

# Adaptive mesh refinement quantum algorithm for Maxwell's equations

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# Content

## I- Context

## II- Classical adaptive mesh refinement

## III- Quantum algorithm for adaptive mesh refinement

### 1- Reformulation of the error estimators

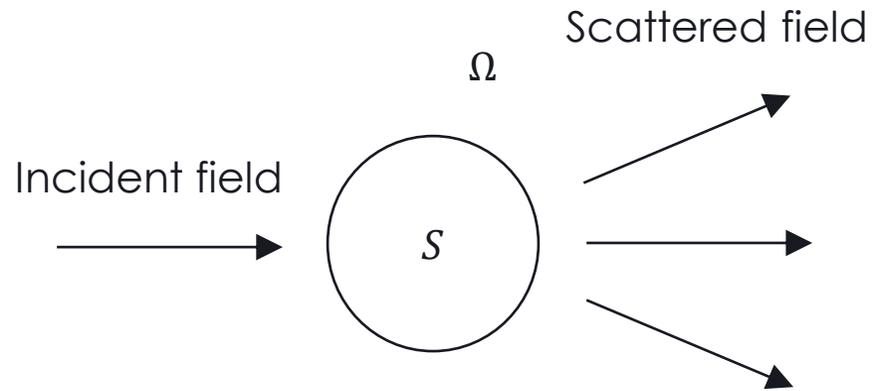
### 2- How to compute these estimators?

### 3- Numerical simulations

# Context (1/3)

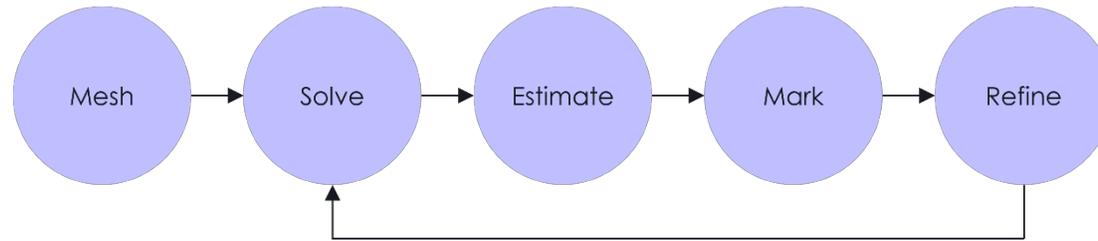
> Electromagnetic simulations for radar design

## Scattering

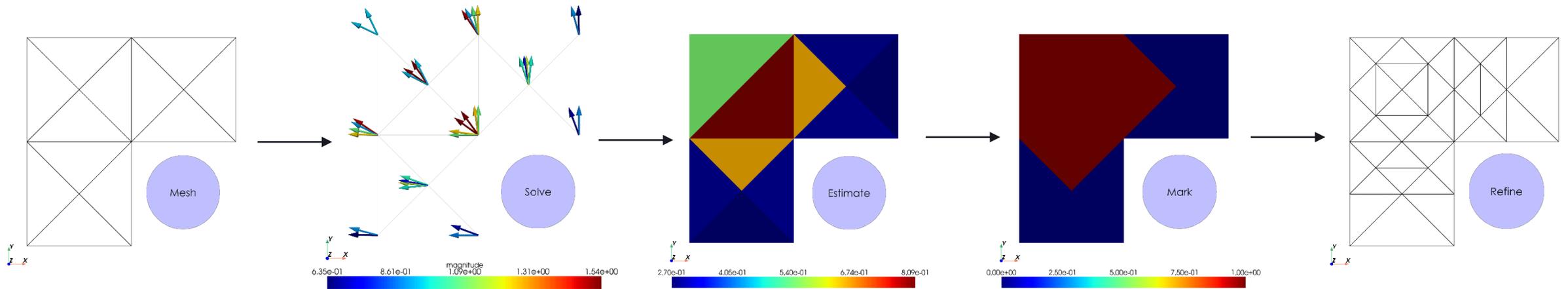


# Context (2/3)

- > Classical strategy: Finite element method (FEM) but finding a solution is expensive.
- > Classical proposition: Adaptive mesh refinement (AMR) [Nochetto 2009].



Estimate = Estimate the error.  
Mark = Mark elements to be refined.



## Context (3/3)

### > Quantum proposition

- ▶ Quantum algorithms to solve linear systems, e.g. HHL [Harrow Hassidim, Lloyd 2009].
- ▶ Application to the FEM [Montanaro, Pallister 2016].
- ▶ Quantum algorithms for electromagnetic simulations [Clader, Jacobs, Sprouse 2013].

> The goal is to study the possibility to introduce quantum computing in an adaptive mesh refinement loop.



