Méthodes Éléments Finis non-conformes adaptées à la conception en temps réel de jumeaux numériques d'organes

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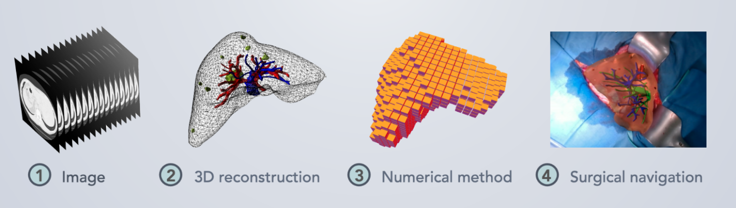
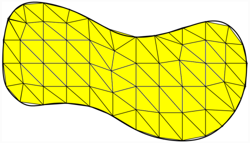
Objectives

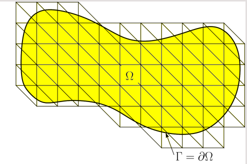
Develop **real-time, patient specific digital twins** for computer-aided surgical interventions.



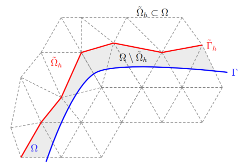
- Simulation of the deformations of organs : PDEs $\longrightarrow$ FEMs,
- Complex geometries $\longrightarrow$ Unfitted FEMs,
- Real-time constructions $\longrightarrow$ Machine learning techniques.



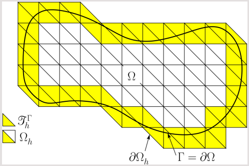
(a) Standard FEM (Clough 60s).



(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**

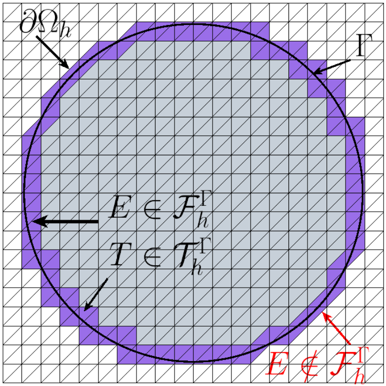
Problems on complex shapes $\longrightarrow$ unfitted FEMs

Level-set function

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

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 $\mathcal{T}_h^\Gamma$.

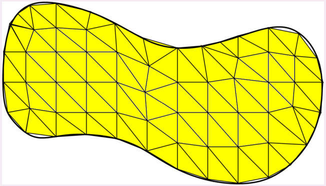


Example with $\varphi(x, y) = -1 + x^2 + y^2$.

Example (Poisson-Dirichlet equation)

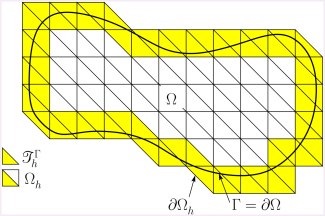
Standard FEM

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



φ-FEM

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



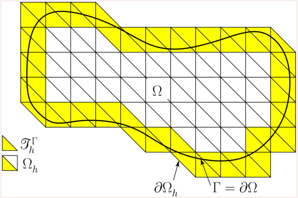
Example (Poisson-Dirichlet equation)

$$-\Delta(\varphi w + g) = f \quad \text{in } \Omega_h\,.$$

φ-FEM scheme (Duprez, Lozinski. 2020.)

Find w_h such that for all v_h,

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



Example (Poisson-Dirichlet equation)

$$-\Delta(\varphi w + g) = f \quad \text{in } \Omega_h \, .$$

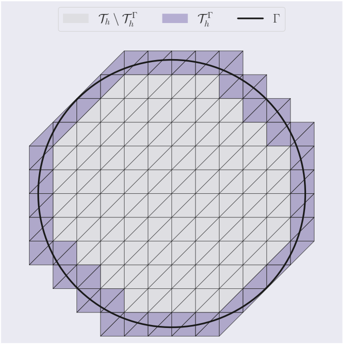
$$\int_{\Omega_h} \nabla(\varphi_h w_h + g_h) \cdot \nabla(\varphi_h v_h) - \int_{\partial\Omega_h} \frac{\partial}{\partial n}(\varphi_h w_h + g_h)\varphi_h v_h$$
$$\underbrace{+ \sigma h \sum_{F \in \mathcal{F}_h^\Gamma} \int_F \left[\frac{\partial}{\partial n}(\varphi_h w_h + g_h)\right] \left[\frac{\partial}{\partial n}(\varphi_h v_h)\right]}_{(\text{Stab1}) : \text{jump over the facets, Ghost penalty [1]}}$$
$$\underbrace{+ \sigma h^2 \sum_{T \in \mathcal{T}_h^\Gamma} \int_T (\Delta(\varphi_h w_h + g_h) + f_h)\Delta(\varphi_h w_h)}_{(\text{Stab2}) : \text{least square imposition of the governing equation}} = \int_{\Omega_h} f_h \varphi_h v_h \, .$$

1. E. Burman, Ghost penalty, 2010.

Main idea

Use the idea of the previous method (*direct variant*) only in the "boundary cells" (purple cells) :

$$u_h = \varphi_h p_h + g_h \,, \text{ in } \Omega_h^\Gamma \,.$$



Main idea

Use the idea of the previous method (*direct variant*) only in the "boundary cells" (purple cells) :

$$u_h = \varphi_h p_h + g_h \,, \text{ in } \Omega_h^\Gamma \,.$$

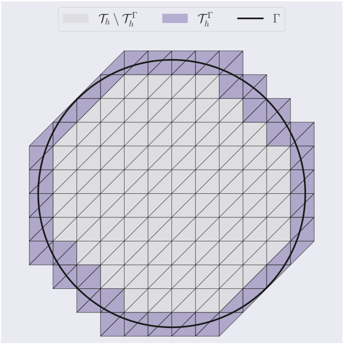
The scheme is given by : find $(u_h, p_h) \in V_h \times Q_h$ such that

$$\int_{\Omega_h} \nabla u_h \cdot \nabla v_h - \int_{\partial\Omega_h} \frac{\partial u_h}{\partial n} v_h$$

$$+ \overbrace{\frac{\gamma}{h^2} \int_{\Omega_h^\Gamma} \left(u_h - \frac{1}{h}\varphi_h p_h - g_h\right)\left(v_h - \frac{1}{h}\varphi_h q_h\right)}^{\text{Penalization}}$$

$$+ \underbrace{G_h^{lhs}(u_h, v_h) = G_h^{rhs}(v_h)}_{\text{Stabilization}}$$

$$+ \int_{\Omega_h} f v_h \,, \quad \forall v_h \in V_h, q_h \in Q_h \,.$$



Theorem (Duprez, Lleras, Lozinski, Vuillemot. In preparation.)

The solution u_h of the given scheme satisfies

$$|u - u_h|_{1,\Omega_h} \leqslant Ch^k \|f\|_{k,\Omega_h} \quad \textit{and} \quad \|u - u_h\|_{0,\Omega_h} \leqslant Ch^{k+1/2} \|f\|_{k,\Omega_h} .$$

Theorem (Duprez, Lleras, Lozinski, Vuillemot. In preparation.)

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Sketch of proof.

Based on the coercivity of the bilinear form,

$$a_h(u_h, p_h; v_h, q_h) = \int_{\Omega_h} \nabla u_h \cdot \nabla v_h - \int_{\partial\Omega_h} \frac{\partial u_h}{\partial n} v_h + \frac{\gamma}{h^2} \int_{\Omega_h^\Gamma} (u_h - \frac{1}{h}\varphi_h p_h - g_h)(v_h - \frac{1}{h}\varphi_h q_h) + G_h^{lhs}(u_h, v_h) .$$

Main difficulty : absorb the boundary term, which is done using an integration by parts on $\Omega_h \setminus \Omega$ and the stabilization terms.

Theorem (Duprez, Lleras, Lozinski, Vuillemot. In preparation.)

The solution u_h of the given scheme satisfies

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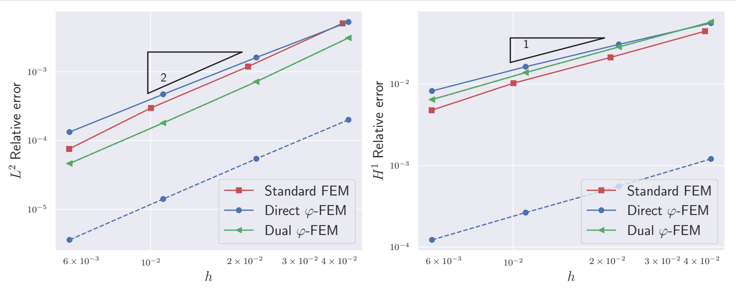
Test case : Poisson on disk

$$\varphi_1(x, y) = -0.3125^2 + (x - 0.5)^2 + (y - 0.5)^2 , \qquad \textit{Dashed lines}$$

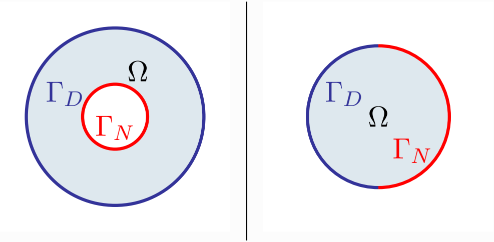
$$\varphi_2(x, y) = -0.3125 + \sqrt{(x - 0.5)^2 + (y - 0.5)^2} . \qquad \textit{Plain lines}$$



The problem

We want to solve

$$\begin{cases} -\Delta u &= f\,, \quad \text{in}\,\Omega\,, \\ u &= 0\,, \ \text{on}\,\Gamma_D\,, \\ \nabla u \cdot n &= 0\,, \ \text{on}\,\Gamma_N\,, \end{cases}$$



Examples of considered situations.

