ϕ-FEM-FNO: a new approach to train a Neural Operator as a fast PDE solver for variable geometries.

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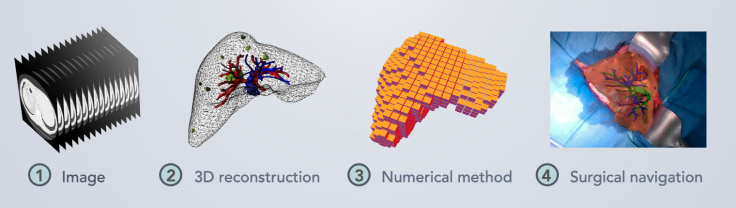
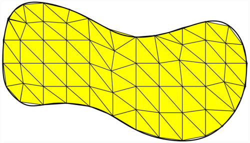
Objectives

Develop **real-time, patient specific digital twins** for computer-aided surgical interventions.

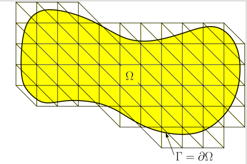


- Simulation of the deformations of organs : PDEs $\longrightarrow$ FEMs,
- Complex geometries $\longrightarrow$ Unfitted FEMs,
- Real-time constructions $\longrightarrow$ machine learning techniques.

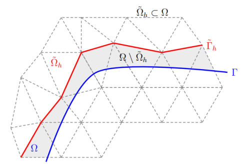
New method : ϕ-FEM, unfitted method, precise, easy to implement.



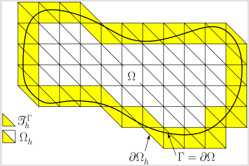
(a) Standard FEM (Clough 60s).



(b) XFEM (Moes and al., 2006)
$\longrightarrow$ Non-classical shape functions,
CutFEM (Burman, Hansbo, 2010-2014)
$\longrightarrow$ cut cells and partial integrals.



(c) Shifted Boundary method (Main, Scovazzi, 2017)
$\longrightarrow$ Taylor development near the boundary.



(d) **ϕ-FEM (Duprez and Lozinski, 2020)**
$\longrightarrow$ **Level-set function**

Problems on complex shapes $\longrightarrow$ unfitted FEMs

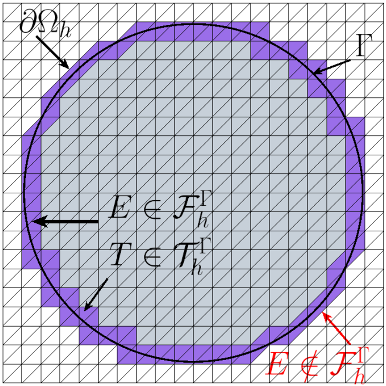
The idea of ϕ-FEM

Level-set function

$$\Omega = \{\phi < 0\} \text{ and } \Gamma = \{\phi = 0\}.$$

The spaces

- $\mathcal{T}_h$: ϕ-FEM mesh,
- $\mathcal{T}_h^\Gamma$: cells of $\mathcal{T}_h$ cut by the boundary (purple triangles),
- $\mathcal{F}_h^\Gamma$: internal facets of $\mathcal{T}_h^\Gamma$.



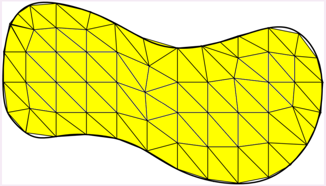
Example with $\phi(x, y) = -1 + x^2 + y^2$.

Example (Poisson-Dirichlet equation)

$$-\Delta u = f \quad \text{in } \Omega, \quad u = g \quad \text{on } \Gamma\,.$$

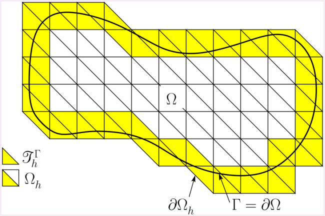
Standard FEM

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



ϕ-FEM

Find w s.t. $\begin{cases} -\Delta u &= f\,, \ \text{in } \Omega_h\,, \\ \quad u &= \phi w + g\,, \ \text{in } \Omega_h\,. \end{cases}$



