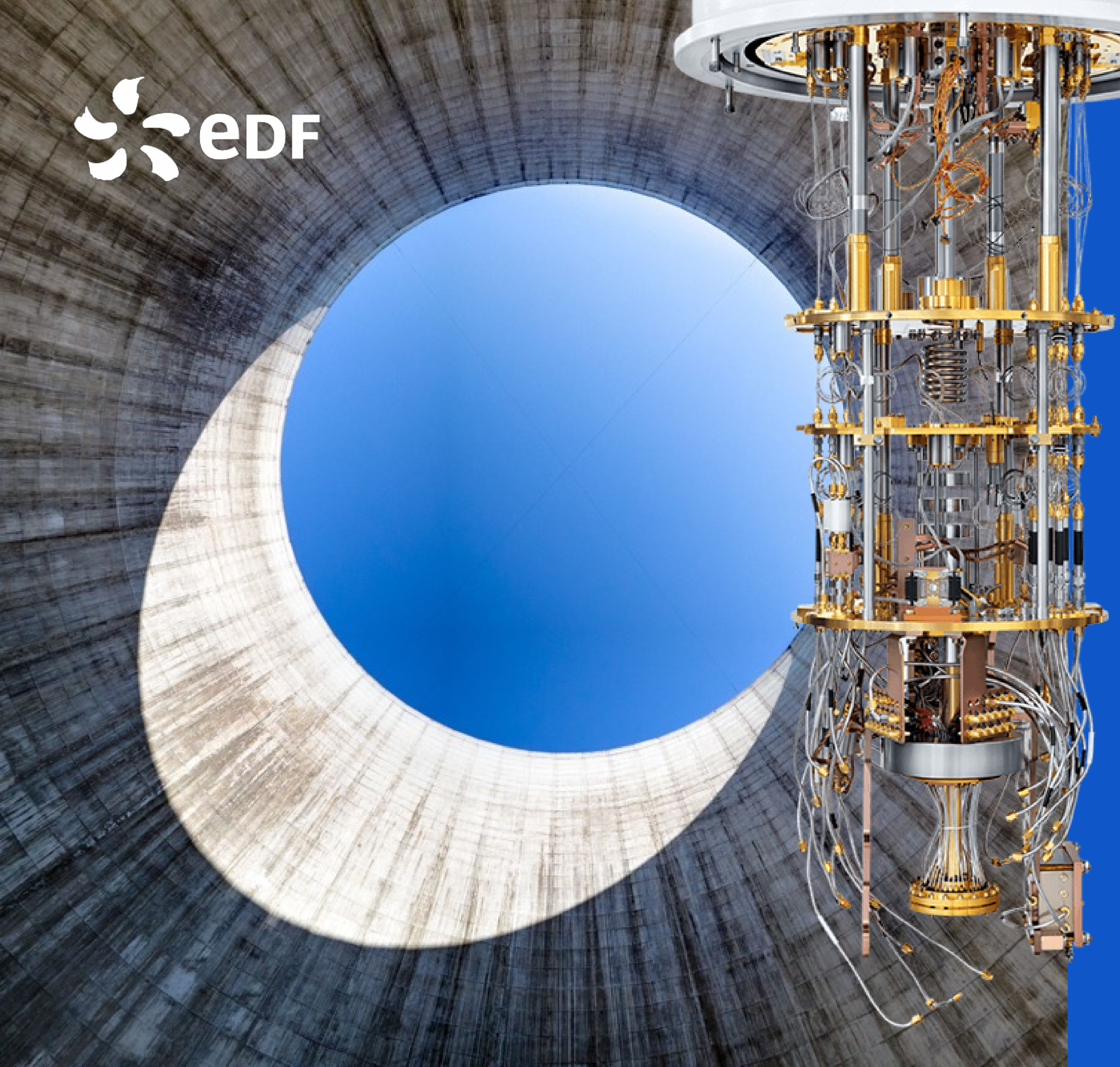
TQCI - Towards industrial applications of quantum algorithms
November 14, 2024 – EDF Lab, Saclay



Quantum Algorithms for Fracture Mechanics

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Solving PDEs

- Substantial differences in length scales within the studied systems.
- Typically involves solving sparse linear systems.
- At EDF : ~ 10^9 CPU hours each year & lots of research work in specific cases
- Goal : any speedup or reduction in power consumption.