Tools to do it : φ-FEM Neumann [a] + φ-FEM *dual* variant.

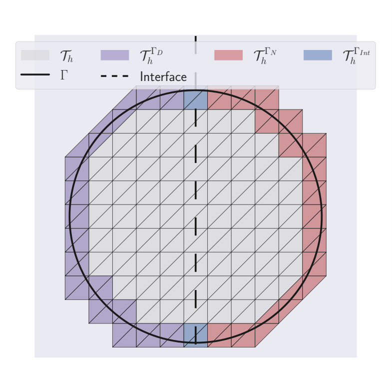
a. A new ϕ-FEM approach for problems with natural boundary conditions. Duprez, Lleras, Lozinski. 2023.

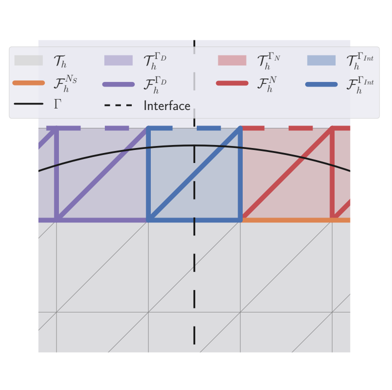
Introduce ψ such that

$$\Gamma_D = \Gamma \cap \{\psi < 0\} \quad \text{and} \quad \Gamma_N = \Gamma \cap \{\psi > 0\}\,.$$

Hence, we can define

$$\mathcal{T}_h^{\Gamma_D} := \{T \in \mathcal{T}_h^{\Gamma} \;:\; \psi_h \leqslant 0 \text{ on } T\} \quad \text{and} \quad \mathcal{T}_h^{\Gamma_N} := \{T \in \mathcal{T}_h^{\Gamma} \;:\; \psi_h \geqslant 0 \text{ on } T\},$$

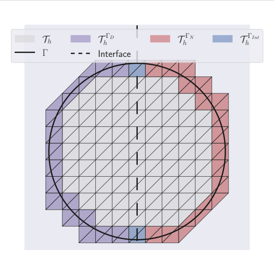




We get 3 new variables and 3 additional equations :

$$u = \varphi p_D \,, \quad \text{in } \Omega_h^{\Gamma_D} \,,$$
$$y + \nabla u = 0 \,, \quad \text{in } \Omega_h^{\Gamma_N} \,,$$
$$y \nabla \varphi + p_N \varphi = 0 \,, \quad \text{in } \Omega_h^{\Gamma_N} \,.$$

(*using that* $n = \nabla \varphi / |\nabla \varphi|$)



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$$u = \varphi p_D\,, \quad \text{in } \Omega_h^{\Gamma_D}\,,$$
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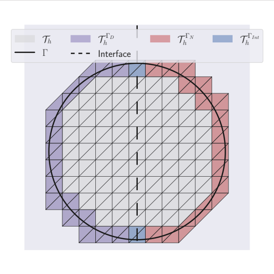
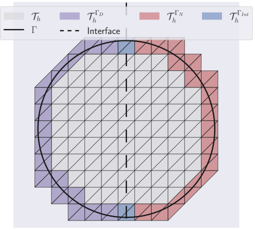


The φ-FEM scheme is given by : find $(u_h, p_{h,D}, y_h, p_{h,N}) \in W_h^{(k)}$ such that for all $(v_h, q_{h,D}, z_h, q_{h,N}) \in W_h^{(k)}$,

$$\int_{\Omega_h} \nabla u_h \cdot \nabla v_h - \int_{\partial\Omega_h \setminus \partial\Omega_{h,N}} \frac{\partial u_h}{\partial n} v_h + a_D(u_h, p_{h,D}; v_h, q_{h,D})$$
$$+ a_N(u_h, y_h, p_{h,N}; v_h, z_h, q_{h,N}) = \int_{\Omega_h} f v_h + l_D(v_h) + l_N(z_h)\,.$$

We want to impose by penalization :

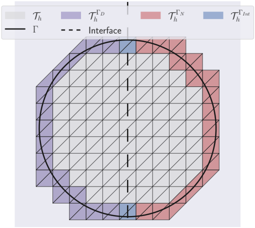
$$u = \varphi p_D \,, \qquad \text{in } \Omega_h^{\Gamma_D} \,.$$



$$a_D(u_h, p_{h,D}; v_h, q_{h,D}) = \overbrace{\frac{\gamma}{h^2}\int_{\Omega_h^{\Gamma_D}} (u_h - \frac{1}{h}\varphi_h p_{h,D})(v_h - \frac{1}{h}\varphi_h q_{h,D})}^{\text{Penalization}}$$

$$\left.\begin{aligned} &+\sigma_D h \sum_{F\in\mathcal{F}_h^{\Gamma_D}\cup\mathcal{F}_h^{\Gamma_{Int}}} \int_F \left[\frac{\partial u_h}{\partial n}\right]\left[\frac{\partial v_h}{\partial n}\right] \\ &+\sigma_D h^2 \int_{\Omega_h^{\Gamma_D}\cup\Omega_h^{\Gamma_{Int}}} \Delta u_h \Delta v_h, \\ l_D(v_h) &= -\sigma_D h^2 \int_{\Omega_h^{\Gamma_D}\cup\Omega_h^{\Gamma_{Int}}} f\Delta v_h \,. \end{aligned}\right\} \text{Stabilization}$$

The scheme : Neumann part



We want to impose by penalization :

$$
\begin{aligned}
y + \nabla u = 0\,, &\quad \text{in } \Omega_h^{\Gamma_N}\,,\\
y\nabla\varphi + p_N\varphi = 0\,, &\quad \text{in } \Omega_h^{\Gamma_N}\,.
\end{aligned}
$$

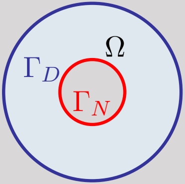
$$
a_N(u_h, y_h, p_{h,N}; v_h, z_h, q_{h,N}) = \overbrace{\int_{\partial\Omega_{h,N}} y_h.n v_h}^{\text{Boundary term}}
$$

$$
\left.
\begin{aligned}
&+\gamma_u \int_{\Omega_h^{\Gamma_N}} (y_h + \nabla u_h)(z_h + \nabla v_h)\\
&+\frac{\gamma_p}{h^2}\int_{\Omega_h^{\Gamma_N}} \left(y_h \cdot \nabla\varphi_h + \frac{1}{h} p_{h,N}\varphi_h\right)\left(z_h \cdot \nabla\varphi_h + \frac{1}{h} q_{h,N}\varphi_h\right)
\end{aligned}
\right\}\ \text{Penalization}
$$

$$
\left.
\begin{aligned}
&+\sigma_N h \sum_{F\in\mathcal{F}_h^{N_S}} \int_F \left[\frac{\partial u_h}{\partial n}\right]\left[\frac{\partial v_h}{\partial n}\right] + \gamma_{div}\int_{\Omega_h^{\Gamma_N}} \operatorname{div} y_h \operatorname{div} z_h\,,\\
&l_N(z_h) = \gamma_{div}\int_{\Omega_h^{\Gamma_N}} f \operatorname{div} z_h\,.
\end{aligned}
\right\}\ \text{Stabilization}
$$

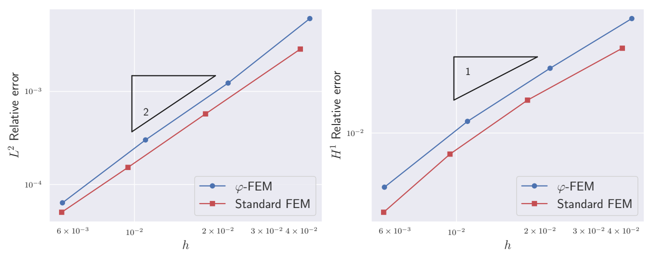
We consider $f = -1$, the domain given by :

$$\begin{cases} \varphi_1(x,y) & = -0.39^2 + (x-0.5)^2 + (y-0.5)^2\,, \\ \varphi_2(x,y) & = -0.14^2 + (x-0.5)^2 + (y-0.5)^2\,, \\ \varphi(x,y) & = \varphi_1(x,y) \times \varphi_2(x,y)\,. \end{cases}$$



and to detect the change of boundary :

$$\psi(x,y) = 0.25^2 - (x-0.5)^2 - (y-0.5)^2\,.$$



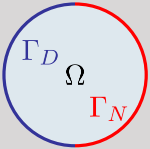
Left : L^2 relative errors. Right : H^1 relative errors.

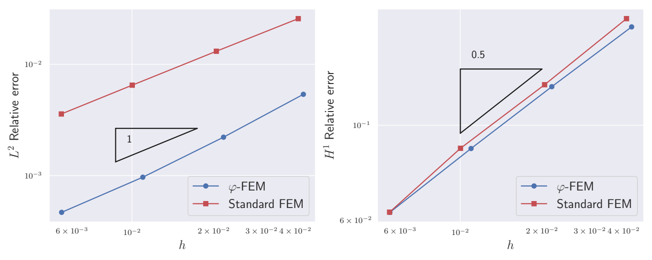
We consider $f = -1$, the domain given by :

$$\varphi(x,y) = -0.31^2 + (x-0.5)^2 + (y-0.5)^2 .$$

and to detect the change of boundary :

$$\psi(x,y) = x - 0.5 .$$





Left : L^2 relative errors. Right : H^1 relative errors.

