beta_1^T} \\
 2 : \quad s &\leftarrow \frac{\beta_2 s + (1 - \beta_2) \nabla^2 f_x}{1 - \beta_2^T} \\
 3 : \quad x &\leftarrow x - \ell \frac{m}{\sqrt{s + \epsilon}}
 \end{aligned}$$

with

- T the number of iteration (starting at 1)
- ϵ a smoothing paramete
- $\beta_i \in]0, 1[$ which convergence quickly to 0.

Our hybrid method

Appendix 7 : ϕ -FEM Method

Appendix 8 : Results

Our hybrid method

Appendix 7 : ϕ -FEM Method

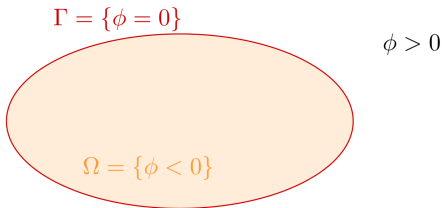
Appendix 8 : Results

Appendix 7 : Problem

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

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

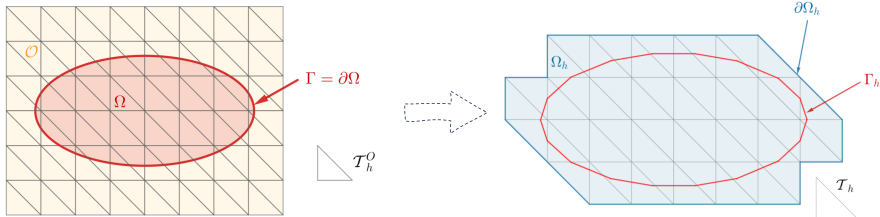
where ϕ is the level-set function and Ω and Γ are given by :



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 conditions on the boundary are respected.

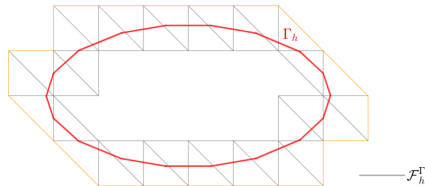
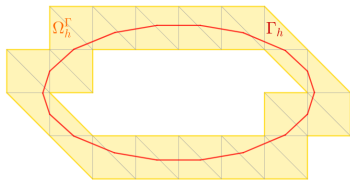
Appendix 7 : Fictitious domain



- 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 for \mathcal{O}

Appendix 7 : Facets and Cells sets



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

Appendix 7 : 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

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

$$l_h(v) = \int_{\Omega_h} f \phi_h v + \boxed{G_h^{hs}(v)} \quad \text{Stabilization terms}$$

and

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

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 .

Appendix 7 : Stabilization terms

Independent parameter of h Jump on the interface E

$$G_h(w, v) = \underbrace{\sigma h \sum_{E \in \mathcal{F}_h^\Gamma} \int_E \left[\frac{\partial}{\partial n}(\phi_h w) \right] \left[\frac{\partial}{\partial n}(\phi_h v) \right]}_{\text{1st order term}} + \underbrace{\sigma h^2 \sum_{T \in \mathcal{T}_h^\Gamma} \int_T \Delta(\phi_h w) \Delta(\phi_h v)}_{\text{2nd order term}}$$

$$G_h^{rhs}(v) = \underbrace{-\sigma h^2 \sum_{T \in \mathcal{T}_h^\Gamma} \int_T f \Delta(\phi_h v)}_{\text{2nd order term}} - \sigma h^2 \sum_{T \in \mathcal{T}_h^\Gamma} \int_T (\Delta(\phi_h w) + f) \Delta(\phi_h v)$$

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

→ 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

Our hybrid method

Appendix 7 : ϕ -FEM Method

Appendix 8 : Results

Appendix 8 : Problem considered

PDE : Poisson problem with Homogeneous Dirichlet conditions

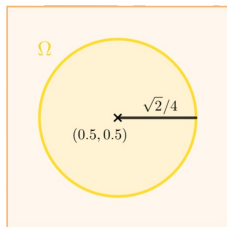
Find $u : \Omega \rightarrow \mathbb{R}^d (d = 1, 2, 3)$ such that

$$\begin{cases} -\Delta u = f, & \text{in } \Omega, \\ u = 0, & \text{on } \Gamma, \end{cases}$$