Agenda

- **1) Classical Simulation of Fracture Mechanics**
- 2) A textbook case study : Pre-cracked plane
- 3) VQA for Fracture Mechanics
- 4) Application to thermodynamics

PDE in structural mechanics at EDF:

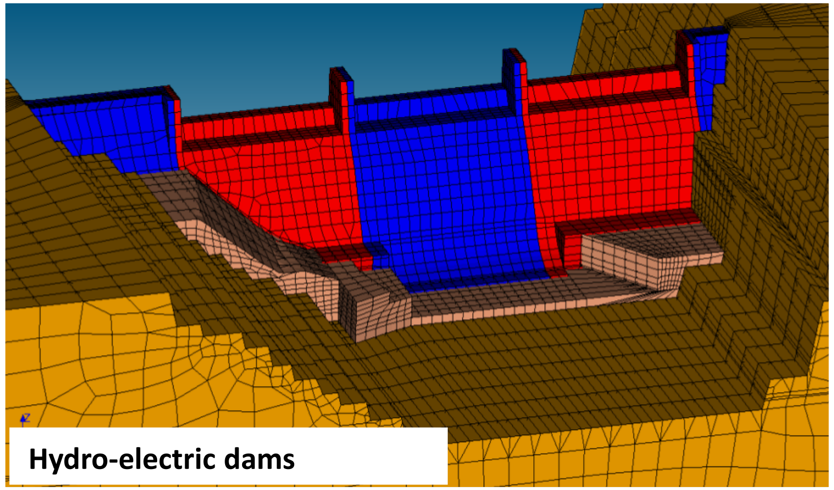
1946 EDF (Electricité de France) was created

1988 Code_Aster, finite elements software

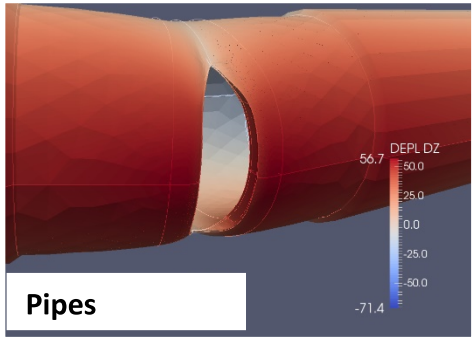
2017 First Quantum project at EDF R&D

2021 PDE with quantum algorithms

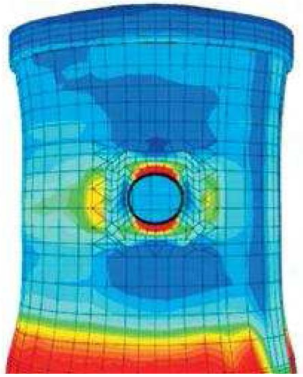
202X Quantum integration in Code_Aster



Hydro-electric dams



Pipes

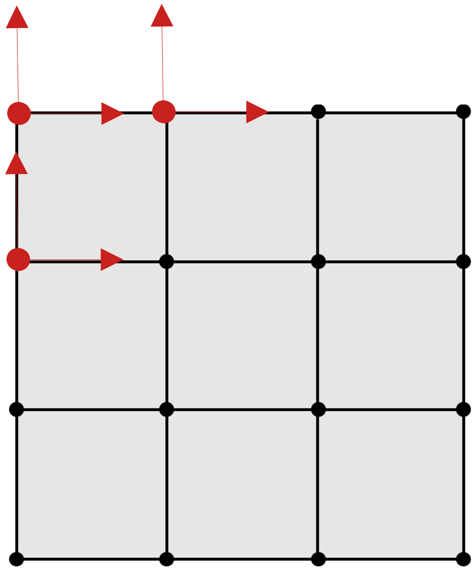


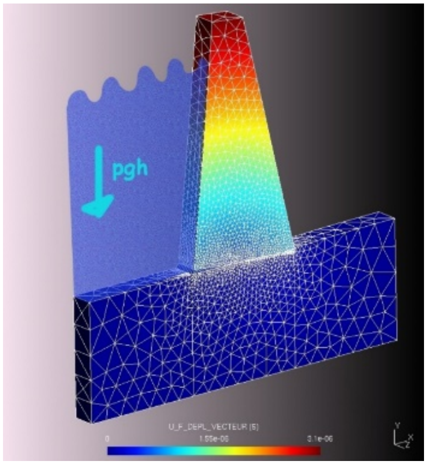
Nuclear power pl.