Model problem

$$\begin{cases} \operatorname{div} \boldsymbol{\sigma}(\boldsymbol{u}) + \boldsymbol{f} & = 0\,, \text{ in } \Omega, \\ \boldsymbol{u} & = \boldsymbol{u}^g\,, \text{ on } \Gamma_D, \\ \boldsymbol{\sigma}(\boldsymbol{u}) \cdot \boldsymbol{n} & = \boldsymbol{g}\,, \text{ on } \Gamma_N. \end{cases}$$

$$\boldsymbol{\sigma}(\boldsymbol{u}) = 2\mu\,\boldsymbol{\varepsilon}(\boldsymbol{u}) + \lambda(\operatorname{div} \boldsymbol{u})\, I$$

Constraints tensor

$$\boldsymbol{\varepsilon}(\boldsymbol{u}) = \tfrac{1}{2}\left(\nabla \boldsymbol{u} + (\nabla \boldsymbol{u})^T\right)$$

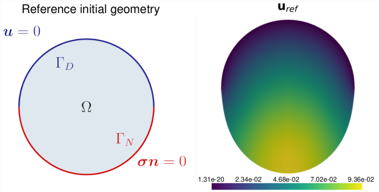
Deformation tensor

$$\mu = \frac{E}{2(1+\nu)}, \quad \lambda = \frac{E\nu}{(1+\nu)(1-2\nu)}$$

Lamé parameters

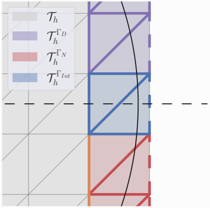
How to construct a φ-FEM scheme to solve this?
Follow the same recipe than before.

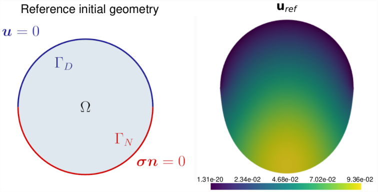
$$-\operatorname{div}\boldsymbol{\sigma}(\boldsymbol{u}) = (0, -\rho g)\,,\ \text{in}\,\Omega\,,\quad \boldsymbol{u} = 0\,,\ \text{on}\,\Gamma_D\,,\quad \boldsymbol{\sigma}(\boldsymbol{u})\cdot\boldsymbol{n} = 0\,,\ \text{on}\,\Gamma_N\,.$$

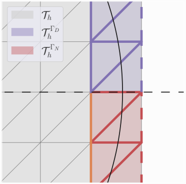


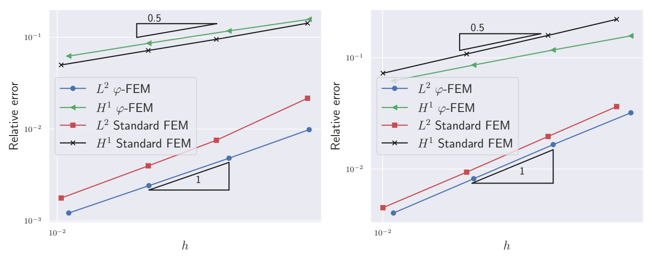
Numerical results

$$-\operatorname{div}\boldsymbol{\sigma}(\boldsymbol{u}) = (0,-\rho g)\,,\ \text{in}\,\Omega\,,\quad \boldsymbol{u}=0\,,\ \text{on}\,\Gamma_D\,,\quad \boldsymbol{\sigma}(\boldsymbol{u})\cdot\boldsymbol{n}=0\,,\ \text{on}\,\Gamma_N\,.$$









Model problem : $\approx$ the same… except non-linear constraints tensor.

$$\begin{cases} -\operatorname{div} \boldsymbol{P}(\boldsymbol{u}) &= \boldsymbol{f}\,, \quad \text{in}\,\Omega\,,\\ \boldsymbol{u} &= \boldsymbol{u}_D\,, \text{ on}\,\Gamma_D\,,\\ \boldsymbol{P}(\boldsymbol{u})\cdot\boldsymbol{n} &= \boldsymbol{g}\,, \quad \text{on}\,\Gamma_N\,,\end{cases}$$

with compressible Neo-Hookean material :

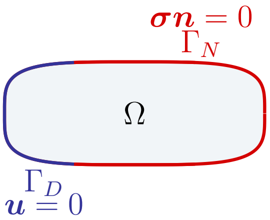
$$\boldsymbol{P} = \frac{\partial W}{\partial F}, \text{ where } W = \frac{\mu}{2}\left(I_1 - 3 - 2\ln(J)\right) + \frac{\lambda}{2}\ln(J)^2,$$

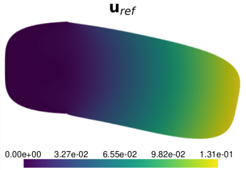
with $F = I + \nabla\boldsymbol{u}, C = F^T\cdot F, I_1 = \mathrm{tr}(C)$, and $J = \det F$.

φ-FEM scheme : $\approx$ the same recipe…

$\boldsymbol{P}$ non-linear $\Longrightarrow$ Stabilization terms non-linear in $\boldsymbol{v}$ $\Longrightarrow$ need to replace $\boldsymbol{P}(v)$ with $D_{\boldsymbol{u}}(\boldsymbol{P})(\boldsymbol{u})\boldsymbol{v}$, the derivative of $\boldsymbol{P}$ evaluated in $\boldsymbol{u}$, in the direction $\boldsymbol{v}$.

$$\varphi(x,y) = \left(\frac{(x-0.5)^4}{0.43^4} + \frac{(y-0.5)^4}{0.17^4} \right)^{0.25} - 1\,, \quad \psi(x,y) = x - 0.3\,.$$





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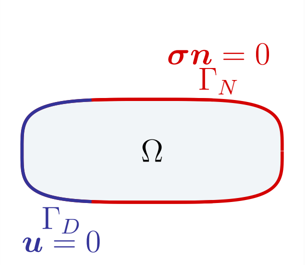

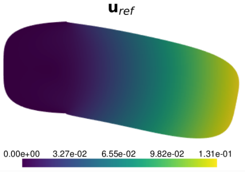

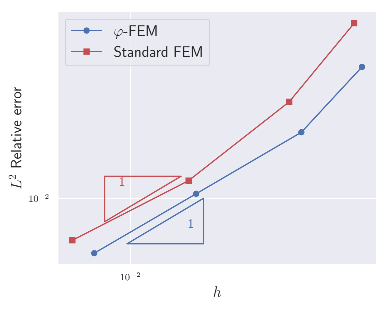

Consider the following problem

$$\begin{cases} \partial_t u - \Delta u &= f\,, \ \text{in}\,\Omega \times (0,T), \\ u &= 0\,, \ \text{on}\,\Gamma \times (0,T), \\ u_{|t=0} &= u^0\,, \qquad\quad \text{in}\,\Omega\,. \end{cases}$$

Consider the following problem

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Time discretization

Implicit Euler scheme : given $u^n = \varphi w^n$, find $u^{n+1} = \varphi w^{n+1}$ such that

$$\frac{\varphi w^{n+1} - \varphi w^n}{\Delta t} - \Delta(\varphi w^{n+1}) = f^{n+1}\,.$$

Considered problem

$$\begin{cases} \partial_t u - \Delta u & = f\,, \ \text{in}\,\Omega \times (0,T), \\ u & = 0\,, \ \text{on}\,\Gamma \times (0,T), \\ u_{|t=0} & = u^0\,, \qquad\qquad \text{in}\,\Omega\,. \end{cases}$$

Time discretization

$$\frac{\varphi w^{n+1} - \varphi w^n}{\Delta t} - \Delta(\varphi w^{n+1}) = f^{n+1}\,.$$

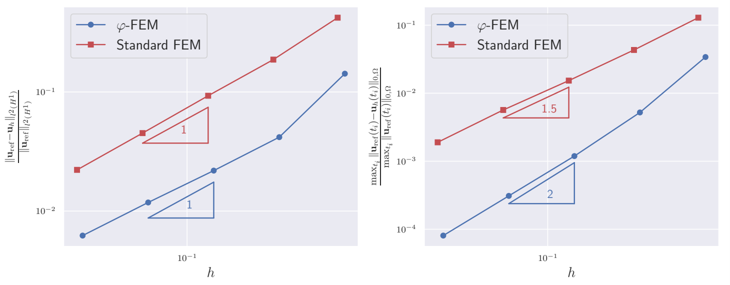
The proposed scheme

$$\int_{\Omega_h} \frac{\varphi_h w_h^{n+1}}{\Delta t} \varphi_h v_h + \int_{\Omega_h} \nabla(\varphi_h w_h^{n+1}) \cdot \nabla(\varphi_h v_h)$$
$$- \int_{\partial\Omega_h} \frac{\partial}{\partial n}(\varphi_h w_h^{n+1}) \varphi_h v_h + \text{stabs} = \int_{\Omega_h} \left(\frac{u_h^n}{\Delta t} + f^{n+1} \right) \varphi_h v_h - \text{stabs}\,.$$

Theorem (Duprez, Lleras, Lozinski, Vuillemot, 2023)

$$\|u-u_h\|_{l^2(H^1)} \leqslant C\|u^0-u_h^0\|_{L^2(\Omega_h)} + C(h^k+\Delta t)\left(\|u\|_{H^2(0,T;H^{k-1}(\Omega))}+\|f\|_{H^1(0,T;H^{k-1}(\Omega_h))}\right),$$

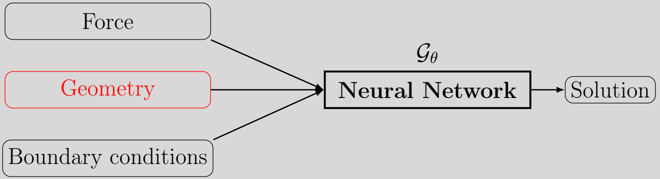
$$\|u-u_h\|_{l^\infty(L^2)} \leqslant C\|u^0-u_h^0\|_{L^2(\Omega_h)} + C(h^{k+\frac{1}{2}}+\Delta t)\left(\|u\|_{H^2(0,T;H^{k-1}(\Omega))}+\|f\|_{H^1(0,T;H^{k-1}(\Omega_h))}\right).$$



Left : $l^2(H^1)$ relative errors. Right : $l^\infty(L^2)$ relative errors.

