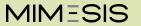
### **Macaron/Tonus retreat presentation**

# Mesh-based methods and physically informed learning

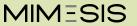
**Authors:** LECOURTIER Frédérique

Supervisors: DUPREZ Michel FRANCK Emmanuel LLERAS Vanessa

February 6-7, 2024



# Introduction

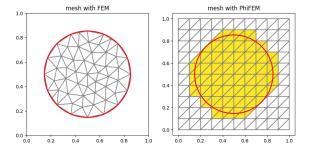


### Scientific context

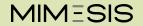
**Context**: Create real-time digital twins of an organ (such as the liver).

 $\phi$ -**FEM Method**: New fictitious domain finite element method.

- ightharpoonup 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

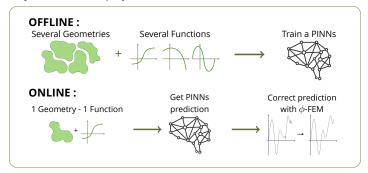


Practical case: Real-time simulation, shape optimization...



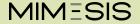
# **Objective**

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



#### **Evolution:**

- Geometry : 2D, simple, fixed (as circle, ellipse..)  $\,
  ightarrow\,$  3D / complex / variable
- PDE : simple, static (Poisson problem)  $\, o \,$  complex / dynamic (elasticity, hyper-elasticity)
- Neural Network : simple and defined everywhere (PINNs)  $\,
  ightarrow\,$  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  $\Delta$  the Laplace operator,  $\Omega$  a smooth bounded open set and  $\Gamma$  its boundary.

### Weak formulation:

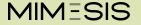
Find 
$$u \in V$$
 such that  $a(u, v) = I(v) \forall v \in V$ 

with

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

$$I(v) = \int_{\Omega} f(x)v(x) dx$$

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



### **Numerical methods**

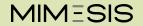
**Objective:** Show that the philosophy behind most ofd the methods are the same.

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
$f \rightarrow \theta_f$	$\theta_f \to \theta_u$	$\theta_u \rightarrow u_{\theta}$



### Mesh-based methods

Encoding/Decoding Approximation



### Mesh-based methods

Encoding/Decoding



# **Encoding/Decoding-FEMs**

• **Decoding :** Linear combination of piecewise polynomial function  $\varphi_i$ .

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

- $\Rightarrow$  linear decoding  $\Rightarrow$  approximation space  $V_N$  = vectorial space
- $\Rightarrow$  existence and uniqueness of the orthogonal projector
- **Encoding :** Orthogonal projection on vector space  $V_N = \textit{Vect}\{\varphi_1, \dots, \varphi_N\}$ .

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

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

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

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

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

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

with J a functional to minimize.

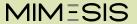
Variants: Depends on the problem form used for projection.

### **Spatial PDE**

Problem - Energetic form Galerkin projection

### Any type of PDE

Problem - Least-square form Galerkin Least-square projection



# **Energetic form**

#### **Minimization Problem:**

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

with

$$J_{in}(\mathbf{v}) = rac{1}{2} \int_{\Omega} \mathcal{L}(\mathbf{v}) \mathbf{v} - \int_{\Omega} \mathbf{f} \mathbf{v} \quad ext{ and } \quad J_{bc}(\mathbf{v}) = rac{1}{2} \int_{\Omega} \mathcal{R}_{bc}(\mathbf{v})^2$$

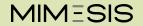
Remark: This form of the problem is due to the Lax-Milgram theorem as a is symmetrical.