Fracture structural mechanics

- PDE Navier-Cauchy for linear elasticity

$$\nabla(\nabla\cdot\vec{u})+(1-2\nu)\nabla^2\vec{u}=\vec{u}$$





Fracture structural mechanics

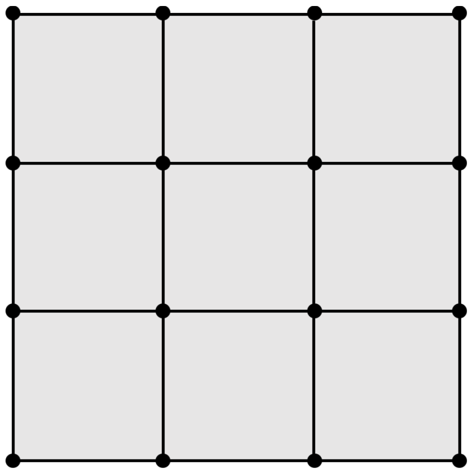
- PDE Navier-Cauchy for linear elasticity

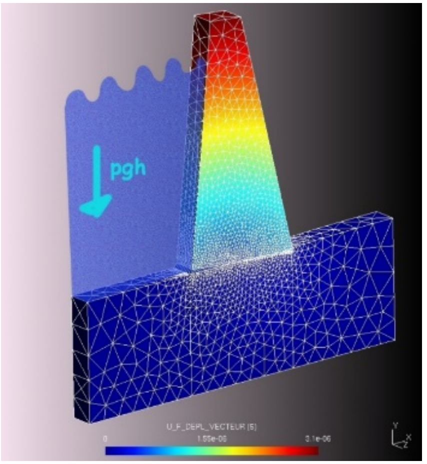
$$\nabla(\nabla \cdot \vec{u}) + (1-2\nu)\,\nabla^2 \vec{u} = \vec{u}$$

- Finite elements discretization (mesh)

$$K\,\vec{u} = \vec{f} \Leftrightarrow \min_{\vec{u}}\left(\left(\vec{u}\,K\,\vec{u}\right)/2 - \left(\vec{f}, \vec{u}\right)\right)$$

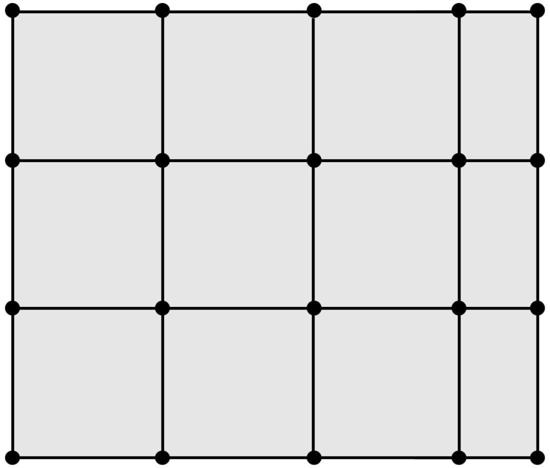
- Linear algebra problem with
  large sparse mechanical stiffness matrix

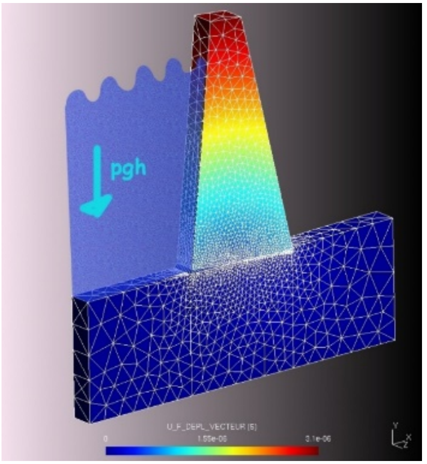




Classical Workflow

- Define a discretization
- Define spots of interest (remeshing)





- Get the entire displacements or some black-box “observable”

