Macaron/Tonus retreat presentation

Mesh-based methods and physically informed learning

Authors:
LECOURTIER Frédérique

Supervisors:
DUPREZ Michel
FRANCK Emmanuel
LLERAS Vanessa

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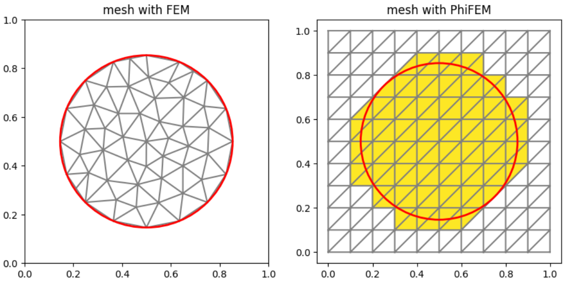
Introduction

Scientific context

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

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

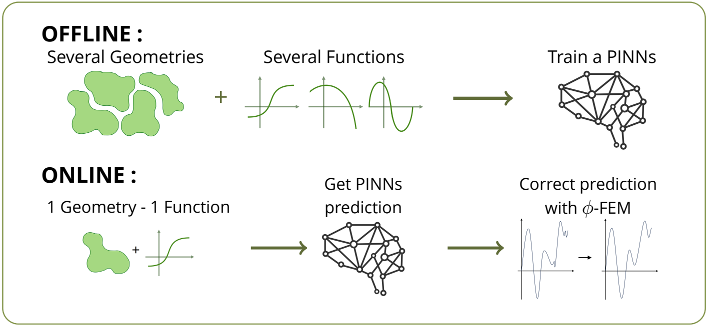
- domain given by a level-set function $\Rightarrow$ don't require a mesh fitting the boundary
- allow to work on complex geometries
- ensure geometric quality



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

Objective

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



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

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

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.
Weak formulation :

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

with

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

$$l(v) = \int_\Omega f(x)v(x)\, dx$$

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

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Numerical methods

Objective : Show that the philosophy behind most ofd 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
$f \rightarrow \theta_f$	$\theta_f \rightarrow \theta_u$	$\theta_u \rightarrow u_\theta$

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Mesh-based methods

Encoding/Decoding

Approximation

Mesh-based methods

Encoding/Decoding

Approximation

Encoding/Decoding - FEMs

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

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

$\Rightarrow$ linear decoding $\Rightarrow$ approximation space V_N = vectorial space
$\Rightarrow$ existence and uniqueness of the orthogonal projector

- **Encoding :** Orthogonal projection on vector space $V_N = Vect\{\varphi_1, \dots, \varphi_N\}$.

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

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

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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

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

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.

Problem - Energetic form	Problem - Least-square form
Galerkin projection	Galerkin Least-square projection

Energetic form

Minimization Problem :

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

with

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

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

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

Min pb **PDE**

Galerkin Projection

Discrete minimization Problem :

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

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

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

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**

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Least-Square form

Minimization Problem :

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

with

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

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

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

Min pb **PDE**

A modifier !

Least-Square Galerkin Projection

Discrete minimization Problem :

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

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

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

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

u_θ sol of (1)	$\Leftrightarrow$	u_θ sol of (5)	$\Leftrightarrow$	u_θ sol of (6)	$\Leftrightarrow$	$\nabla_\theta J(\theta) = 0$	$\Leftrightarrow$	u_θ sol of (7)
PDE		**Min pb**		**Discrete min pb**				**LS Galerkin projection**

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Steps Decomposition - FEMs

<table>
<tr><th>Encoding</th><th colspan="2">Approximation</th><th>Decoding</th></tr>
<tr><td>$f \rightarrow \theta_f$</td><td colspan="2">$\theta_f \rightarrow \theta_u$</td><td>$\theta_u \rightarrow u_\theta$</td></tr>
<tr><td rowspan="2">$\theta_f = \mathcal{E}(f) = M^{-1}b(f)$</td><td>Galerkin
$\langle R(u_\theta), \varphi_i \rangle_{L^2} = 0$</td><td>LS Galerkin
$\langle R(u_\theta), (\nabla_\theta R(u_\theta))_i \rangle_{L^2} = 0$</td><td rowspan="2">$u_\theta(x) = \mathcal{D}_\theta(x) = \sum_{i=1}^{N} (\theta_u)_i \varphi_i$</td></tr>
<tr><td colspan="2">$A\theta_u = B$</td></tr>
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Example : Galerkin projection.
For $i \in \{1, \dots, N\}$,

$$
\begin{aligned}
& \langle R(u_\theta), \varphi_i \rangle_{L^2} = 0 \\
\iff & \int_\Omega L(u_\theta)\varphi_i = \int_\Omega f\varphi_i \\
\iff & \sum_{j=1}^{N} (\theta_u)_j \int_\Omega \varphi_i L(\varphi_j) = \int_\Omega f\varphi_i
\end{aligned}
$$

$A\theta_u = B$ with

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

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Physically Informed Learning

Encoding/Decoding
Approximation

Physically Informed Learning

Encoding/Decoding

Approximation

Encoding/Decoding - NNs

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Non-Linear Decoder - Advantages

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Physically Informed Learning

Encoding/Decoding

Approximation

Approximation

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Deep-Ritz

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Standard PINNs

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In practice...

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Steps Decomposition - NNs

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 $\langle R(u_\theta), \varphi_i \rangle_{L^2} = 0$	LS Galerkin $\langle R(u_\theta), (\nabla_\theta R(u_\theta))_i \rangle_{L^2} = 0$	$u_\theta(x) = \mathcal{D}_\theta(x) = \sum_{i=1}^{N} (\theta_u)_i \varphi_i$
	$A\theta_u = B$		

A compléter !

Hybrid method

ϕ-FEM Method

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Impose exact boundary conditions in PINNs

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Correct PINNs prediction with ϕFEM

A compléter !

Conclusion

Conclusion

A compléter !

Bibliography

Bibliography

Appendix 1 : Encoding - FEMs

A compléter !

Appendix 2 : Energetic form

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Appendix 3 : Galerkin Projection

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Appendix 4 : Least-Square form

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Appendix 5 : LS Galerkin Projection

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