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# FEM: From time-harmonic Maxwell's equation to a linear system (1/2)

## Time harmonic Maxwell's equation

Problem : Find the electric field  $\mathbf{E}$  such that :

$$\nabla \times (\mu_r^{-1} \nabla \times \mathbf{E}) - k^2 \epsilon_r \mathbf{E} = \mathbf{F} \quad \text{in } \Omega$$

$$\mathbf{v} \times \mathbf{E} = 0 \quad \text{on } \Gamma$$

$\Omega \subset \mathbb{R}^d$  ( $d=2,3$ ) domain  
 $\Gamma$  boundary of the domain  
 $\mathbf{v}$  outward unit normal  
 $\mathbf{F}$  source term with  $\nabla \cdot \mathbf{F} = 0$

$\epsilon_r$  relative permittivity  
 $\mu_r$  relative permeability  
 $k$  wave number

## Finite element method (FEM)

### Weak formulation

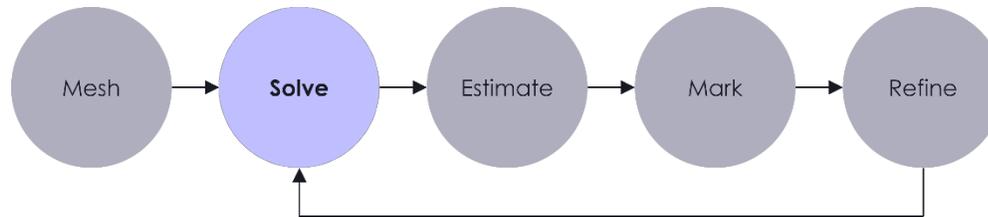
Find  $\mathbf{E} \in V$ , such that

$$a(\mathbf{E}, \mathbf{u}) = b(\mathbf{u}) \quad \forall \mathbf{u} \in V,$$

with  $a(\mathbf{E}, \mathbf{u}) := \int_{\Omega} \mu_r^{-1} \nabla \times \mathbf{E} \cdot \nabla \times \bar{\mathbf{u}} - k^2 \int_{\Omega} \epsilon_r \mathbf{E} \cdot \bar{\mathbf{u}}$ ,  $b(\mathbf{u}) := \int_{\Omega} \mathbf{F} \cdot \bar{\mathbf{u}}$  and

$$V = \mathbf{H}_0(\text{curl}, \Omega) := \left\{ \mathbf{u} \in (L^2(\Omega))^3, \nabla \times \mathbf{u} \in (L^2(\Omega))^3 \mid \mathbf{v} \times \mathbf{u} = 0 \text{ on } \Gamma \right\}.$$

Denote  $\mathbf{E}$  this solution.



# FEM: From time-harmonic Maxwell's equation to a linear system (2/2)

Finite element space on mesh  $\mathcal{T}_h$ :  $V_h = \text{span}\{\boldsymbol{\phi}_i, 1 \leq i \leq N\}$

**Nédélec** finite elements [Nédélec 1980]

## Discretized weak formulation

Find  $\mathbf{E}_h \in V_h$  such that  $a(\mathbf{E}_h, \mathbf{u}_h) = b(\mathbf{u}_h) \forall \mathbf{u}_h \in V_h$ .

## Linear system

Write  $\mathbf{E}_h = \sum_{i=1}^N \alpha_i \boldsymbol{\phi}_i$  with  $\alpha_i \in \mathbb{C}$  and choose  $\mathbf{u}_h = \boldsymbol{\phi}_j$ .

Let  $A = [a(\boldsymbol{\phi}_i, \boldsymbol{\phi}_j)]_{1 \leq i, j \leq N}$  and  $\underline{F} = [b(\boldsymbol{\phi}_j)]_{1 \leq j \leq N}$

Find  $\underline{E}_h = (\alpha_1 \dots \alpha_N)^T \in \mathbb{C}^N$  such that  $A \underline{E}_h = \underline{F}$ .

A is an **indefinite** and possibly **non-Hermitian** matrix.

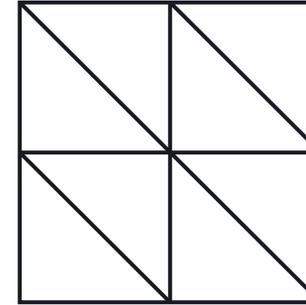


Fig: Possible mesh  $\mathcal{T}_h$  of a square.

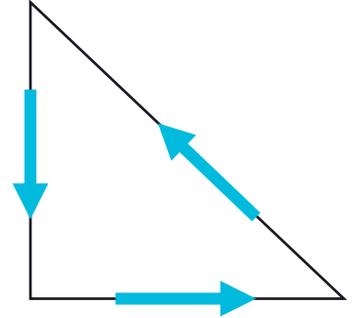


Fig: Degrees of freedom for lowest order Nédélec finite elements are integrals of the tangential component.