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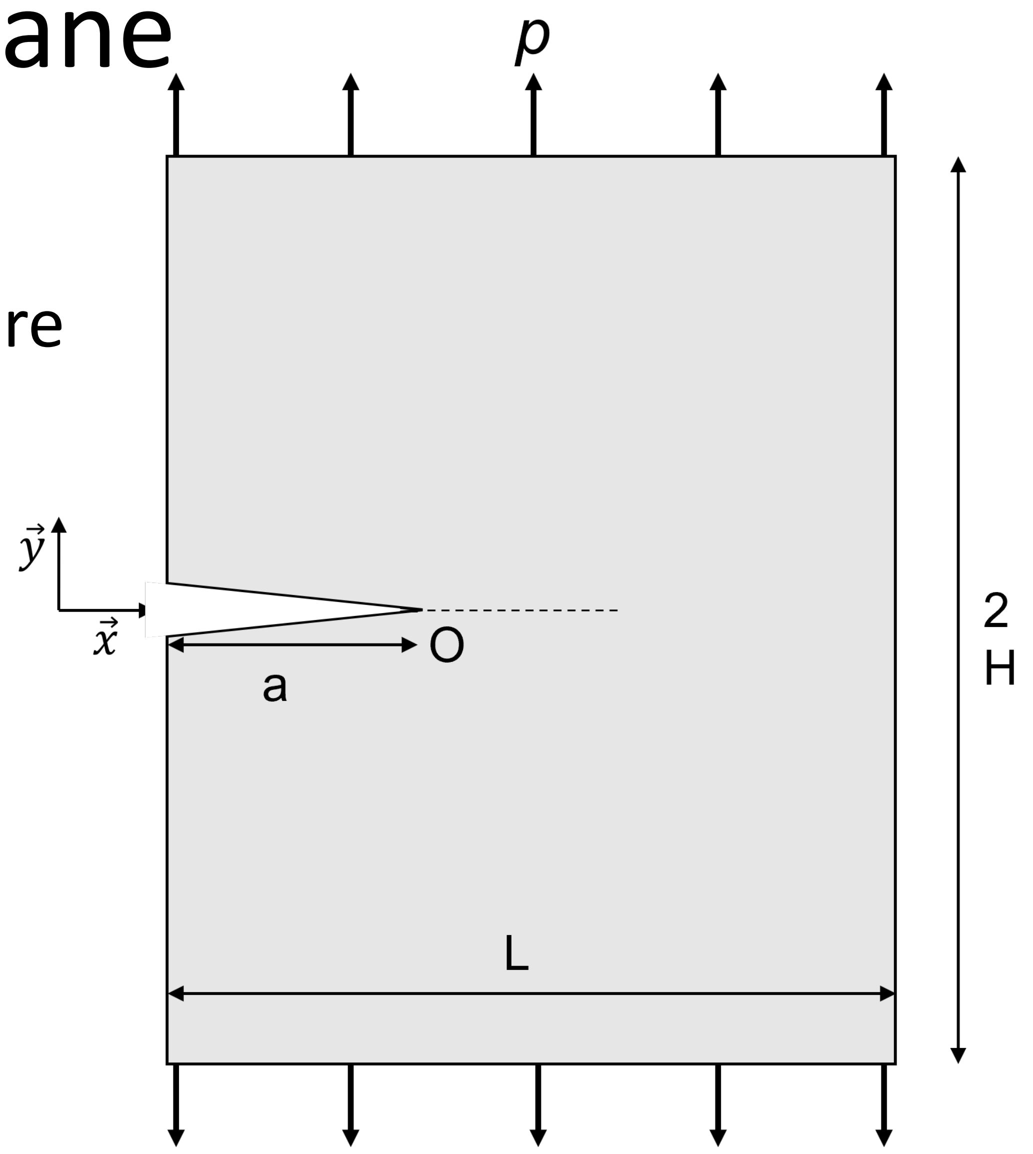