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

Geometry : Circle - center = $(0.5, 0.5)$, radius = $\sqrt{2}/4$

$$\mathcal{O} = [0, 1]^2$$



→ **Level-set function :**

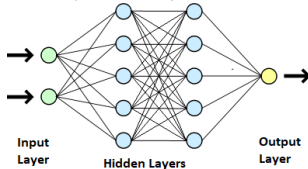
$$\phi(x, y) = -1/8 + (x - 1/2)^2 + (y - 1/2)^2$$

→ **Exact solution :**

$$u_{ex}(x, y) = \phi(x, y) \sin(x) \exp(y)$$

Appendix 8 : Networks

PINNs : Multi-Layer Perceptron (MLP, Fully connected) with a physical loss



$$loss = mse(\Delta(\phi(x_i, y_i)w_{\theta, i}) + f_i)$$

$$\begin{aligned} \text{inputs} &= \{(x_i, y_i)\} \\ \text{outputs} &= \{u_i\} \\ &\quad i = 1, \dots, n_{pts} \\ u_i &= \phi(x_i, y_i)w_{\theta, i} \end{aligned}$$

- n_layers=4
- n_neurons=20 (in each layer)
- n_epochs=10000
- n_pts=2000 (randomly drawn in the square $[0, 1]^2$)

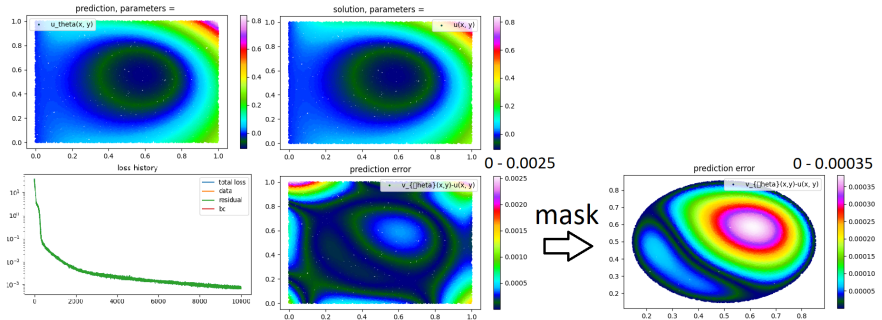
Some important points :

- Need $u_{NN} \in \mathbb{P}^k$ of high degree (PINNs Ok)
- Need the derivatives to be well learn (PINNs Ok)
- For the correction : Need a correct solution on Ω_h , not on Ω (training on the square for the moment).

with $(x_i, y_i) \in \mathcal{O}$.

Remark : We impose exact boundary conditions.

Appendix 8 : Training

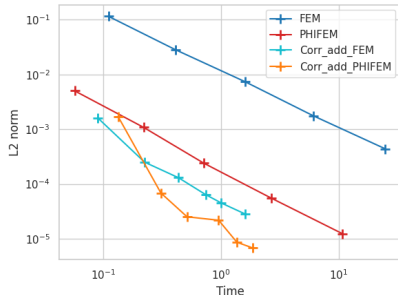


⚠ We consider a single problem (f fixed) on a single geometry (ϕ fixed).

$$||u_{ex} - u_\theta||_{L^2(\Omega)}^{(rel)} \approx 2.81e-3$$

Appendix 8 : Correction

$$u_\theta \in \mathbb{P}^{10} \rightarrow \tilde{u} \in \mathbb{P}^1$$



FEM / ϕ -FEM : $n_{vert} \in \{8, 16, 32, 64, 128\}$

Corr : $n_{vert} \in \{5, 10, 15, 20, 25, 30\}$

Remark : The stabilisation parameter σ of the ϕ -FEM method has a major impact on the error obtained.

Calculation time (to reach an error of 1e-4)

	mesh	u_PINNs	assemble	solve	TOTAL
FEM	0,08832		29,55516	0,07272	29,71621
PhiFEM	0,33222		1,86924	0,00391	2,20537
Corr_add_FEM	0,00183	0,11187	0,46195	0,00061	0,57626
Corr_add_PhiFEM	0,03213	0,05351	0,22006	0,00040	0,30609

Remark : Problem with assemble and solve time

+ mesh time for ϕ -FEM would be parallelized

- **mesh** - FEM : construct the mesh
(ϕ -FEM : construct cell/facet sets)
- **u_PINNs** - get u_θ in \mathbb{P}^{10} freedom degrees
- **assemble** - assemble the FE matrix
- **solve** - resolve the linear system