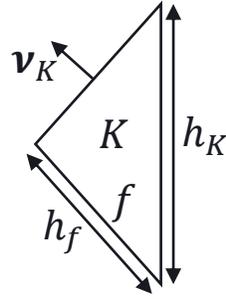
# Residual-based a posteriori error estimation

## Notation

$h_K$  diameter of element  $K$

$\mathbf{v}_K$  outward unit normal for  $K$

$h_f$  diameter of face  $f$



tangential jump operator  $[\mathbf{v}]_T = \mathbf{v}|_{K_1} \times \mathbf{v}_{K_1} + \mathbf{v}|_{K_2} \times \mathbf{v}_{K_2}$

normal jump operator  $[\mathbf{v}]_N = \mathbf{v}|_{K_1} \cdot \mathbf{v}_{K_1} + \mathbf{v}|_{K_2} \cdot \mathbf{v}_{K_2}$

## Local a posteriori error estimator [Chen, Wang, Zheng 2007]

For each  $K \in \mathcal{T}_h$ , the local error estimator  $\eta_K$  is defined by

$$\eta_K^2 := \eta_{1K}^2 + \eta_{2K}^2 + \eta_{3K}^2 + \eta_{4K}^2,$$

$$\text{with } \eta_{1K}^2 := h_K^2 \|\mathbf{F} - \nabla \times \mu_r^{-1} \nabla \times \mathbf{E}_h + k^2 \epsilon_r \mathbf{E}_h\|_{(L^2(K))^3}^2,$$

$$\eta_{2K}^2 := h_K^2 \|k^2 \nabla \cdot (\epsilon_r \mathbf{E}_h)\|_{L^2(K)}^2,$$

$$\eta_{3K}^2 := \frac{1}{2} \sum_{f \in \partial K \setminus \Gamma} h_f \|\mu_r^{-1} \nabla \times \mathbf{E}_h\|_{(L^2(f))^3}^2,$$

$$\eta_{4K}^2 := \frac{1}{2} \sum_{f \in \partial K \setminus \Gamma} h_f \|k^2 [\epsilon_r \mathbf{E}_h]_N\|_{(L^2(f))^3}^2.$$

It does not depend on the exact solution  $\mathbf{E}$ .

# Application of adaptive mesh refinement (1/2)

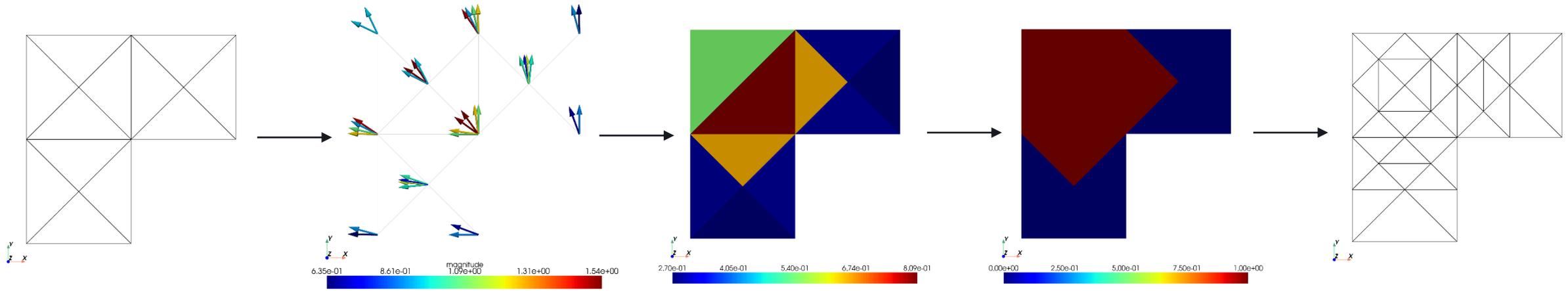
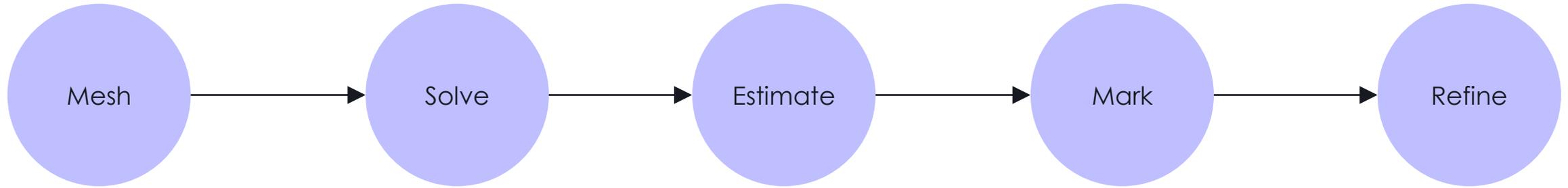