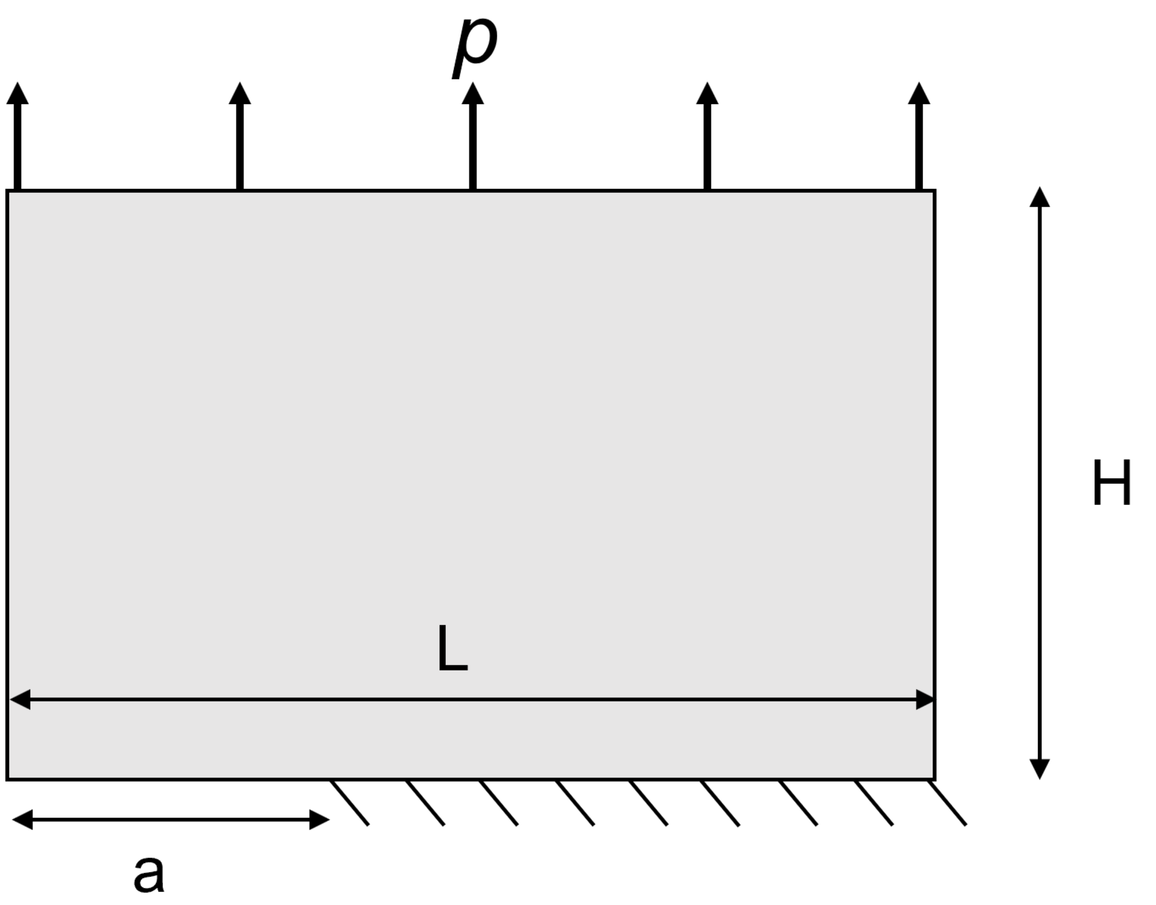
Pre-cracked plane