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
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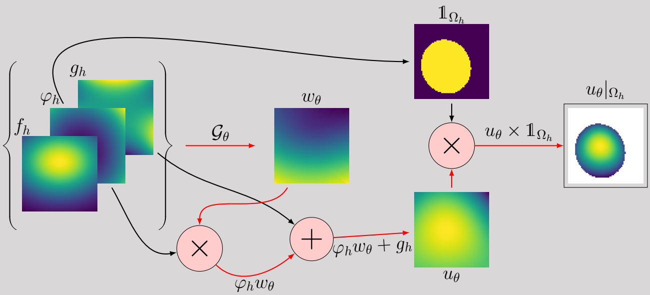
- φ-FEM $+$ Neural Networks $\longrightarrow$ Precise and real-time method?

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.[a]

[a]. Z. Li, N. Kovachki, K. Azizzadenesheli, B. Liu, K. Bhattacharya, A. Stuart, and A. Anandkumar. Fourier neural operator for parametric partial differential equations, 2021

Why choose the FNO ?

- Neural operator : learns a mapping, not a solution,
- Uses FFT $\longrightarrow$ requires Cartesian grid, as φ-FEM does,
- Can be implemented easily,
- 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 : $X = (f_h, \varphi_h, g_h) \to w_h$, 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 », $n_d >> 3$.

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

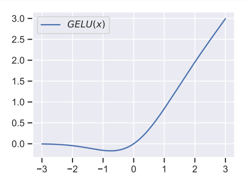
$\longrightarrow$ from « hidden dimension » n_d to final dimension 1.

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 :

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



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

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.

First test case

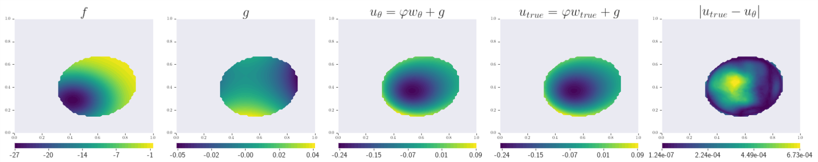
$$-\Delta u = f\,,\ \text{in}\,\Omega,\ u = g\,,\ \text{on}\,\Gamma\,,$$

- Ω : random rotated ellipse,
- f : random gaussian force with variable amplitude

$$f(x,y) = A\exp\left(-\frac{(x-\mu_0)^2}{2\sigma_x^2} - \frac{(y-\mu_1)^2}{2\sigma_y^2}\right)\,,$$

- $g_{(\alpha,\beta)}(x,y) = \alpha\left((x-0.5)^2 - (y-0.5)^2\right)\cos\left(\beta y\pi\right).$

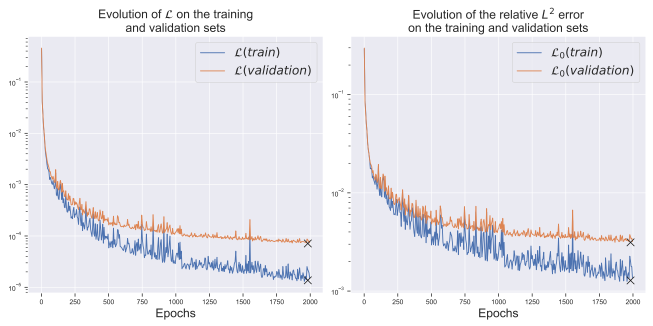
Dataset : 1500 training data, 300 validation data, 300 test data.
Random parameters : ellipses parameters and $(A, \mu_0, \mu_1, \sigma_x, \sigma_y, \alpha, \beta)$.



We try to approximate the operator :

$$\begin{array}{rccc} \mathcal{G}^\dagger : & \mathbb{R}^{n_x \times n_y \times 3} & \to & \mathbb{R}^{n_x \times n_y \times 1} \\ & (f_h, \varphi_h, g_h) & \mapsto & w_h \, . \end{array}$$

Convergence of the loss function $\approx \| \cdot \|_{1,\Omega_h}$



We compare the following techniques :

- Standard-FEM, φ-FEM and φ-FEM-FNO.
- φ-FEM-FNO 2 : φ-FEM-FNO predicting directly u_θ :

$$\begin{aligned} \mathcal{G}_\theta : \quad \mathbb{R}^{n_x \times n_y \times 3} &\to \mathbb{R}^{n_x \times n_y \times 1}, \\ (f_h, \varphi_h, g_h) &\mapsto u_\theta . \end{aligned}$$

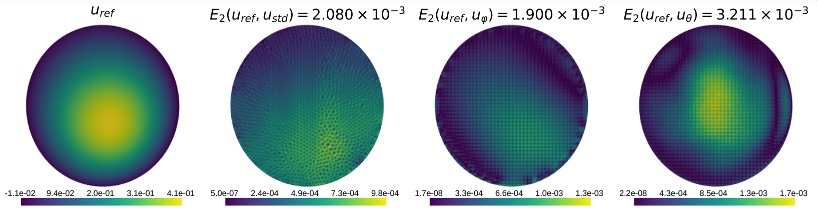
- φ-FEM-UNET : φ-FEM-FNO, but using a U-NET.
- Standard-FEM-FNO : FNO trained with standard $\mathbb{P}^1$ FEM solutions, extrapolated on Cartesian grids as data.
- Geo-FNO.[a]

a. Z. Li, D. Huang, B. Liu, A. Anandkumar : Fourier Neural Operator with Learned Deformations for PDEs on General Geometries. Codes : `https://github.com/neuraloperator/Geo-FNO`

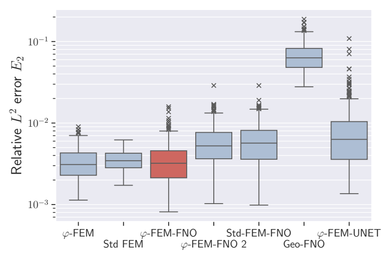
Using the relative L^2 error :

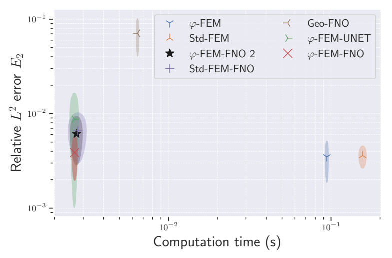
$$E_2(u_{\text{ref}}, u_\theta) := \frac{\|\Pi_{\Omega_{\text{ref}}} u_\theta - u_{\text{ref}}\|_{0,\Omega_{\text{ref}}}}{\|u_{\text{ref}}\|_{0,\Omega_{\text{ref}}}} = \sqrt{\frac{\int_{\Omega_{\text{ref}}} (\Pi_{\Omega_{\text{ref}}} u_\theta - u_{\text{ref}})^2 \, \mathrm{d}x}{\int_{\Omega_{\text{ref}}} u_{\text{ref}}^2 \, \mathrm{d}x}} .$$

φ-FEM-FNO VS OTHER TECHNIQUES



Outputs of Standard-FEM, φ-FEM and φ-FEM-FNO compared to the reference solution.





Errors of the methods.

Second test case

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

where Ω is defined using Gaussian functions,

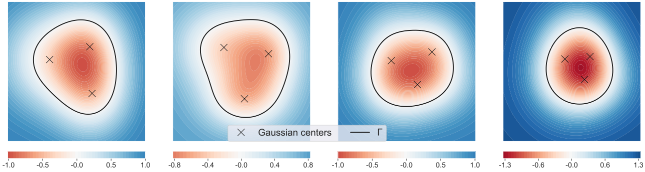
$$\varphi(x,y) = -\psi(x,y) + 0.5 \max_{(x,y)\in[0,1]^2} \psi(x,y)\,,$$

with

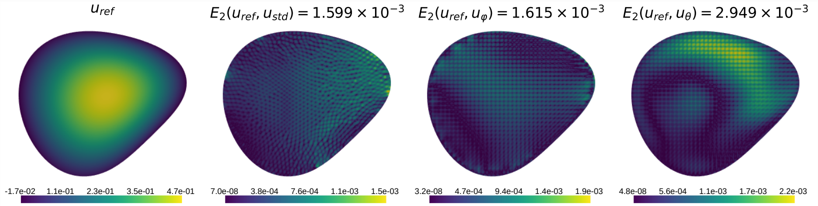
$$\psi(x,y) = \sum_{k=1}^{3} \exp\left(-\frac{(x-x_k)^2}{2\sigma_k} - \frac{(y-y_k)^2}{2\gamma_k}\right)\,,$$

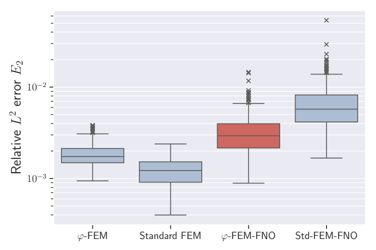
$\Longrightarrow$ 500 training data, 300 validation data, 300 test data.