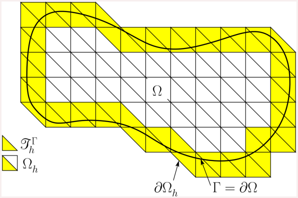
Example (Poisson-Dirichlet equation)

$$-\Delta u = f \quad \text{in } \Omega, \qquad u = g \quad \text{on } \Gamma\,.$$

ϕ-FEM scheme

Find w_h such that for all v_h,

$$\int_{\Omega_h} \nabla(\phi_h w_h + g_h) \cdot \nabla(\phi_h v_h) - \int_{\partial\Omega_h} \frac{\partial}{\partial n}(\phi_h w_h + g_h)\phi_h v_h + \text{stabs} = \int_{\Omega_h} f_h \phi_h v_h - \text{stabs}\,.$$



Who are « stabs » ?

- First order : Ghost penalty $(\mathcal{S}_1)$,
- Second order : least square imposition of the strong formulation on $\mathcal{T}_h^\Gamma$ $(\mathcal{S}_2)$.

$$\int_{\Omega_h} \nabla(\phi_h w_h + g_h) \cdot \nabla(\phi_h v_h) - \int_{\partial\Omega_h} \frac{\partial}{\partial n}(\phi_h w_h + g_h)\phi_h v_h$$

$$\underbrace{+\, \sigma h \sum_{E \,\in\, \mathcal{F}_\Gamma} \int_E \left[\frac{\partial}{\partial n}(\phi_h w_h + g_h)\right] \left[\frac{\partial}{\partial n}(\phi_h v_h)\right]}_{(\mathcal{S}_1)\text{ : Ghost penalty, jump over the facets}}$$

$$\underbrace{+\, \sigma h^2 \sum_{T \,\in\, \mathcal{T}_h^\Gamma} \int_T \Delta(\phi_h w_h + g_h)\Delta(\phi_h w_h)}_{(\mathcal{S}_2)\text{ : least square imposition of the governing equation}} = \int_{\Omega_h} f_h \phi_h v_h$$

$$\underbrace{-\sigma h^2 \sum_{T \,\in\, \mathcal{T}_h^\Gamma} \int_T f \Delta(\phi_h w_h)}_{\mathcal{S}_2\text{'s friend}} .$$

Interests of the method

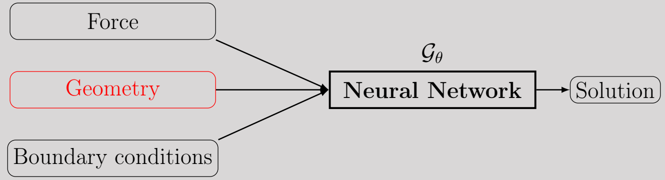
- Optimal convergence in L^2 and H^1 norms,
- Easy to implement : standard shape functions, no cut cells $\longrightarrow$ standard quadrature rules,
- Acceptable conditioning of the finite element matrix,
- No need to generate a conforming mesh.

Other schemes

- Dirichlet or Neumann boundary conditions,
- Linear elasticity problems,
- Stokes problem,
- Heat equation.

In the context of real-time simulations, we need
quasi-instantaneous results.

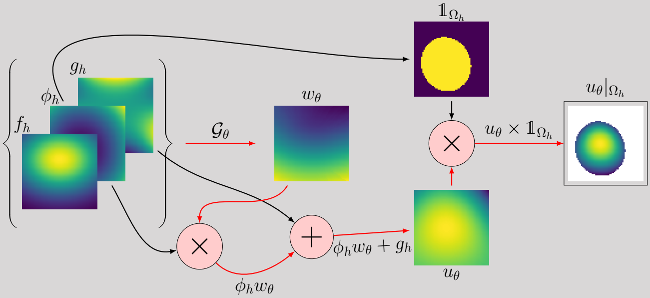
- ϕ-FEM : precise but slow $\longrightarrow$ Not real-time
- Neural Networks $\longrightarrow$ Real time
- ϕ-FEM $+$ Neural Networks $\longrightarrow$ Precise and real-time method ?