Minimization Problem (2) 
$$\Leftrightarrow$$
 PDE (1): 
$$\nabla_{v} J(v) = R(v)$$
 Appendix 2

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

Min pb

PDE



# **Galerkin Projection**

#### **Discrete minimization Problem:**

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

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

Galerkin projection: Consists in resolving

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

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

$$\nabla_{\theta} J(\theta) = \left( \int_{\Omega} R_{in}(v_{\theta}) \varphi_{i} \right)_{i=1,...,N} \qquad \text{Appendix 3}$$

$$\begin{matrix} u_{\theta} \text{ sol} \\ \text{of (1)} \end{matrix} \Leftrightarrow \begin{matrix} u_{\theta} \text{ sol} \\ \text{of (2)} \end{matrix} \Leftrightarrow \begin{matrix} u_{\theta} \text{ sol} \\ \text{of (3)} \end{matrix} \Leftrightarrow \nabla_{\theta} J(\theta) = 0 \Leftrightarrow \begin{matrix} u_{\theta} \text{ sol} \\ \text{of (4)} \end{matrix}$$

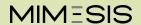
$$\begin{matrix} \text{PDE} \end{matrix}$$

$$\begin{matrix} \text{Min pb} \end{matrix}$$

$$\begin{matrix} \text{Discrete} \\ \text{min pb} \end{matrix}$$

$$\begin{matrix} \text{Discrete} \\ \text{min pb} \end{matrix}$$

$$\begin{matrix} \text{projection} \end{matrix}$$



# **Least-Square form**

#### **Minimization Problem:**

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

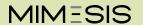
with

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

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

$$\begin{array}{ll} \text{Minimization Problem (5)} \Leftrightarrow \text{PDE (1):} \\ \nabla_{v} J(v) = L(R(v)) \mathbb{1}_{\Omega} + (v-g) \mathbb{1}_{\partial \Omega} & \text{Appendix 4} \\ \\ u_{\theta} \text{ sol} \\ \text{of (5)} & \Leftrightarrow \nabla_{u_{\theta}} J(u_{\theta}) = 0 \ \Leftrightarrow \begin{cases} L(R(u_{\theta})) = 0 \text{ in } \Omega \\ R(u_{\theta}) = 0 \text{ on } \partial \Omega \end{cases} \Leftrightarrow R(u_{\theta}) = 0 \ \Leftrightarrow \begin{cases} u_{\theta} \text{ sol of (1)} \\ R(u_{\theta}) = 0 \text{ on } \partial \Omega \end{cases} \\ \\ \text{PDE} \end{array}$$

A modifier!



# **Least-Square Galerkin Projection**

#### **Discrete minimization Problem:**

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

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

Galerkin projection: Consists in resolving

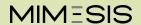
Least-Square Galerkin Projection (7)  $\Leftrightarrow$  PDE (1):

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

$$\nabla_{\theta} J(\theta) = \left(\int_{\Omega} L(R_{in}(v_{\theta})) \varphi_{i}\right)_{i=1,...,N} \qquad \text{Appendix 5}$$

$$\begin{array}{c} u_{\theta} \text{ sol} \\ \text{of (1)} \end{array} \Leftrightarrow \begin{array}{c} u_{\theta} \text{ sol} \\ \text{of (5)} \end{array} \Leftrightarrow \begin{array}{c} u_{\theta} \text{ sol} \\ \text{of (6)} \end{array} \Leftrightarrow \nabla_{\theta} J(\theta) = 0 \Leftrightarrow \begin{array}{c} u_{\theta} \text{ sol} \\ \text{of (7)} \end{array}$$

$$\text{PDE} \qquad \begin{array}{c} \text{Discrete} \\ \text{min pb} \end{array} \qquad \begin{array}{c} \text{LS Galerkin} \\ \text{projection} \end{array}$$



# **Steps Decomposition - FEMs**

Encoding	Арр	Decoding	
$f  o  heta_f$	$ heta_f   o  heta_u$		$\theta_u \rightarrow u_{ heta}$
0 (6)	Galerkin	LS Galerkin	$u_{\theta}(x) = \mathcal{D}_{\theta}(x)$
$\theta_f = \mathcal{E}(f) \\ = M^{-1}b(f)$	$\langle R(u_{\theta}), \varphi_i \rangle_{L^2} = 0$	$\langle R(u_{\theta}), (\nabla_{\theta}R(u_{\theta}))_i \rangle_{L^2} = 0$	$=\sum_{i=1}^{N}(\theta_{u})_{i}\varphi_{i}$
20)	$A\theta_u = B$		i=1

**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**

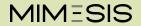
• **Decoding**: Implicit neural representation.