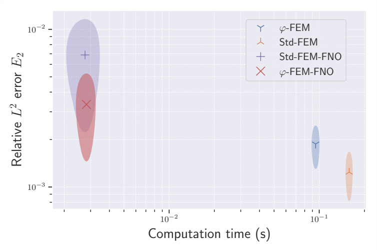
Examples of considered geometries and corresponding φ



φ-FEM-FNO : COMPLEX SHAPES



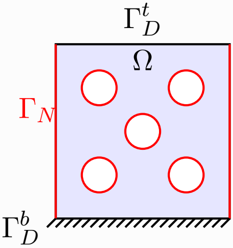


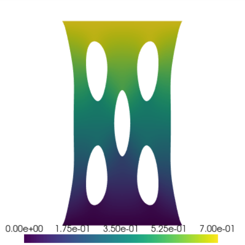


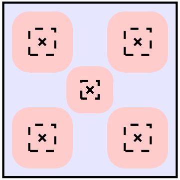
Outputs and errors of the methods.

φ-FEM-FNO : NON-LINEAR ELASTICITY

$$-\operatorname{div} \boldsymbol{P}(\boldsymbol{u}) = 0\,, \text{ in } \Omega\,,\ \ \boldsymbol{u} = \boldsymbol{u}_D\,, \text{ on } \Gamma_D^t\,,\ \ \boldsymbol{u} = 0\,, \text{ on } \Gamma_D^b\,,\ \ \boldsymbol{P}(\boldsymbol{u})\cdot\boldsymbol{n} = 0\,, \text{ on } \Gamma_N\,.$$







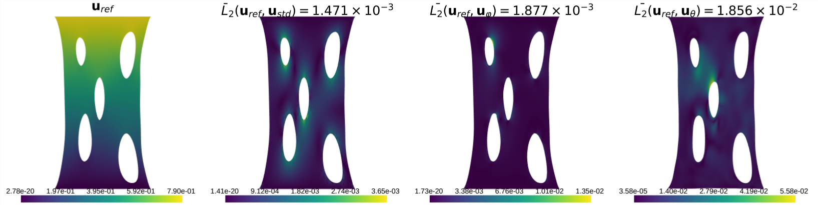
Training :

- New operator to approximate :

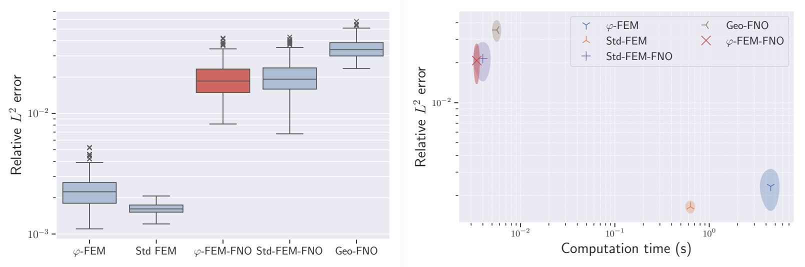
$$\begin{array}{rccc} \mathcal{G}^\dagger : & \mathbb{R}^{n_x \times n_y \times 2} & \rightarrow & \mathbb{R}^{n_x \times n_y \times 2} \\ & (\varphi_h, g_{h,y}) & \mapsto & \boldsymbol{u}_h = (u_{h,x}, u_{h,y})\,. \end{array}$$

- Loss function : $\mathcal{L} \approx |\cdot|_{1,\Omega_h}$
- 200 training data, 300 validation data, 300 test data.

Random parameters : imposed displacement $\boldsymbol{u}_D$ and centers and radii of the holes.



Outputs of Standard-FEM, φ-FEM and φ-FEM-FNO compared to the reference solution.



Errors of the methods.

What's φ-FD?

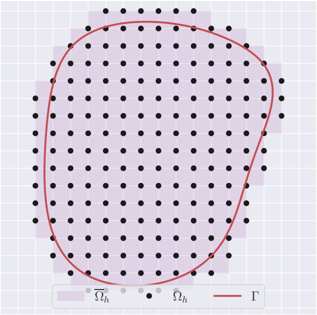
Extension of the φ-FEM dual scheme to finite difference.

Advantages :

- faster and easier to implement than φ-FEM,
- well conditioned compared to the Shortley-Weller approach.[1]

Consider the case $n = 2$

$$\Omega_h = \{x_\alpha \in \mathcal{O}_h : x_\alpha \in \Omega \text{ or } x_{\alpha \pm d} \in \Omega,\ d \in \{(1,0),(0,1)\}\},$$
$$\Omega_h^{\text{int}} = \{x_\alpha \in \mathcal{O}_h : x_\alpha \in \Omega\}.$$



1. G. H. Shortley and R. Weller. The numerical solution of Laplace's equation. 1938.

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$$\Omega_h^{\text{int}} = \{x_\alpha \in \mathcal{O}_h : x_\alpha \in \Omega\}.$$

The scheme is given by : Find $u_h = (u_\alpha)_{\alpha : x_\alpha \in \Omega_h}$, s.t.

$$(-\Delta_h u_h, v_h) + b_h(u_h, v_h) + j_h(u_h, v_h) = \sum_{\alpha : x_\alpha \in \Omega_h^{\text{int}}} \sum_{d \in D} f_\alpha v_\alpha(v_h),$$

with

$$(-\Delta_h u_h, v_h) = \sum_{\alpha : x_\alpha \in \Omega_h^{\text{int}}} \sum_{d \in D} \frac{-u_{\alpha-d} + 2u_\alpha - u_{\alpha+d}}{h^2} v_\alpha,$$

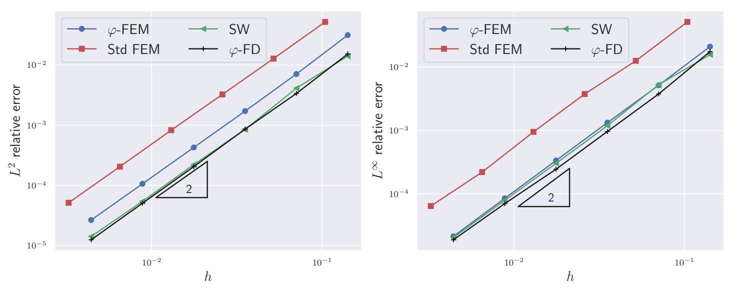
$$b_h(u_h, v_h) = \frac{\gamma}{2h^2} \sum_{(\alpha,d) \in B} \frac{1}{\varphi_\alpha^2 + \varphi_{\alpha+d}^2} (\varphi_{\alpha+d} u_\alpha - \varphi_\alpha u_{\alpha+d})(\varphi_{\alpha+d} v_\alpha - \varphi_\alpha v_{\alpha+d}),$$

$$j_h(u_h, v_h) = \sigma \sum_{(\alpha,d) \in J} \frac{-u_{\alpha-d} + 2u_\alpha - u_{\alpha+d}}{h} \times \frac{-v_{\alpha-d} + 2v_\alpha - v_{\alpha+d}}{h}.$$

Theorem (Duprez, Lleras, Lozinski, Vigon, Vuillemot, 2025.)

Under some assumptions on the domain ($\approx$ should be smooth*), assuming that* $u \in \mathcal{C}^4(\Omega)$*, and denoting by* $U = (u(x_\alpha))_{\alpha : x_\alpha \in \Omega_h^{int}}$*, one has*

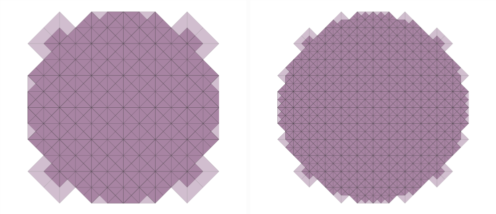
$$\|U - u_h\|_{h,0} + \|U - u_h\|_{h,\infty} + |U - u_h|_{h,1} + \leqslant Ch^{3/2}\|u\|_{\mathcal{C}^4(\Omega)}.$$



2D test case. Relative L^2 error (left) and L^∞ error (right), where SW stands for the Shortley-Weller approach.