In the context of real-time simulations, we need **quasi-instantaneous results.**

- ϕ-FEM : precise but slow $\longrightarrow$ Not real-time
- Neural Networks $\longrightarrow$ Real time
- ϕ-FEM $+$ Neural Networks $\longrightarrow$ Precise and real-time method ?

The idea : construct an operator $\mathcal{G}_\theta$



How to combine ϕ-FEM and neural networks to obtain fast and precise results ?

$\longrightarrow$ the Fourier Neural Operator.

Why choose the FNO ?

- Neural operator : learns a mapping, not a solution,
- Uses FFT $\longrightarrow$ requires Cartesian grid, as ϕ-FEM does,
- According to the authors, more accurate than other ML-methods :

	NN	PCANN	DeepOnet	GNO	LNO	FNO
Darcy Flow	0.17	0.02	0.04	0.03	0.05	**0.01**
1D Burgers	0.47	0.04	0.06	0.06	0.02	**0.001**

L^2 errors of different methods **[Kovachki et al, 2023]**.

- Almost no need to change the underlying architecture when changing the governing PDE.

Parametric application :

$$\mathcal{G}_\theta : \mathbb{R}^{n_x \times n_y \times 3} \xrightarrow{N} \mathbb{R}^{n_x \times n_y \times 3} \xrightarrow{P_\theta} \mathbb{R}^{n_x \times n_y \times n_d} \xrightarrow{\mathcal{H}_\theta^1} \mathbb{R}^{n_x \times n_y \times n_d} \xrightarrow{\mathcal{H}_\theta^2}$$
$$\dots \xrightarrow{\mathcal{H}_\theta^4} \mathbb{R}^{n_x \times n_y \times n_d} \xrightarrow{Q_\theta} \mathbb{R}^{n_x \times n_y \times 1} \xrightarrow{N^{-1}} \mathbb{R}^{n_x \times n_y \times 1} .$$

- In and out dimensions : $X = (f_h, \phi_h, g_h) \to w_h$, with f_h, ϕ_h, g_h and w_h images of shape (n_x, n_y).
- N and N^{-1} : standardization and unstandardization (channel by channel),
- P_θ and Q_θ : « embedding and projection »,

$$P_\theta(X)_{ijk} = \sum_{k'=1}^{3} W_{kk'}^{P_\theta} X_{ijk'} + B_k^{P_\theta} \in \mathbb{R}^{n_d} ,$$

$\longrightarrow$ from original dimension 3 to « hidden dimension », $n_d >> 3$.

$$Q_\theta(X)_{ij} = \left[\sum_{k=1}^{n_Q} W_{1k}^{Q_\theta,2} \sigma \left(\sum_{k'=1}^{n_d} W_{kk'}^{Q_\theta,1} X_{ijk'} + B_k^{Q_\theta,1} \right) \right] + B^{Q_\theta,2} \in \mathbb{R}$$

$\longrightarrow$ from « hidden dimension » n_d to final dimension 1.

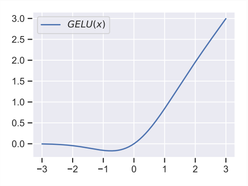
Parametric application :

$$\mathcal{G}_\theta : \mathbb{R}^{n_x \times n_y \times 3} \xrightarrow{N} \mathbb{R}^{n_x \times n_y \times 3} \xrightarrow{P_\theta} \mathbb{R}^{n_x \times n_y \times n_d} \xrightarrow{\mathcal{H}_\theta^1} \mathbb{R}^{n_x \times n_y \times n_d} \xrightarrow{\mathcal{H}_\theta^2}$$

$$\dots \xrightarrow{\mathcal{H}_\theta^4} \mathbb{R}^{n_x \times n_y \times n_d} \xrightarrow{Q_\theta} \mathbb{R}^{n_x \times n_y \times 1} \xrightarrow{N^{-1}} \mathbb{R}^{n_x \times n_y \times 1}.$$

Each layer $\mathcal{H}_\theta^\ell$ is defined by :

$$\mathcal{H}_\theta^\ell = \sigma\Big(\mathcal{C}_\theta^\ell(X) + \mathcal{B}_\theta^\ell(X) \Big)$$



$$\mathcal{C}_\theta^\ell(X) \longrightarrow \mathcal{F}^{-1}\left(W^{\mathcal{C}_\theta^\ell}\mathcal{F}(X)\right)$$

with $\mathcal{F}$ the real-FFT and $\mathcal{F}^{-1}$ its inverse.