- A 2D plane under some sort of vertical pressure
- A crack is already present
- Useful problem using linear elasticity



Pre-cracked plane

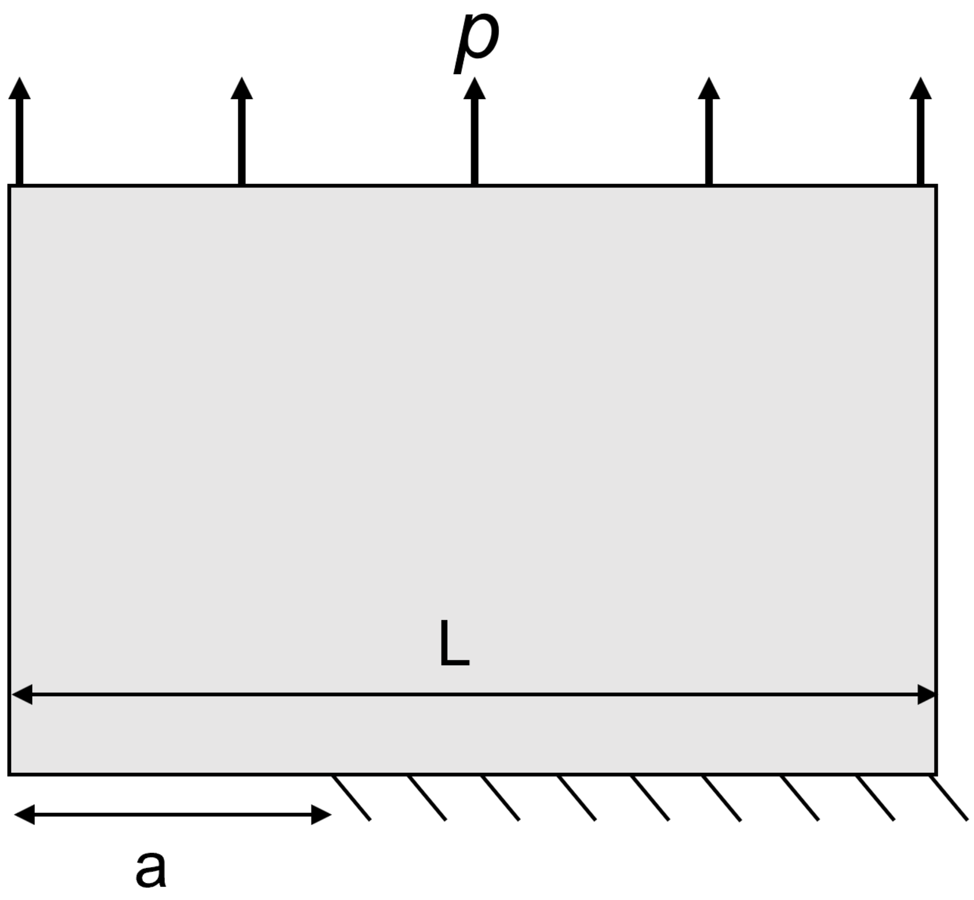
- A 2D plane under some sort of pressure
- A crack is already present
- Useful problem using linear elasticity
- Both Dirichlet and Neumann boundary conditions
- Symmetric problem



Pre-cracked plane

- K coming from the stiffness conditions
- f coming from the boundary conditions

$$K\vec{u}=\vec{f} \Leftrightarrow \min_{\vec{u}}\left(\left(\vec{u}\,K\,\vec{u}\right)/2-\left(\vec{f},\vec{u}\right)\right)$$



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Various Main Goals:

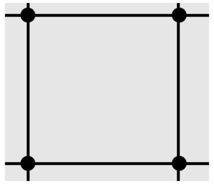
- Explore quantum advantage for solving **sparse linear systems**
- **Oracle** issue : efficient encoding of classical data into quantum system
- Identification of **observables**
- Adapt algorithms to different **boundary conditions**
- **Test-cases** relevant for EDF
- **Scaling and complexity**
- **NISQ to FTQC** transition

Any reduction in electricity consumption during these computations would offer a long-term advantage

Fracture structural mechanics

First solution : naive Qiskit HHL (2008)

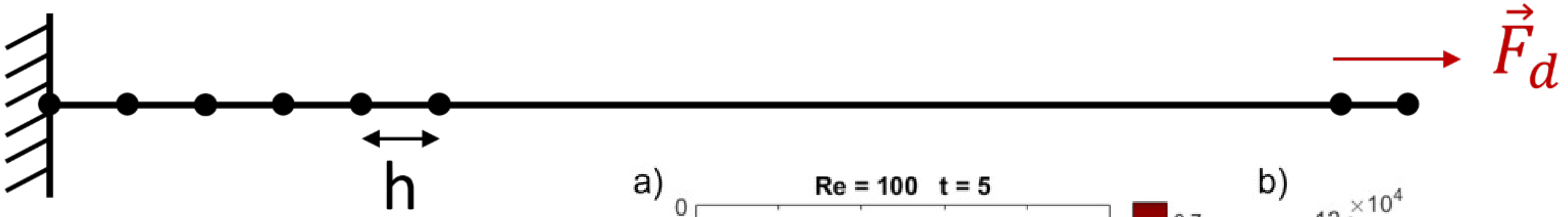
Size	2x2	4x4	8x8
CPU time, sec	0.1	1.3	184
# gates	335	5331	314 753
# qubits	5	8	11