Motivation

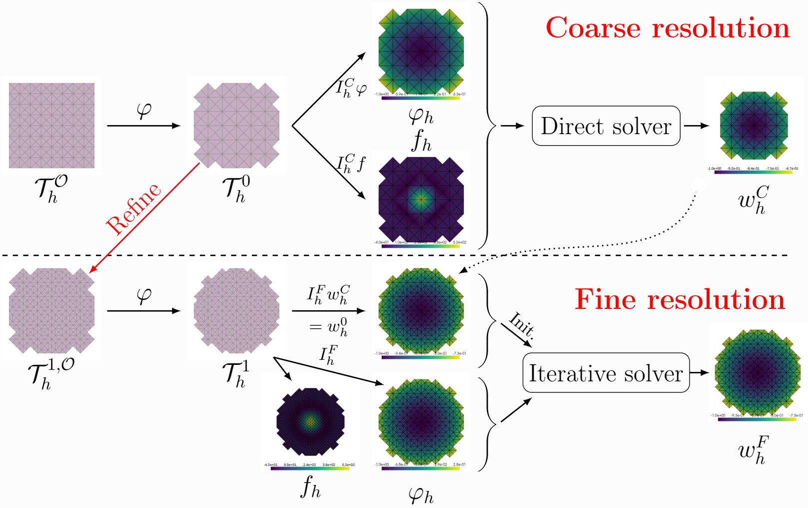
We want to reduce the computationnal cost of φ-FEM preserving its accuracy.

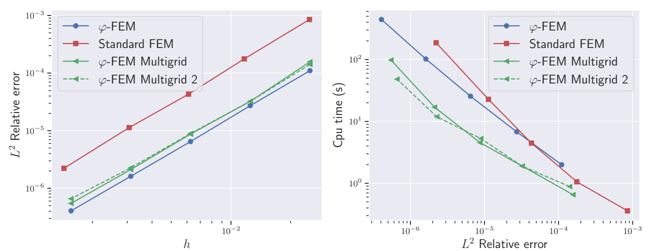


Coarse resolution $\longrightarrow$
- Fast mesh generation
- Fast system resolution
- Good approximation of the solution

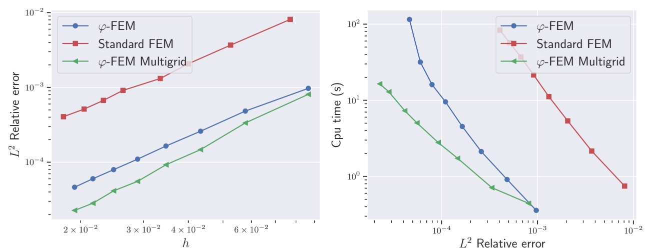
$+$ Fine resolution with initial guess $\longrightarrow$
- No mesh to generate (only refine)
- Interpolate coarse solution
- Iterative solver with good initialization

$$-\nabla\cdot(q(u)\nabla u)=f\,,\ \text{in}\,\Omega\,(\text{a disk})\ ,u=0\,,\ \text{on}\,\Gamma\,.$$



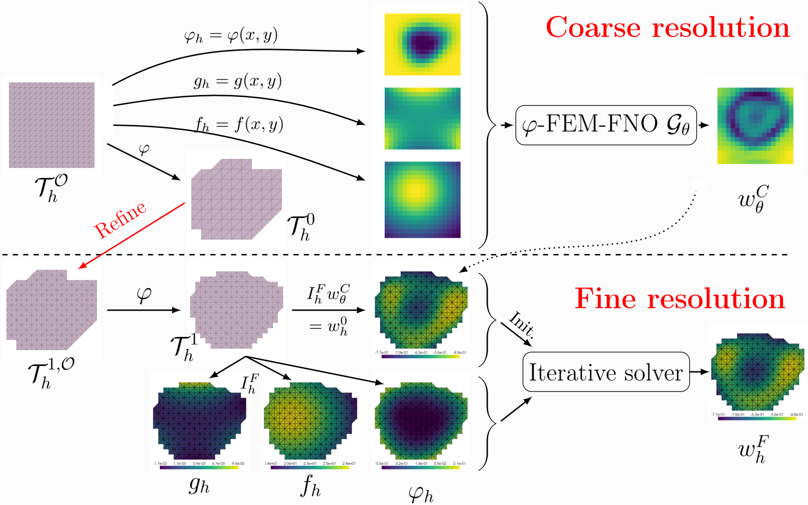


2D test case.



3D test case.

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



Test case

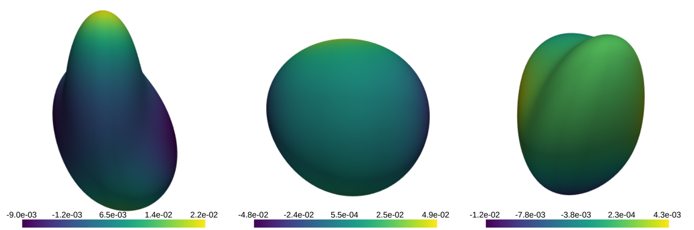
We want to solve

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

We consider domains defined by

$$\varphi(x,y,z) = (-1)^3 \prod_{j=1}^{3} \left(-1 + \exp\left(-\frac{x_j^2}{2l_{x,j}^2} - \frac{y_j^2}{2l_{y,j}^2} - \frac{z_j^2}{2l_{z,j}^2} \right) \right),$$

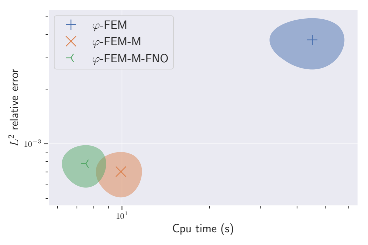
with $(x_j, y_j, z_j)^T = R_z(\theta_z)\, R_y(\theta_y)\, R_x(\theta_x)\, (x-\mu_x, y-\mu_y, z-\mu_z)^T$.

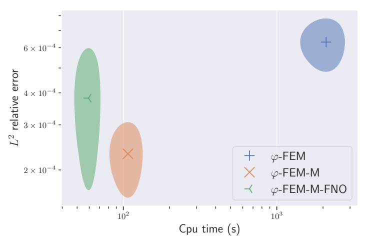


Examples of considered situations.

FNO training

- Generate 250 data (200 training + 50 validation), with $20 \times 20 \times 20$ grids.
- Train φ-FEM-FNO for 200 epochs.





Comparison on 6 test cases : average L^2 relative error. Left : 80^3 grids. Right : 160^3 grids.

Results

- φ-FEM is a powerful tool capable of solving many problems and easy to understand.
- The method offers many evolutions : can be adapted to finite difference, combined to neural networks, to multigrid approach, etc.
- In particular, we proposed φ-FEM-FNO :
  - Combination that bypasses the main limitations of FNOs,
  - Real-time : ≈ 100 times faster than FEM solvers,
  - ≈ 5 times faster and more precise than Geo-FNO on test case 1.
  - Adapted to non-linear elastic materials.
- Its combination with φ-FEM-M is very promising.

Perspectives :

- Explore the theoretical aspects of φ-FEM mixed bcs and elasticity.
- Adapt φ-FEM-FNO and φ-FEM-M-FNO to Mixed Dirichlet-Neumann boundary conditions, Time-Dependant PDE's, ...
- 3D problems : validation on organ geometries and realistic test cases.

Thank you for your attention !

Contributions

φ**-FEM-FNO : a new approach to train a Neural Operator as a fast PDE solver for variable geometries.** M. Duprez, V. Lleras, A. Lozinski, V. Vigon, **K. Vuillemot**. 2026.

φ**-FD : A well-conditioned finite difference method inspired by** φ**-FEM for general geometries on elliptic PDEs.** M. Duprez, V. Lleras, A. Lozinski, V. Vigon, **K. Vuillemot**. 2025.

φ**-FEM for the heat equation : optimal convergence on unfitted meshes in space.** M. Duprez, V. Lleras, A. Lozinski, **K. Vuillemot**. 2023.

φ**-FEM : an efficient simulation tool using simple meshes for problems in structure mechanics and heat transfer.** S. Cotin, M. Duprez, V. Lleras, A. Lozinski, **K. Vuillemot**. 2022.

How to impose Neumann boundary conditions?

- Introduce y such that
$$y = -\nabla u \text{ on } \Omega_h^{\Gamma_N}\,.$$
- Allows to rewrite (on $\Omega_h^{\Gamma_N}$ and Γ_N) :
$$-\Delta u = f \;\Rightarrow \operatorname{div} y = f\,, \quad \nabla u \cdot n = 0 \Rightarrow y \cdot n = 0\,.$$
- Using that $n = \nabla\varphi / |\nabla\varphi|$ gives,
$$y \cdot n = 0 \;\Rightarrow y \cdot \frac{\nabla\varphi}{|\nabla\varphi|} = 0\,.$$
- Introduce p_N such that
$$y \cdot \nabla\varphi + p_N\varphi = 0\,.$$
- This can finally be sum up in :
$$\begin{aligned} y + \nabla u = 0\,, &\quad \text{in } \Omega_h^{\Gamma_N}\,, \\ y\nabla\varphi + p_N\varphi = 0\,, &\quad \text{in } \Omega_h^{\Gamma_N}\,. \end{aligned}$$

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The variables are discretized using the following spaces :

$$
\begin{aligned}
p_{h,D} \in Q_h^{(k)}(\Omega_h^{\Gamma_D}) &:= \left\{ q_h : \Omega_h^{\Gamma_D} \to \mathbb{R} : q_{h|T} \in \mathbb{P}^k(T) \; \forall T \in \mathcal{T}_h^{\Gamma_D} \right\}, \\
z_h \in Z_h^{(k)}(\Omega_h^{\Gamma_N}) &:= \left\{ z_h : \Omega_h^{\Gamma_N} \to \mathbb{R}^d \; : z_{h|T} \in \mathbb{P}^k(T)^d \, \forall T \in \mathcal{T}_h^{\Gamma_N} \right\} \\
p_{h,N} \in Q_h^{(k-1)}(\Omega_h^{\Gamma_N}) &:= \left\{ q_h : \Omega_h^{\Gamma_N} \to \mathbb{R} : q_{h|T} \in \mathbb{P}^{k-1}(T) \; \forall T \in \mathcal{T}_h^{\Gamma_N} \right\}.
\end{aligned}
$$