Fig: Initial mesh

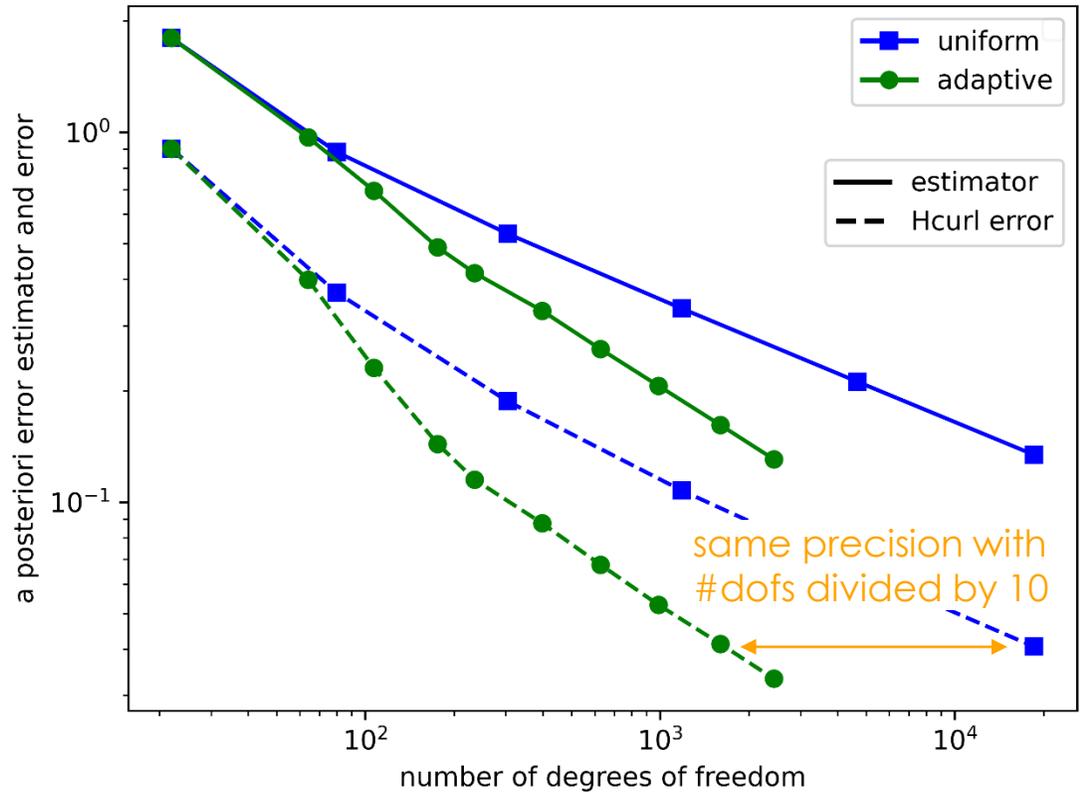
Fig:  $E_h$  at iteration 0

Fig: Local error estimators at iteration 0

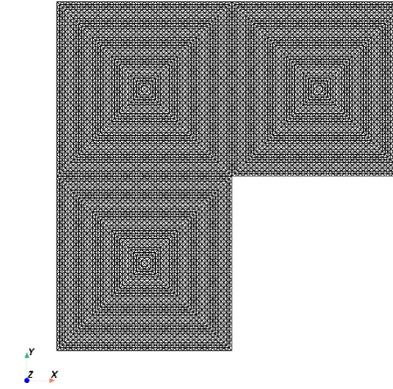
Fig: Marked elements at iteration 0

Fig: Refined mesh

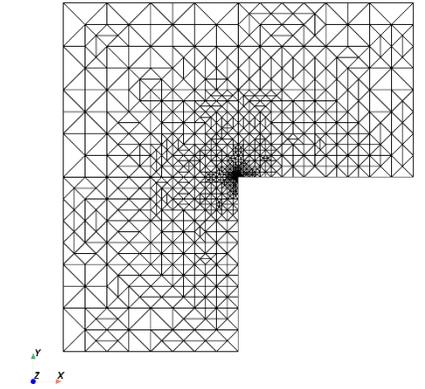
# Application of adaptive mesh refinement (2/2)



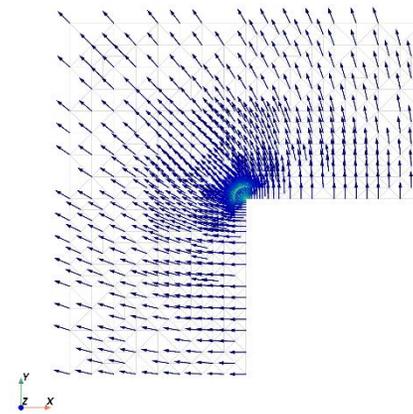
Uniformly refined mesh



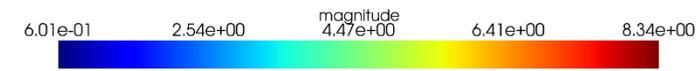
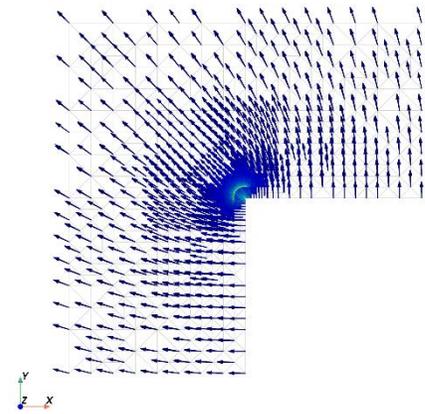
Adaptively refined mesh