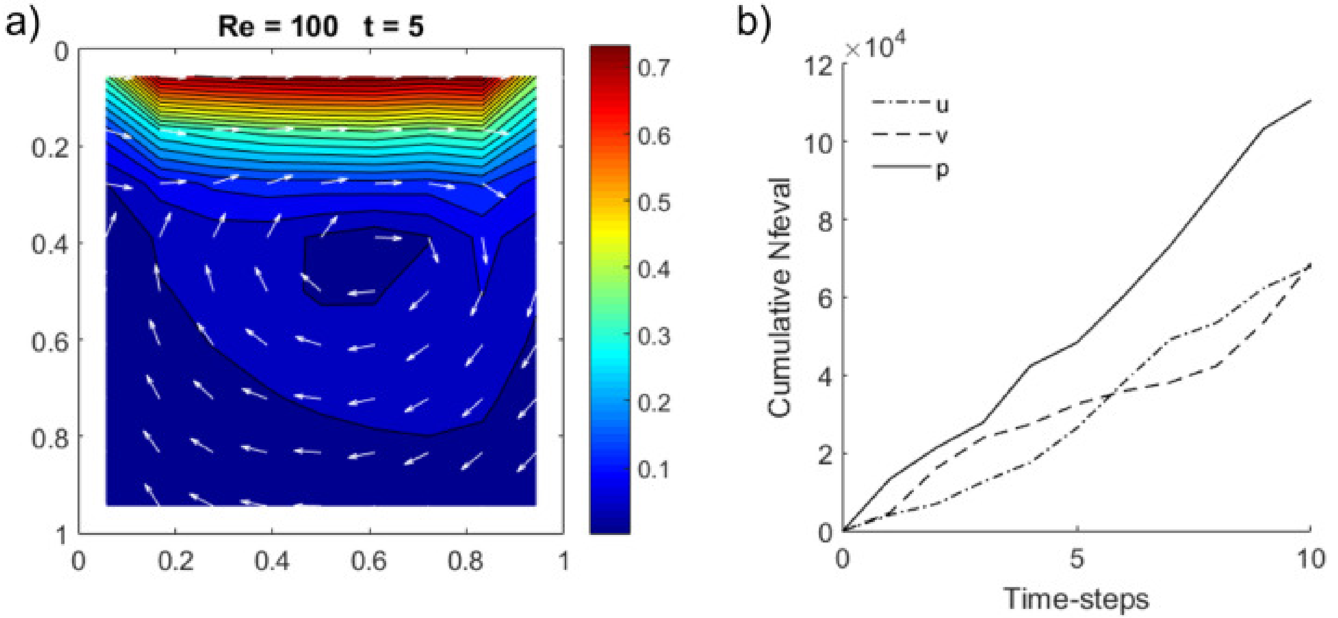
$$K\vec{u}=\vec{f} \Leftrightarrow \min_{\vec{u}}\left(\left(\vec{u}K\vec{u}\right)/2-\left(\vec{f},\vec{u}\right)\right)$$

State of the Art

- Improvements of HHL ([Childs 15], [Wossnig 17], …)
- VQA for 1D structural mechanics [Liu 20]