We introduce the FE space :

$$
W_h^{(k)} := V_h^{(k)} \times Q_h^{(k)}(\Omega_h^{\Gamma_D}) \times Z_h^{(k)}(\Omega_h^{\Gamma_N}) \times Q_h^{(k-1)}(\Omega_h^{\Gamma_N}).
$$

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Back to the results

Let p_1 and p_2 defined on $\Omega_h^{\Gamma_N}$ and consider

$$\tilde{u}(p_1, p_2) = p_1 + \varphi(g - \nabla p_1 \cdot \nabla\varphi + p_2\varphi) \quad \text{in } \Omega_h^{\Gamma_N} .$$

Hence $\dfrac{\partial \tilde{u}(p_1, p_2)}{\partial n} = g$ on Γ_N, and $u = p_1 + \varphi(g - \nabla p_1 \cdot \nabla\varphi + p_2\varphi)$ with $p_1 = u$ and $p_2 = p$. The scheme is given by : find $(u_h, p_{h,D}, p_{h,1}, p_{h,2}) \in W_h^{(k)}$ s.t.

$$\begin{aligned}
&\int_{\Omega_h} \nabla u_h \cdot \nabla v_h - \int_{\partial\Omega_h^N} \nabla \widetilde{u}_h \cdot n v_h - \int_{\partial\Omega_h^D \cup \partial\Omega_h^I} \nabla u_h \cdot n v_h + \gamma \frac{1}{h^2} \int_{\Omega_h^{\Gamma_N}} (u_h - \widetilde{u}_h)(v_h - \widetilde{v}_h) \\
&\quad + \frac{\sigma_N}{h} \sum_{F \in \mathcal{F}_h^N} \int_F [\nabla \tilde{u}_h \cdot n][\nabla \tilde{v}_h \cdot n] + \gamma \int_{\Omega_h^{\Gamma_N}} (\mathrm{div}(\nabla \widetilde{u}_h) + f_h)\mathrm{div}(\nabla \widetilde{v}_h) \\
&+ \sigma_N h \sum_{F \in \mathcal{F}_h^{N_s}} \int_F [\nabla u_h \cdot n][\nabla v_h \cdot n] + \frac{\gamma_D}{h^2} \int_{\Omega_h^{\Gamma_D}} (u_h - \frac{1}{h}\varphi_h p_{h,D} - u_D)(v_h - \frac{1}{h}\varphi_h q_{h,D}) \\
&+ \sigma_D h \sum_{F \in \mathcal{F}_h^{\Gamma_D}} \int_F [\nabla u_h \cdot n][\nabla v_h \cdot n] + \gamma_D h^2 \int_{\Omega_h^{\Gamma_D}} (\Delta u_h + f_h)\Delta v_h = \int_{\Omega_h} f_h v_h ,
\end{aligned}$$

$$\forall (v_h, q_{h,D}, q_{h,1}, q_{h,2}) \in W_h^{(k)} .$$

Back to the recipe

Find $\boldsymbol{u}_h \in \boldsymbol{V}_h, \boldsymbol{p}_{h,D} \in \boldsymbol{Q}_h^k(\Omega_h^{\Gamma_D}), \boldsymbol{y}_h \in \boldsymbol{Z}_h(\Omega_h^{\Gamma_N})$ and $\boldsymbol{p}_{h,N} \in \boldsymbol{Q}_h^{k-1}(\Omega_h^{\Gamma_N})$ s.t.

$$\int_{\Omega_h} \boldsymbol{\sigma}(\boldsymbol{u}_h) : \nabla \boldsymbol{v}_h - \int_{\partial\Omega_h \setminus \partial\Omega_{h,N}} \boldsymbol{\sigma}(\boldsymbol{u}_h)\boldsymbol{n} \cdot \boldsymbol{v}_h + \int_{\partial\Omega_{h,N}} \boldsymbol{y}_h \boldsymbol{n} \cdot \boldsymbol{v}_h$$

$$+ \gamma_u \int_{\Omega_h^{\Gamma_N}} (\boldsymbol{y}_h + \boldsymbol{\sigma}(\boldsymbol{u}_h)) : (\boldsymbol{z}_h + \boldsymbol{\sigma}(\boldsymbol{v}_h))$$

$$+ \frac{\gamma_p}{h^2} \int_{\Omega_h^{\Gamma_N}} \left(\boldsymbol{y}_h \nabla \varphi_h + \frac{1}{h} \boldsymbol{p}_{h,N} \varphi_h \right) \cdot \left(\boldsymbol{z}_h \nabla \varphi_h + \frac{1}{h} \boldsymbol{q}_{h,N} \varphi_h \right)$$

$$+ \frac{\gamma}{h^2} \int_{\Omega_h^{\Gamma_D}} (\boldsymbol{u}_h - \frac{1}{h} \varphi_h \boldsymbol{p}_{h,D}) \cdot (\boldsymbol{v}_h - \frac{1}{h} \varphi_h \boldsymbol{q}_{h,D}) + G_h(\boldsymbol{u}_h, \boldsymbol{v}_h)$$

$$+ J_h^{lhs,D}(\boldsymbol{u}_h, \boldsymbol{v}_h) + J_h^{lhs,N}(\boldsymbol{y}_h, \boldsymbol{z}_h) = \int_{\Omega_h} \boldsymbol{f} \cdot \boldsymbol{v}_h$$

$$+ \frac{\gamma}{h^2} \int_{\Omega_h^D} \boldsymbol{u}_h^g \cdot (\boldsymbol{v}_h - \frac{1}{h} \varphi_h \boldsymbol{q}_{h,D}) - \frac{\gamma_p}{h^2} \int_{\Omega_h^{\Gamma_N}} \boldsymbol{g} \cdot |\nabla \varphi_h| (\boldsymbol{z}_h \cdot \nabla \varphi_h + \frac{1}{h} \boldsymbol{q}_{h,N} \varphi_h)$$

$$+ J_h^{rhs,D}(\boldsymbol{v}_h) + J_h^{rhs,N}(\boldsymbol{z}_h)$$

$$\forall \boldsymbol{v}_h \in \boldsymbol{V}_h, \boldsymbol{q}_{h,D} \in \boldsymbol{Q}_h^k(\Omega_h^{\Gamma_D}), \boldsymbol{z}_h \in \boldsymbol{Z}_h(\Omega_h^{\Gamma_N}), \boldsymbol{q}_{h,N} \in \boldsymbol{Q}_h^{k-1}(\Omega_h^{\Gamma_N}).$$

Find $\boldsymbol{u}_h \in \boldsymbol{V}_h^k, \boldsymbol{p}_{h,N} \in \boldsymbol{Q}_h^{(k-1)}(\Omega_h^{\Gamma_N}), \boldsymbol{y}_h \in \boldsymbol{Z}_h(\Omega_h^{\Gamma_N})$ et $\boldsymbol{p}_{h,D} \in \boldsymbol{Q}_h^{(k)}(\Omega_h^{\Gamma_D})$ s.t.

$$\int_{\Omega_h} \boldsymbol{P}(\boldsymbol{u}_h) : \nabla \boldsymbol{v}_h + \int_{\partial\Omega_h^{\Gamma_N}} \boldsymbol{y}_h \boldsymbol{n} \cdot \boldsymbol{v}_h - \int_{\partial\Omega_h \setminus \partial\Omega_h^{\Gamma_N}} \nabla \boldsymbol{u}_h \boldsymbol{n} \cdot \boldsymbol{v}_h - \int_{\Omega_h} \boldsymbol{f}_h \boldsymbol{v}_h$$

$$+ \gamma_D \int_{\Omega_h^{\Gamma_D}} (\boldsymbol{u}_h - \frac{1}{h}\varphi_h \boldsymbol{p}_{h,D} - \boldsymbol{u}_{h,D})(\boldsymbol{v}_h - \frac{1}{h}\varphi_h \boldsymbol{q}_{h,D})$$

$$+ \sigma_D h^2 \sum_{T \in \mathcal{T}_h^{\Gamma_D} \cup \mathcal{T}_h^{\Gamma_{Int}}} \int_T (\operatorname{div} \boldsymbol{P}(\boldsymbol{u}_h) + \boldsymbol{f}_h) \operatorname{div}(D_{\boldsymbol{u}}(\boldsymbol{P})(\boldsymbol{u}_h)\boldsymbol{v}_h)$$

$$+ \gamma_u \int_{\Omega_h^{\Gamma_N}} (\boldsymbol{y}_h + \boldsymbol{P}(\boldsymbol{u}_h)) : (\boldsymbol{z}_h + D_{\boldsymbol{u}}(\boldsymbol{P})(\boldsymbol{u}_h)\boldsymbol{v}_h)$$

$$+ \frac{\gamma_p}{h^2} \int_{\Omega_h^{\Gamma_N}} (\boldsymbol{y}_h \nabla\varphi_h + \frac{1}{h}\boldsymbol{p}_{h,N}\varphi_h + \boldsymbol{g}|\nabla\varphi_h|) \cdot (\boldsymbol{z}_h \nabla\varphi_h + \frac{1}{h}\boldsymbol{q}_{h,N}\varphi_h)$$

$$+ \gamma_{div} \int_{\Omega_h^{\Gamma_N}} (\operatorname{div} \boldsymbol{y}_h + \boldsymbol{f}_h) \cdot \operatorname{div} \boldsymbol{z}_h + G_h(\boldsymbol{u}_h, \boldsymbol{v}_h) = 0\,,$$

$$\forall \boldsymbol{v}_h \in \boldsymbol{V}_h^k,\ \boldsymbol{q}_{h,N} \in \boldsymbol{Q}_h^{(k-1)}(\Omega_h^{\Gamma_N}),\ \boldsymbol{z}_h \in \boldsymbol{Z}_h(\Omega_h^{\Gamma_N}), \boldsymbol{q}_{h,D} \in \boldsymbol{Q}_h^{(k)}(\Omega_h^{\Gamma_D})\,.$$

Back to the test case

- Standardization (channel by channel) :

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

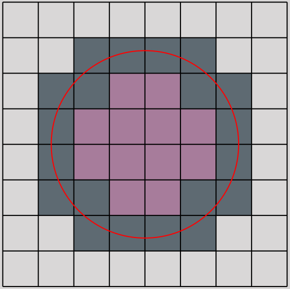
where the mean and standard-deviation are computed only on Ω_h, since all the values are 0 outside Ω_h.