The coefficients of $W^{\mathcal{C}_\theta^\ell}$ are complex trainable parameters.

$$\mathcal{B}_\theta^\ell(X)_{ijk} = \sum_{k'=1}^{n_d} W_{kk'}^{\mathcal{B}_\theta^\ell} X_{ijk'} + B_k^{\mathcal{B}_\theta^\ell}$$

The coefficients of $W^{\mathcal{B}_\theta^\ell}$ and $B^{\mathcal{B}_\theta^\ell}$ are real trainable parameters.

Question :

How many trainable parameters for ϕ-FEM-FNO?

$$\mathcal{C}_\theta^l \;:\; 2 \times \overbrace{n_d}^{\text{Number of in channels}} \times \underbrace{n_d}_{\text{Number of out channels}} \times \overbrace{m_x \times m_y}^{\text{Number of Fourier modes}}$$

- $\mathcal{F}(X)$: RFFT $\to$ low frequencies stored in NW and SW corners,
- High frequencies negligible $\Longrightarrow W = 0$ outside NW and SW corners,
- Size of the corners = « number of modes » $= m_x, m_y$,
- Finally, for each corner : $n_d \times n_d \times m_x \times m_y$ parameters $\longrightarrow \times 2$.

Total number :

$$\overbrace{4 \times n_d}^{P_\theta : 3 \times n_d + n_d} + 4 \times \underbrace{(\overbrace{2 \times n_d^2 \times m_x \times m_y}^{\mathcal{C}_\theta^l \text{ : by truncation of high frequencies}} + \overbrace{n_d^2 + n_d}^{\mathcal{B}_\theta^l})}_{\mathcal{H}_\theta^l} + \overbrace{(n_d + 2) \times n_Q + 1}^{Q_\theta : n_d \times n_Q + n_Q + n_Q \times 1 + 1} .$$

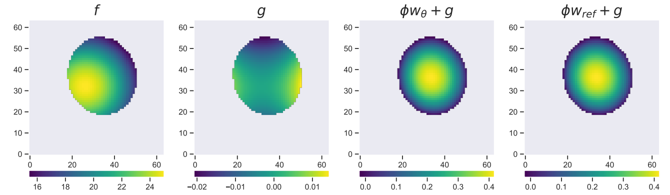
Does not depend on the resolution of the images!

First test case

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

- Ω is a random rotated ellipse defined using the signed distance ϕ,
- f is a random gaussian force centered in Ω with constant amplitude $\implies f \in [0, 25]\,,$
- $g_{(\alpha,\beta)}(x, y) = \alpha\left((x-0.5)^2 - (y-0.5)^2\right)\cos(\beta y \pi)$ $\implies g \in [-0.17, 0.15]\,,$
- $\implies u \in [-0.17, 0.87]\,.$

Dataset : 1500 training data, 300 validation data.

