

## Macaron/Tonus retreat presentation

# Mesh-based methods and physically informed learning

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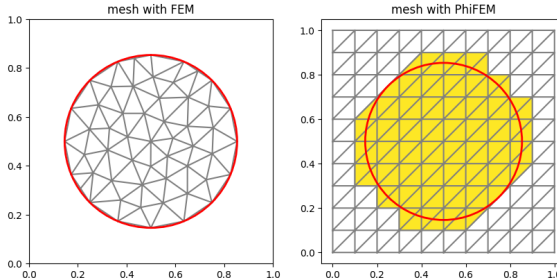
# Introduction

# Scientific context

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

**$\phi$ -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



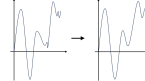
+



Get PINNs prediction



Correct prediction with  $\phi$ -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  $\Delta$  the Laplace operator,  $\Omega$  a smooth bounded open set and  $\Gamma$  its boundary.

## Weak formulation :

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

with

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

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

# 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
$f \rightarrow \theta_f$	$\theta_f \rightarrow \theta_u$	$\theta_u \rightarrow u_\theta$

# Mesh-based methods

Encoding/Decoding  
Approximation

# Mesh-based methods

Encoding/Decoding

Approximation



# 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  $V_N = \text{vectorial space}$

$\Rightarrow$  existence and uniqueness of the orthogonal projector

- **Encoding** : 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  $\Omega$  and on the boundary  $\partial\Omega$ .

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

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

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

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

*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

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

**Min pb**

**PDE**

# Galerkin Projection

## Discrete minimization Problem :

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

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

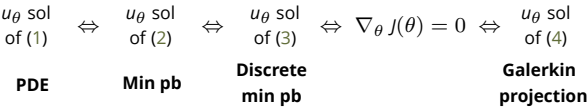
**Galerkin projection :** Consists in resolving

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

**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



# 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

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

*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 :

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

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

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

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

$$\begin{aligned} &A\theta_u = B \text{ with} \\ A_{i,j} = \int_{\Omega} \varphi_i L(\varphi_j) \quad , \quad B_i = \int_{\Omega} f \varphi_i \end{aligned}$$



# 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

$\Rightarrow$  there is no unique projector

- **Encoding**: Optimization process.

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

# Non-Linear Decoder

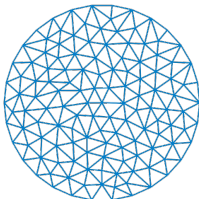
## Advantages :

- 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

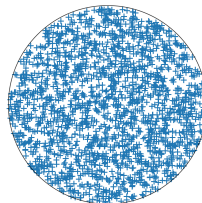
⇒ use meshes



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

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

with

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

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

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

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

- $(y_1, \dots, y_{n_b})$  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

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

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

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

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

- $(y_1, \dots, y_{n_b})$  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	
	$\theta_u = \arg \min_{\theta \in \mathbb{R}^N} J(\theta)$		

# Hybrid method

# $\phi$ -FEM Method

A compléter !

# Impose exact BC in PINNs

A compléter !

# Correct PINNs prediction with $\phi$ FEM

A compléter !

# Conclusion

# Conclusion

A compléter !



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# Bibliography

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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

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

- 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  $v$ .

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

Then

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

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  $\theta$  with

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

First, we define

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

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

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

- 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  $v$ .

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

Then

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

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  $\theta$  with

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

First, we define

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

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

A compléter !