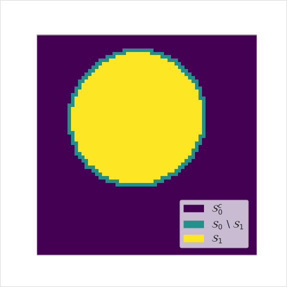
- Unstandardization :

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

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

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





Back to the test case

Test cases 1 and 2

$$\mathcal{L}\left(U_{\text{true}};U_\theta\right)=\frac{1}{N_{\text{data}}}\sum_{n=0}^{N_{\text{data}}}\left(\mathcal{E}_0(u^n_{\text{true}};u^n_\theta)+\mathcal{E}_1(u^n_{\text{true}};u^n_\theta)\right)\ ,$$

where

$$\mathcal{E}_0(u^n_{\text{true}};u^n_\theta)=\|u^n_{\text{true}}-u^n_\theta\|^2_{0,\mathcal{S}^n_0}\ ,$$

and

$$\mathcal{E}_1(u^n_{\text{true}};u^n_\theta)=\|\nabla^h_x u^n_{\text{true}}-\nabla^h_x u^n_\theta\|^2_{0,\mathcal{S}^n_1}+\|\nabla^h_y u^n_{\text{true}}-\nabla^h_y u^n_\theta\|^2_{0,\mathcal{S}^n_1}\ .$$

Test case 3

$$\mathcal{L}\left(U_{\text{true}};U_\theta\right)=\frac{1}{N_{\text{data}}}\sum_{n=0}^{N_{\text{data}}}\left(\mathcal{E}_1(u^n_{\text{true},x};u^n_{\theta,x})+\mathcal{E}_1(u^n_{\text{true},y};u^n_{\theta,y})\right)\ ,$$

where

$$\mathcal{E}_1(u^n_{\text{true},\cdot};u^n_{\theta,\cdot})=\|\nabla^h_x u^n_{\text{true},\cdot}-\nabla^h_x u^n_{\theta,\cdot}\|^2_{0,\mathcal{S}^n_1}+\|\nabla^h_y u^n_{\text{true},\cdot}-\nabla^h_y u^n_{\theta,\cdot}\|^2_{0,\mathcal{S}^n_1}\ .$$

Find $u_h = (u_{ij})_{ij}$ s.t. $\tilde{a}_h(u_h, v_h) = l_h(v_h)$, with

$$\tilde{a}_h(u_h, v_h) = (-\Delta_h u_h, v_h) + \tilde{b}_h(u_h, v_h) + \tilde{j}_h(u_h, v_h),$$

where

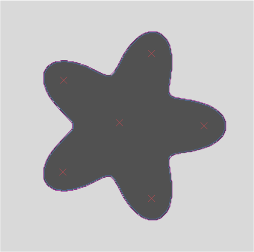
$$\tilde{b}_h(u_h, v_h) = \frac{\gamma}{2h^2}\left(\sum_{ij} \frac{u^{\varphi}_{(i-1,j)-(i+1,j)} \times v^{\varphi}_{(i-1,j)-(i+1,j)}}{4\varphi^2_{i+1,j}\varphi^2_{i-1,j} + \varphi^2_{ij}\varphi^2_{i-1,j} + \varphi^2_{ij}\varphi^2_{i+1,j}} + \sum_{ij} \frac{u^{\varphi}_{(i,j-1)-(i,j+1)} \times v^{\varphi}_{(i,j-1)-(i,j+1)}}{4\varphi^2_{i,j+1}\varphi^2_{i,j-1} + \varphi^2_{ij}\varphi^2_{i,j-1} + \varphi^2_{ij}\varphi^2_{i,j+1}}\right),$$

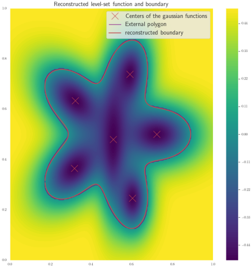
$$u^{\varphi}_{(i-1,j)-(i+1,j)} := 2\varphi_{i+1}\varphi_{i-1}u_i - \varphi_i\varphi_{i-1}u_{i+1} - \varphi_i\varphi_{i+1}u_{i-1},$$

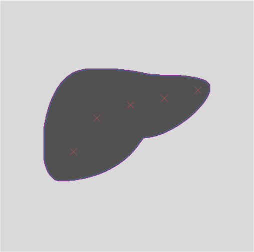
with $u^{\varphi}_{(i,j-1)-(i,j+1)}$ and $v^{\varphi}_{(i,j-1)-(i,j+1)}$ defined similarly, and

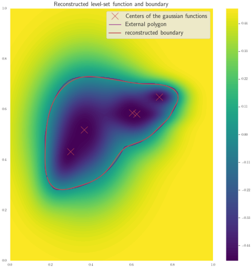
$$\tilde{j}_h(u_h, v_h) = \sigma\left(\sum_{i,j} \frac{-u_{i-1,j} + 3u_{ij} - 3u_{i+1,j} + u_{i+2,j}}{h} \times \frac{-v_{i-1,j} + 3v_{ij} - 3v_{i+1,j} + v_{i+2,j}}{h} + \text{resp in } j\right).$$

A4 – How to construct φ









- First idea : signed distance.
  - Pros : fast and easy
  - Cons : Non smooth function, non smooth boundary, in practice no analytical expression
- Second idea : product of Gaussian functions
  - Pros : smooth expression, smooth boundary, analytical expression, easy to derivate
  - Cons : not so easy to get, available only for smooth geometries

$$\varphi(x,y) = (-1)^n \prod_j^n \left(-1 + \exp\left(-\frac{x_j^2}{2l_{x,j}^2} - \frac{y_j^2}{2l_{y,j}^2} \right) \right),$$

with

$$x_j = \cos(\theta_j)(x - x_{0,j}) - \sin(\theta_j)(y - y_{0,j}),$$
$$y_j = \sin(\theta_j)(x - x_{0,j}) + \cos(\theta_j)(y - y_{0,j}).$$

We minimize the following functionnal :

$$F(\varphi) = \alpha f_1(\varphi) + \beta f_2(\varphi) + \gamma f_3(\varphi) + \delta f_4(\varphi)\,,$$

where :

$$f_1(\varphi) = \frac{1}{n_x n_y} \sum_{(x,y)\in B} \left(\frac{\partial^2}{\partial x^2}\varphi(x,y)^2 + 2\frac{\partial^2}{\partial x \partial y}\varphi(x,y)^2 + \frac{\partial^2}{\partial y^2}\varphi(x,y)^2 \right)\,,$$

$\rightarrow$ *Function enery*

$$f_2(\varphi) = \sum_{(x,y)\in B_i} \varphi(x,y)^2\,,$$ $\rightarrow$ *values at the inside polygon nodes*

$$f_3(\varphi) = \sum_{(x,y)\in B_e} \varphi(x,y)^2\,,$$ $\rightarrow$ *values at the outside polygon nodes*

$$f_4(\varphi) = \frac{1}{n_x n_y} \sum_{(x,y)\in B} \left(1 - \left(\frac{\partial}{\partial x}\varphi(x,y)^2 + \frac{\partial}{\partial y}\varphi(x,y)^2 \right) \right)^2\,.$$ $\rightarrow$ *Eikonal equation*

A4 – Numerical results

	Reference	Nanomesh	Signed distance	Gaussian
Min	0.0	2.3×10^{-5}	4.5×10^{-6}	2.0×10^{-6}
Avg	8.0×10^{-16}	2.9×10^{-3}	1.2×10^{-3}	1.2×10^{-3}
Max	9.9×10^{-15}	7.7×10^{-3}	4.3×10^{-3}	4.1×10^{-3}

Boundary reconstruction errors ($|\varphi_{ex}(x, y)|$).

Standard-FEM (red) :

- exact expression of φ (***plain lines***) ;
- signed distance (***dashed lines***) ;
- Nanomesh (***dotted***) ;

φ-FEM direct (blue) and dual (green) :

- exact expression of φ (***plain lines***) ;
- signed distance (***dashed lines***) ;
- Gaussian product (***dotted***) ;