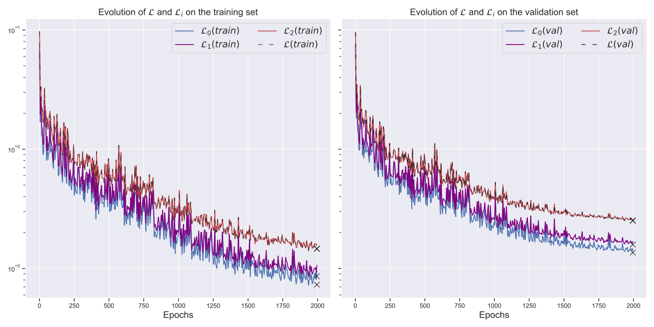


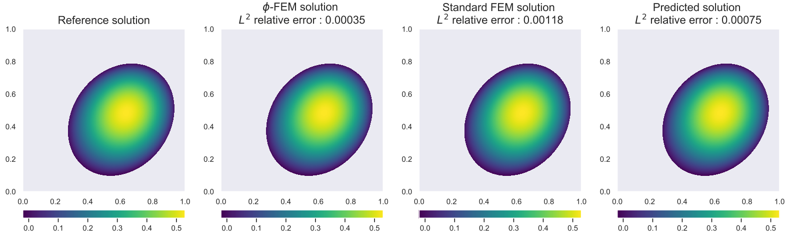
First test case

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

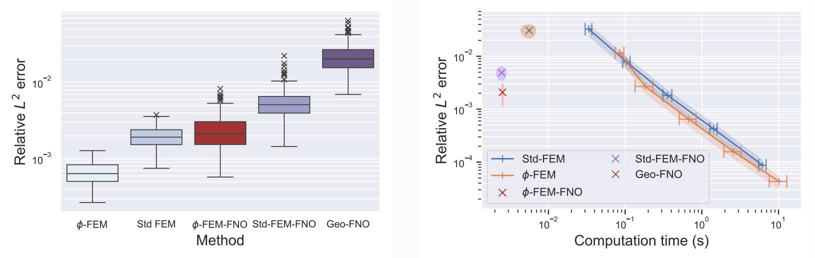
where Ω is a random rotated ellipse.

Convergence of the loss function : $\approx \|\cdot\|_{2,\Omega_h}$





Outputs of the first three methods.



Errors of the methods.

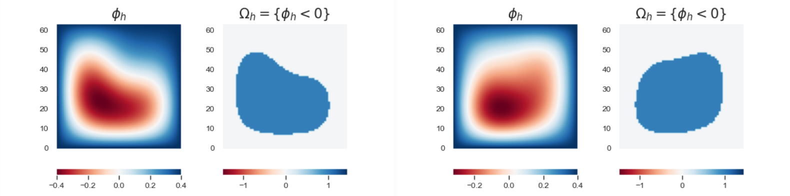
Second test case

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

where Ω is defined using Fourier series,

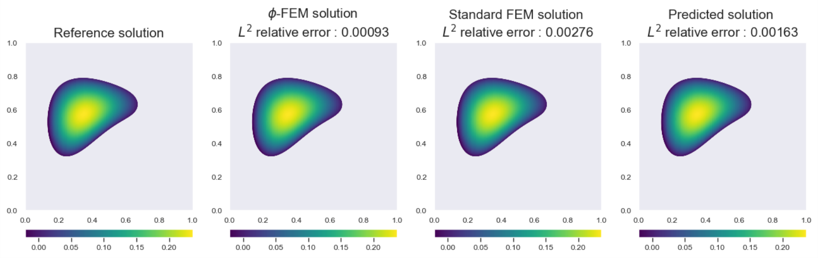
$$\phi(x, y) = 0.4 - \sum_{k=1}^{3} \sum_{l=1}^{3} \alpha_{kl} \sin(k\pi x) \sin(l\pi y),$$

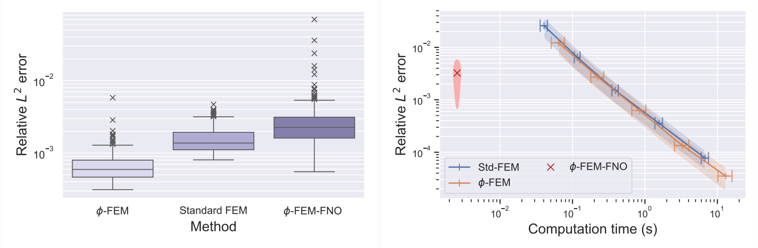
Dataset : 2200 training data, 467 validation data.



Examples of level-set functions and corresponding domains.

ϕ-FEM and FNO : complex shapes





Results

- Real-time : $\approx$ 100 times faster than FEM solvers,
- $\approx$ 5 times faster and more precise than the previous work Geo-FNO.

Perspectives :

- More realistic test cases,
- Mixed Dirichlet-Neumann boundary conditions, Time-Dependant PDE's, Linear and non-linear elasticity, ...
- 3D problems,
- Validation on organ geometries.

Thanks for your attention!