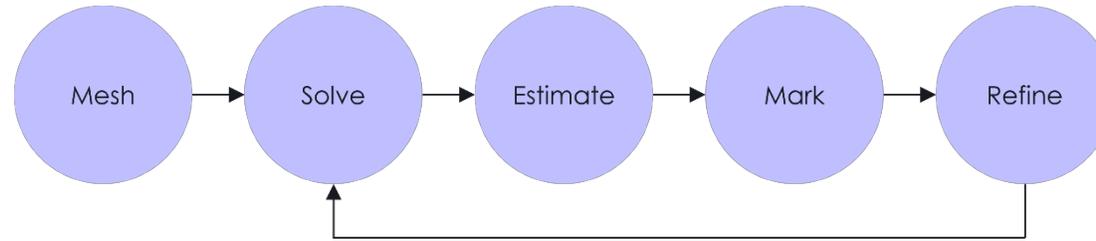
Exact solution



Approximate solution



# Classical adaptive mesh refinement



## > Solve

The FEM solves the linear system associated with the initial problem.

## > Estimate

A posteriori error estimation to define local error estimators .

## > Is there a quantum algorithm to compute the error estimators ?



# Content

## I- Context

## II- Classical adaptive mesh refinement

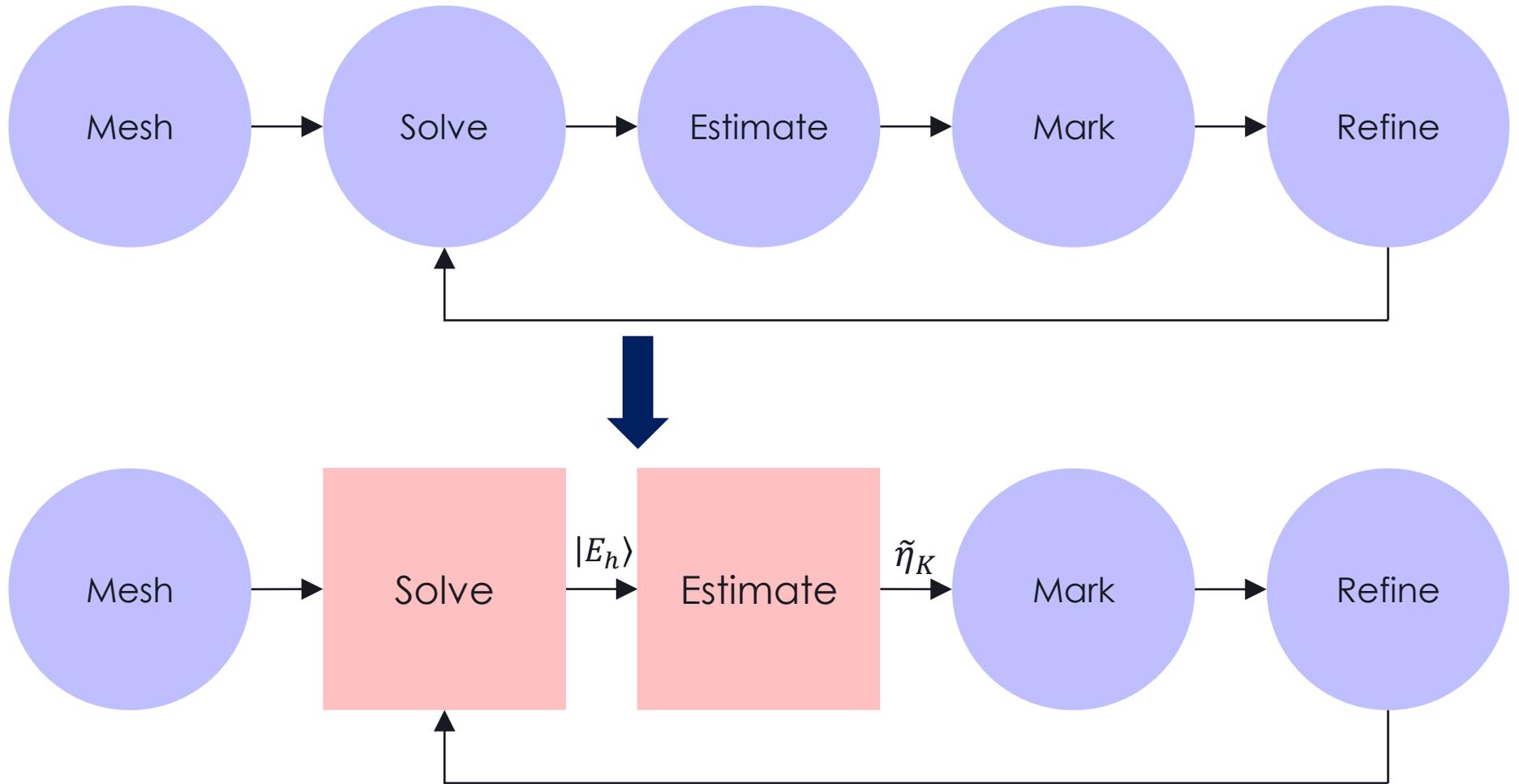
## III- Quantum algorithm for adaptive mesh refinement