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

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

- $\Rightarrow$  non-linear decoding  $\Rightarrow$  approximation space  $V_N$  = finite-dimensional variety
- ⇒ there is no unique projector
- Encoding: Optimization process.

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



### **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  $\Rightarrow$  local precision

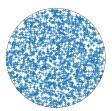
⇒ use meshes

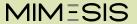


NN models

⇒ global precision

 $\Rightarrow$  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)

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

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

with

$$J_{in}( heta) = rac{1}{2} \int_{\Omega} \mathit{L}(\mathsf{v}_{ heta}) \mathsf{v}_{ heta} - \int_{\Omega} \mathit{fv}_{ heta} \quad ext{ and } \quad \mathit{J}_{bc}( heta) = rac{1}{2} \int_{\Omega} (\mathsf{v}_{ heta} - \mathsf{g})^2$$

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

•  $(\mathbf{x}_1,\ldots,\mathbf{x}_n)$  randomly drawn according to  $\mu(\mathbf{x})$  defined on  $\Omega$ 

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

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

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



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

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

with

$$J_{\mathit{in}}(\theta) = rac{1}{2} \int_{\Omega} (\mathit{L}(\mathit{v}_{ heta}) - \mathit{f})^2 \quad ext{ and } \quad J_{\mathit{bc}}(\theta) = rac{1}{2} \int_{\Omega} (\mathit{v}_{ heta} - \mathit{g})^2$$

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

•  $(x_1, \ldots, x_n)$  randomly drawn according to  $\mu(x)$  defined on  $\Omega$ 

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

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

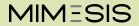
$$J_{bc}(\theta) = \frac{1}{2n_b} \sum_{i=1}^{n_b} (v_{\theta}(y_i) - g(y_i))^2$$

# 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:

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

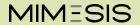


# **Steps Decomposition - NNs**

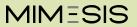
Encoding	Encoding Approximation	
$f  o  heta_f$	$ heta_f   o  heta_u$	$\theta_u \rightarrow u_{\theta}$

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

Physically informed learning					
C	Deep-Ritz	Standard PINNs			
$ heta_f = \min_{ heta \in \mathbb{R}^N} \int_{\Omega}   f_{ heta} - f  ^2$	Energetic Form	LS Form	$u_{\theta}(x) = u_{NN}(x)$		
0 (22 0 32	$ heta_u = \operatorname{argmin}_{\theta \in \mathbb{R}^N} J(\theta)$				



# Our hybrid method



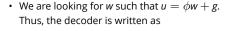
# $\phi$ -FEM Method

#### Main ideas:

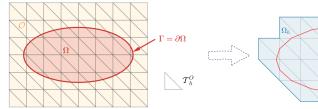
• Domain defined by a LevelSet Function  $\phi$ .

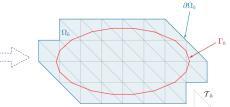


- Mesh of a fictitious domain containing  $\Omega.$ 



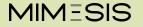
$$u_{\theta}(x) = \mathcal{D}_{\theta_{w}}(x) = \phi(x) \sum_{i=1}^{N} (\theta_{w})_{i} \varphi_{i} + g(x)$$





### **Impose exact BC in PINNs**

A compléter!



# Correct PINNs prediction with $\phi$ FEM

A compléter!

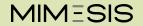


# Conclusion

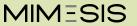


### **Conclusion**

A compléter!



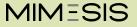
# **Bibliography**



# **Bibliography**



# 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

$$\langle f_{\theta} - f, \varphi_{i} \rangle = 0$$

$$\iff \langle f_{\theta}, \varphi_{i} \rangle = \langle f, \varphi_{i} \rangle$$

$$\iff \sum_{j=1}^{N} (\theta_{f})_{j} \langle \varphi_{j}, \varphi_{i} \rangle = \langle f, \varphi_{i} \rangle$$

$$\iff M\theta_{f} = b(f)$$

$$\iff \theta_{f} = M^{-1}b(f)$$

with

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

## Appendix 2: Energetic form I

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

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

• First, let's calculate the differential of  $I_{in}$  with respect to v.