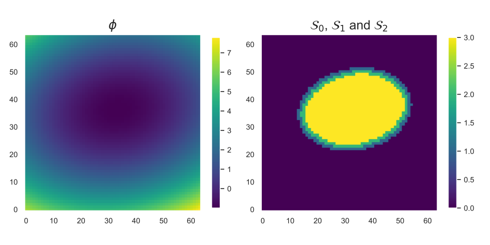
- The standardization and unstandardization operators are applied channel by channel and are given by :

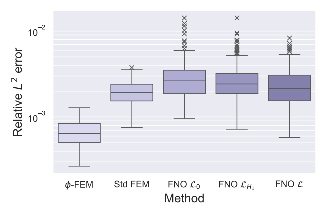
$$C^N = N(C) = \left(\frac{C - \text{mean}(C^{\text{train}})}{\text{std}(C^{\text{train}})} \right), \tag{N}$$

$$N^{-1}(Y) = Y \times \text{std}(Y^{\text{train}}) + \text{mean}(Y^{\text{train}}). \tag{N^{-1}}$$

H^2 norm : $\mathcal{L}^2 \approx \|\cdot\|^2_{0,\mathcal{S}_0} + |\cdot|^2_{1,\mathcal{S}_1} + |\cdot|^2_{2,\mathcal{S}_2}$

- First and second derivatives : finite differences.
- Need to reduce the computational domain :





$$\mathcal{L}\left(U_{\text{true}}; U_\theta\right) = \frac{1}{N_{\text{data}}} \sum_{n=0}^{N_{\text{data}}} \sqrt{\frac{\sum_{i=0}^{2} \mathcal{E}_i(u^n_{\text{true}}; u^n_\theta)}{\sum_{i=0}^{2} \mathcal{N}_i(u^n_{\text{true}})}},$$

where

$$\mathcal{E}_0(u^n_{\text{true}}; u^n_\theta) = \sum_{\mathcal{S}_0} \left\| u^n_{\text{true}}(i,j) - u^n_\theta(i,j) \right\|^2,$$

$$\mathcal{E}_1(u^n_{\text{true}}; u^n_\theta) = \sum_{\mathcal{S}_1} \left(\left\| \nabla^h_x u^n_{\text{true}}(i,j) - \nabla^h_x u^n_\theta(i,j) \right\|^2 + \left\| \nabla^h_y u^n_{\text{true}}(i,j) - \nabla^h_y u^n_\theta(i,j) \right\|^2 \right),$$

$$\mathcal{E}_2(u^n_{\text{true}}; u^n_\theta) = \sum_{\mathcal{S}_2} \left(\left\| \nabla^h_x \nabla^h_x u^n_{\text{true}}(i,j) - \nabla^h_x \nabla^h_x u^n_\theta(i,j) \right\|^2 \right.$$

$$\left. + \left\| \nabla^h_x \nabla^h_y u^n_{\text{true}}(i,j) - \nabla^h_x \nabla^h_y u^n_\theta(i,j) \right\|^2 + \left\| \nabla^h_y \nabla^h_y u^n_{\text{true}}(i,j) - \nabla^h_y \nabla^h_y u^n_\theta(i,j) \right\|^2 \right),$$

and

$$\mathcal{N}_0(u^n_{\text{true}}) = \sum_{\mathcal{S}_0} \left\| u^n_{\text{true}}(i,j) \right\|^2,$$

$$\mathcal{N}_1(u^n_{\text{true}}) = \sum_{\mathcal{S}_1} \left(\left\| \nabla^h_x u^n_{\text{true}}(i,j) \right\|^2 + \left\| \nabla^h_y u^n_{\text{true}}(i,j) \right\|^2 \right),$$

$$\mathcal{N}_2(u^n_{\text{true}}) = \sum_{\mathcal{S}_2} \left(\left\| \nabla^h_x \nabla^h_x u^n_{\text{true}}(i,j) \right\|^2 + \left\| \nabla^h_x \nabla^h_y u^n_{\text{true}}(i,j) \right\|^2 + \left\| \nabla^h_y \nabla^h_y u^n_{\text{true}}(i,j) \right\|^2 \right).$$