### 1- Reformulation of the error estimators

### 2- How to compute these estimators?

### 3- Numerical simulations

# Adaptive mesh refinement with quantum computing



# Reformulation of the local error estimator

Assumptions: -  $k^2 \epsilon_r = \mu_r = 1$

- Efficient state preparation of  $|F\rangle := \frac{1}{\|F\|} \sum_{i=1}^N \underline{F}_i |i\rangle$

- access to  $|E_h\rangle := \frac{1}{\|E_h\|} \sum_{i=1}^N \underline{E}_{hi} |i\rangle$  using a quantum linear system solver (QLSS)

## Decomposition of $\eta_{1K}$

$$\begin{aligned} \eta_{1K}^2 &= h_K^2 \|\mathbf{F} - \nabla \times \nabla \times \mathbf{E}_h + \mathbf{E}_h\|_{(L^2(K))^3}^2 \\ &= h_K^2 \left[ \int_K \mathbf{F} \cdot \bar{\mathbf{F}} + \int_K \nabla \times \nabla \times \mathbf{E}_h \cdot \nabla \times \nabla \times \bar{\mathbf{E}}_h + \int_K \mathbf{E}_h \cdot \bar{\mathbf{E}}_h - 2\mathcal{R}(\int_K \mathbf{F} \cdot \nabla \times \nabla \times \bar{\mathbf{E}}_h) + 2\mathcal{R}(\int_K \mathbf{F} \cdot \bar{\mathbf{E}}_h) - 2\mathcal{R}(\int_K \nabla \times \nabla \times \mathbf{E}_h \cdot \bar{\mathbf{E}}_h) \right] \\ &= \underline{F}^\dagger \underline{M}_K \underline{F} + \underline{E}_h^\dagger \underline{C}_K \underline{E}_h + \underline{E}_h^\dagger \underline{M}_K \underline{E}_h - 2\mathcal{R}(\underline{F}^\dagger \underline{S}_K \underline{E}_h) + 2\mathcal{R}(\underline{F}^\dagger \underline{M}_K \underline{E}_h) - 2\mathcal{R}(\underline{E}_h^\dagger \underline{S}_K \underline{E}_h) \end{aligned}$$

With  $\underline{M}_K := (h_K^2 \int_K \boldsymbol{\phi}_i \cdot \boldsymbol{\phi}_j)_{1 \leq i, j \leq N}$ ,  $\underline{S}_K := (h_K^2 \int_K \boldsymbol{\phi}_i \cdot \nabla \times \nabla \times \boldsymbol{\phi}_j)_{1 \leq i, j \leq N}$ ,  $\underline{C}_K := (h_K^2 \int_K \nabla \times \nabla \times \boldsymbol{\phi}_i \cdot \nabla \times \nabla \times \boldsymbol{\phi}_j)_{1 \leq i, j \leq N}$ .

3 types of terms  $\underline{E}_h^\dagger \underline{W} \underline{E}_h$  (bilinear),  $\underline{E}_h^\dagger \underline{W} \underline{F}$  (linear),  $\underline{F}^\dagger \underline{W} \underline{F}$  (constant)

2 issues: matrices are **not unitary** and the FEM vectors are **not normalized**.

# Block-encoding for non-unitary matrices

**Block-encoding** [Gilyén, Su, Low, Wiebe 2019, Lin 2022]

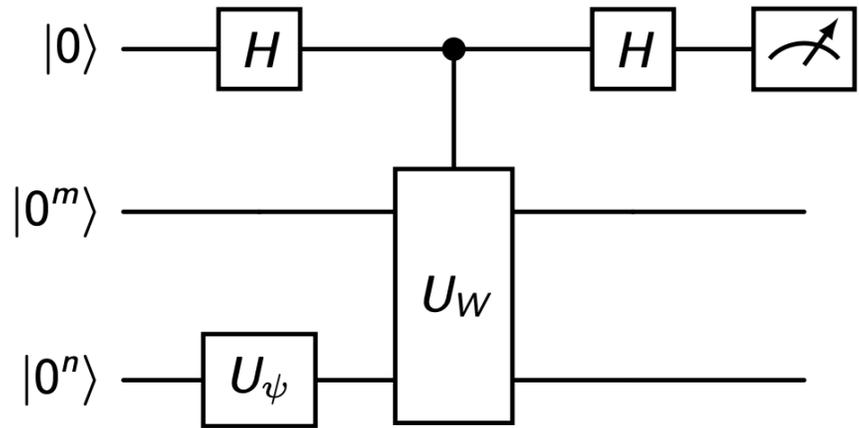
Given an  $n$ -qubit matrix  $W$ , an  $(\alpha, m, \varepsilon)$ -block-encoding of  $W$  is an  $(m + n)$ -qubit matrix  $U_W$  such that