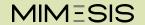
$$J_{in}(v + \epsilon h) = \frac{1}{2} \int_{\Omega} (A\nabla(v + \epsilon h)) \cdot \nabla(v + \epsilon h) + c(v + \epsilon h)^{2} - \int_{\Omega} f(v + \epsilon h)$$

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

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

And thus

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



### Appendix 2: Energetic form II

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

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

Then

$$\mathcal{D}J_{bc}(v) \cdot h = \lim_{\epsilon \to 0} \frac{J_{bc}(v + \epsilon h) - J_{bc}(v)}{\epsilon} = \int_{\Omega} v^2 - hg$$

And thus

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

$$abla_{v} J(v) = 
abla_{v} J_{i}(v) + 
abla_{v} J_{bc}(v) = R(v)$$

### **Appendix 3: Galerkin Projection**

Let's compute the gradient of I with respect to  $\theta$  with

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

First, we define

$$v_{\theta} = \sum_{i=1}^{N} \theta_{i} \varphi_{i} = \theta \cdot \varphi$$
 and  $v_{\theta + \epsilon h} = (\theta + \epsilon h) \cdot \varphi = v_{\theta} + \epsilon v_{h}$ 

Then since A is symmetric

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

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

## Appendix 4: Least-Square form I

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

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

First, let's calculate the differential of J<sub>in</sub> with respect to v.

$$\mathcal{D}J_{in}(v) \cdot h = \langle \nabla \cdot (A\nabla h), \nabla \cdot (A\nabla v) - cv + f \rangle + \langle ch, -\nabla \cdot (A\nabla v) + cv - f \rangle$$

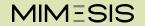
$$= -\langle \nabla \cdot (A\nabla h), R_{in}(v) \rangle + \langle ch, R_{in}(v) \rangle$$

$$= \langle -\nabla \cdot (A\nabla R_{in}(v)) + cR_{in}(v), h \rangle$$

$$= \langle L(R_{in}(v)), h \rangle$$

And thus

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



### **Appendix 4: Least-Square form II**

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

$$J_{b\epsilon}(\textit{v}+\epsilon\textit{h}) = rac{1}{2}\int_{\Omega} \textit{v}^2 + 2\epsilon\textit{v}\textit{h} + \epsilon^2\textit{h}^2 - 2\textit{v}\textit{g} - 2\epsilon\textit{h}\textit{g} + \emph{g}^2$$

Then

$$\mathcal{D}J_{bc}(v) \cdot h = \lim_{\epsilon \to 0} \frac{J_{bc}(v + \epsilon h) - J_{bc}(v)}{\epsilon} = \int_{\Omega} v^2 - hg$$

And thus

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

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

### **Appendix 5: LS Galerkin Projection**

Let's compute the gradient of I with respect to  $\theta$  with

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

First, we define

$$v_{\theta} = \sum_{i=1}^{N} \theta_{i} \varphi_{i} = \theta \cdot \varphi$$
 and  $v_{\theta + \epsilon h} = (\theta + \epsilon h) \cdot \varphi = v_{\theta} + \epsilon v_{h}$ 

Then since A is symmetric

$$\mathcal{D}J(\theta) \cdot h = \int_{\Omega} L(R(\nu_{\theta})) \nu_{h} = \sum_{i=1}^{N} h_{i} \int_{\Omega} L(R(\nu_{\theta})) \varphi_{i}$$