$$\| W - \alpha(\langle 0^m | \otimes I_n) U_W (| 0^m \rangle \otimes I_n) \| \leq \varepsilon.$$

- $\alpha$  subnormalization factor
- $m$  number of ancilla qubits
- $\varepsilon$  target accuracy

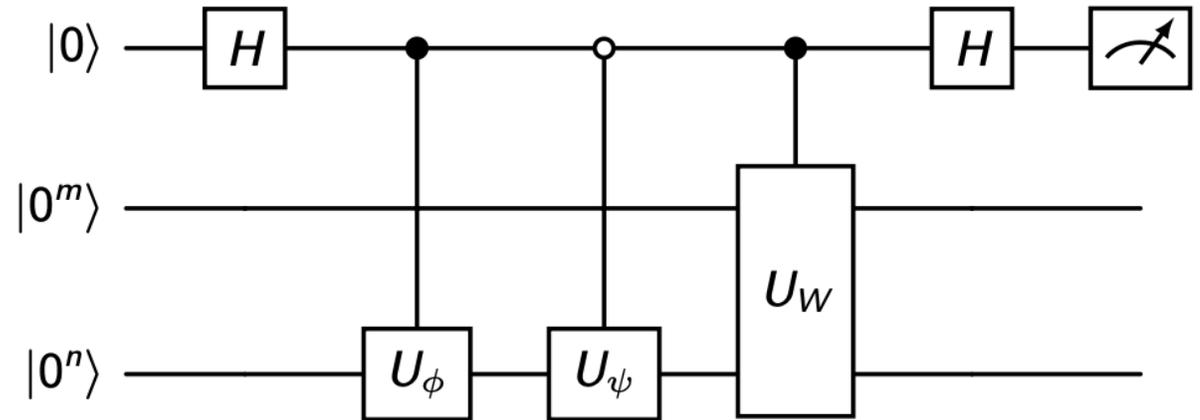
$$U_W \sim \begin{pmatrix} W & * \\ \alpha & * \\ * & * \end{pmatrix}$$

# Hadamard tests for non unitary matrices [Tong, An, Wiebe, Lin 2022]



$$\mathbb{P}(|0\rangle) = \frac{1}{2} \left( 1 + \mathcal{R} \left( \left\langle \psi \left| \frac{W}{\alpha} \right| \psi \right\rangle \right) \right)$$

For  $\frac{1}{\alpha} \mathcal{R}(\langle E_h | W | E_h \rangle)$  or  $\frac{1}{\alpha} \mathcal{R}(\langle F | W | F \rangle)$ .



$$\mathbb{P}(|0\rangle) = \frac{1}{2} \left( 1 + \mathcal{R} \left( \left\langle \phi \left| \frac{W}{\alpha} \right| \psi \right\rangle \right) \right)$$

For  $\frac{1}{\alpha} \mathcal{R}(\langle E_h | W | F \rangle)$ .

# Computation of the error estimator with quantum computing

$$\underline{E}_h^\dagger W \underline{E}_h = \frac{1}{\alpha} \mathcal{R}(\langle \underline{E}_h | W | \underline{E}_h \rangle) * || \underline{E}_h ||^2 * \alpha$$

$$\underline{E}_h^\dagger W \underline{F} = \frac{1}{\alpha} \mathcal{R}(\langle \underline{E}_h | W | \underline{F} \rangle) * || \underline{E}_h || * || \underline{F} || * \alpha$$

$$\underline{F}^\dagger W \underline{F} = \frac{1}{\alpha} \mathcal{R}(\langle \underline{F} | W | \underline{F} \rangle) * || \underline{F} ||^2 * \alpha$$

## Hadamard tests

Quantum procedure to estimate the norm of the solution [Thm 33, Chakraborty, Gilyén, Jeffery 2019, Bravo-Prieto, LaRose, Cerezo, Subaşı, Cincio, Coles 2023]

Normalization constant supposed known (depends on the norm of the matrix and the block encoding procedure)

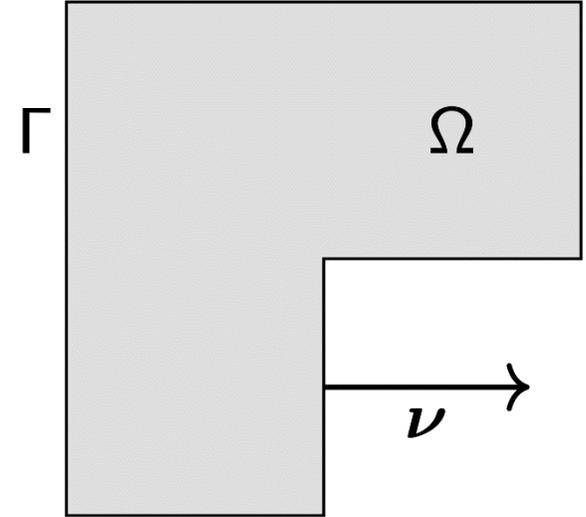
# Numerical simulations in a 2D L-shaped domain (1/2)

Test case

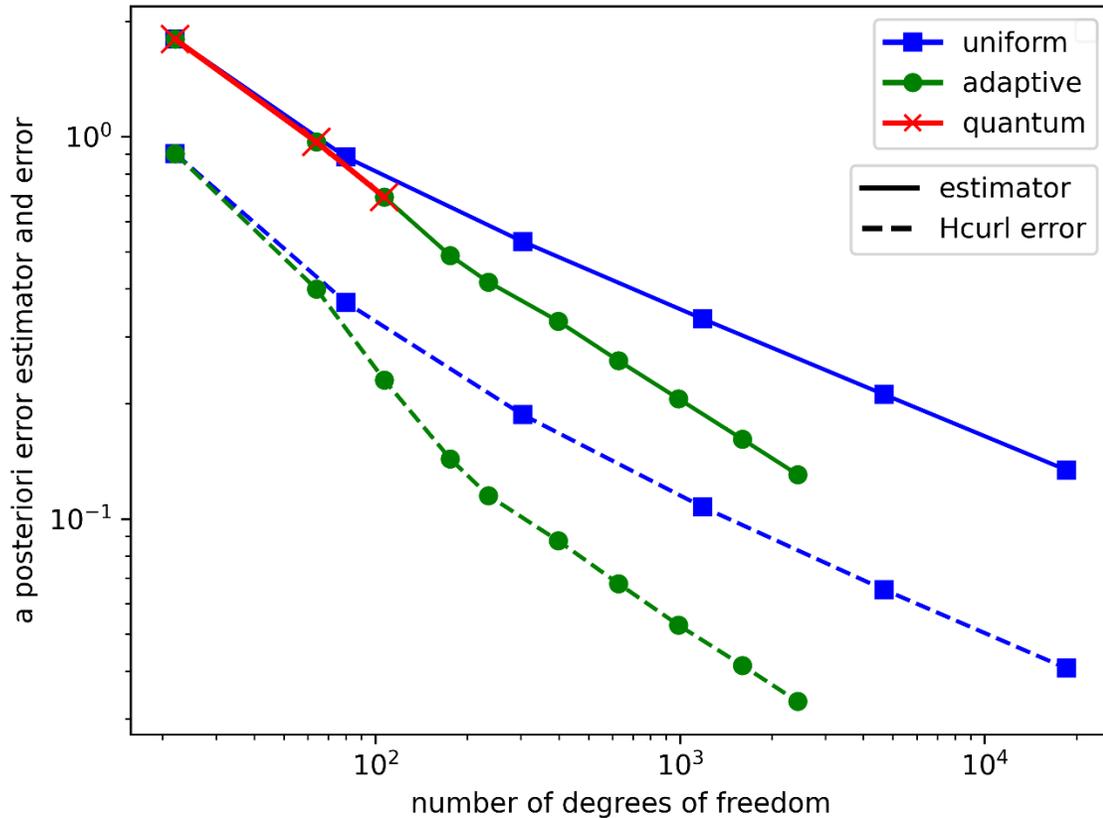
Domain  $\Omega = [-1,1]^2 \setminus [0,1] \times [-1,0]$

Exact solution  $\mathbf{E} = \nabla \left( r^{2/3} \sin \left( \frac{2\phi}{3} \right) \right)$

Python libraries: gmsh (mesh), dolfinx (FEM), PETSc (solve)  
qiskit (quantum circuits) and FABLE (block-encoding)



# Numerical simulations in a 2D L-shaped domain (2/2)



Recall

- The a posteriori error estimator is a good estimator of the  $\mathbf{H}(\text{curl})$  error.
- Adaptive mesh refinement is more efficient than uniform mesh refinement.

→ **Without sampling error**, the error estimator computed with the quantum circuits is **overlaid** with the one computed classically.

Fig:  $\mathbf{H}(\text{curl})$  error and a posteriori error estimator  $\eta$  as a function of the number of degrees of freedom  $N$ .

# Conclusion and perspectives

- We have proposed a hybrid adaptive mesh refinement algorithm.
- Simulations without sampling error validate the procedure.
- Future work: strategy to only compute a subset of the local estimators.

# Thank you!