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

# **Physically Informed Learning**



# Appendix 6: ADAM Method

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

1: 
$$m \leftarrow \frac{\beta_1 m + (1 - \beta_1) \nabla f_x}{1 - \beta_1^T}$$

$$2: \qquad \mathbf{s} \leftarrow \frac{\beta_2 \mathbf{s} + (1 - \beta_2) \nabla^2 f_{\mathbf{x}}}{1 - \beta_2^{\mathsf{T}}}$$

$$3: \qquad x \leftarrow x - \ell \frac{m}{\sqrt{s + \epsilon}}$$

#### with

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

# Our hybrid method

Appendix 7 :  $\phi ext{-FEM Method}$ 



# Our hybrid method

Appendix 7 :  $\phi$ -FEM Method

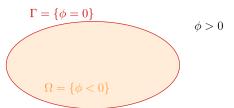


## **Appendix 7: Problem**

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

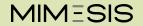
$$\begin{cases} -\Delta u = f, \text{ in } \Omega, \\ u = g, \text{ on } \Gamma, \end{cases}$$

where  $\phi$  is the level-set function and  $\Omega$  and  $\Gamma$  are given by :

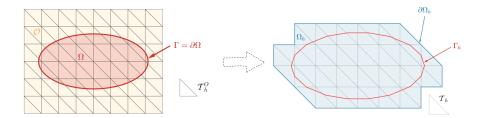


The level-set function  $\phi$  is supposed to be known on  $\mathbb{R}^d$  and sufficiently smooth. For instance, the signed distance to  $\Gamma$  is a good candidate.

*Remark*: Thanks to  $\phi$  and g, the conditions on the boundary are respected.

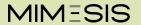


# **Appendix 7: Fictitious domain**

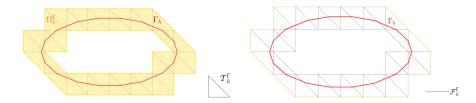


- $\rightarrow$   $\phi_h$ : approximation of  $\phi$
- ightharpoonup  $\Gamma_{\it h}=\{\phi_{\it h}=0\}$  : approximate boundary of  $\Gamma$
- $\rightarrow \Omega_h$ : computational mesh
- $\rightarrow \partial \Omega_h$ : boundary of  $\Omega_h$  ( $\partial \Omega_h \neq \Gamma_h$ )

*Remark : n\_{vert}* will denote the number of vertices in each direction for  ${\cal O}$ 



## **Appendix 7: Facets and Cells sets**



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



### Appendix 7: Poisson problem

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

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

where

$$a_h(w, v) = \int_{\Omega_h} \nabla(\phi_h w) \cdot \nabla(\phi_h v) - \int_{\partial\Omega_h} \frac{\partial}{\partial n} (\phi_h w) \phi_h v + \boxed{G_h(w, v)},$$
 $I_h(v) = \int_{\Omega} f \phi_h v + \boxed{G_h^{rhs}(v)}$  Stabilization terms

and

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

For the non homogeneous case, we replace

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

by supposing that g is currently given over the entire  $\Omega_h$ .

## **Appendix 7: Stabilization terms**

Independent parameter of h Jump on the interface E 
$$G_h(w,v) = \begin{bmatrix} \sigma h \sum_{E \in \mathcal{F}_h^{\Gamma}} \int_{\mathcal{E}} \left[ \frac{\partial}{\partial n} (\phi_h w) \right] \left[ \frac{\partial}{\partial n} (\phi_h v) \right] + \sigma h^2 \sum_{T \in \mathcal{T}_h^{\Gamma}} \int_{\mathcal{T}} \Delta(\phi_h w) \Delta(\phi_h v) \\ I^{\text{st}} \text{ order term} \\ G_h^{\text{rhs}}(v) = \begin{bmatrix} -\sigma h^2 \sum_{T \in \mathcal{T}_h^{\Gamma}} \int_{\mathcal{T}} f \Delta(\phi_h v) \\ \sigma h^2 \sum_{T \in \mathcal{T}_h^{\Gamma}} \int_{\mathcal{T}} (\Delta(\phi_h w) + f) \Delta(\phi_h v) \end{bmatrix}$$

<u>1st term</u>: ensure continuity of the solution by penalizing gradient jumps.

→ Ghost penalty [Burman, 2010]

<u>2nd term</u>: require the solution to verify the strong form on  $\Omega_h^{\Gamma}$ .

#### 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