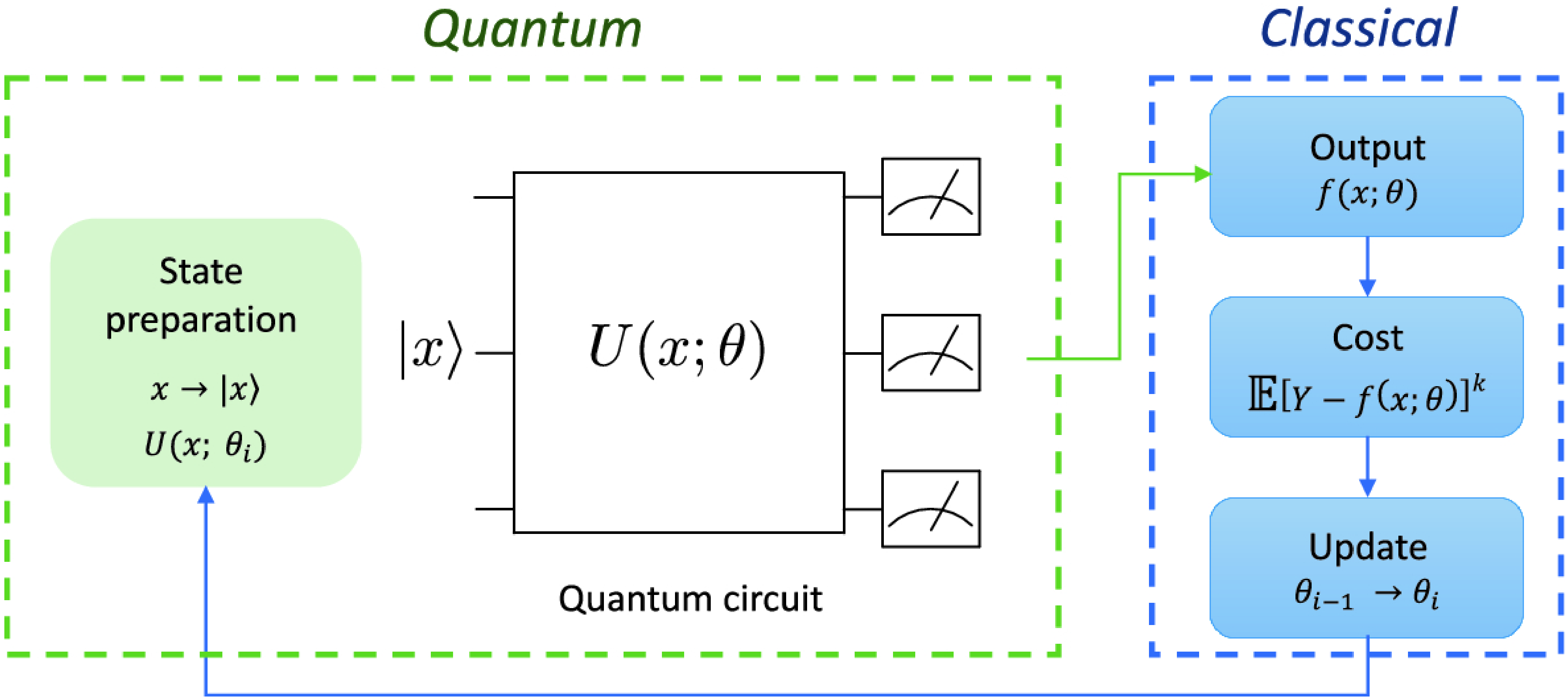


- VQA for 2D heat conduction & Incompressible Navier-Stokes [Leong 22]



VQA general scheme

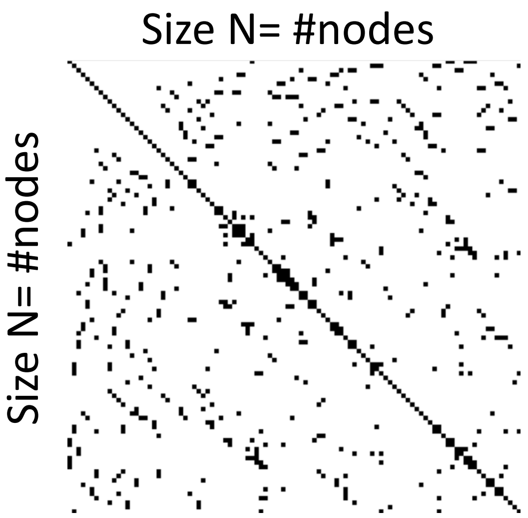
- We encode the displacements as quantum amplitudes : $|u\rangle = \Sigma a|x, y, d\rangle$
- We minimize the elastic energy obsevable to find the correct displacements.

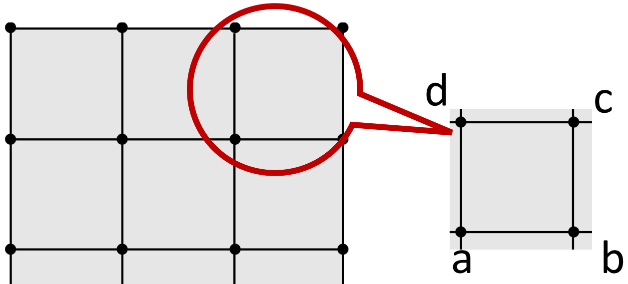


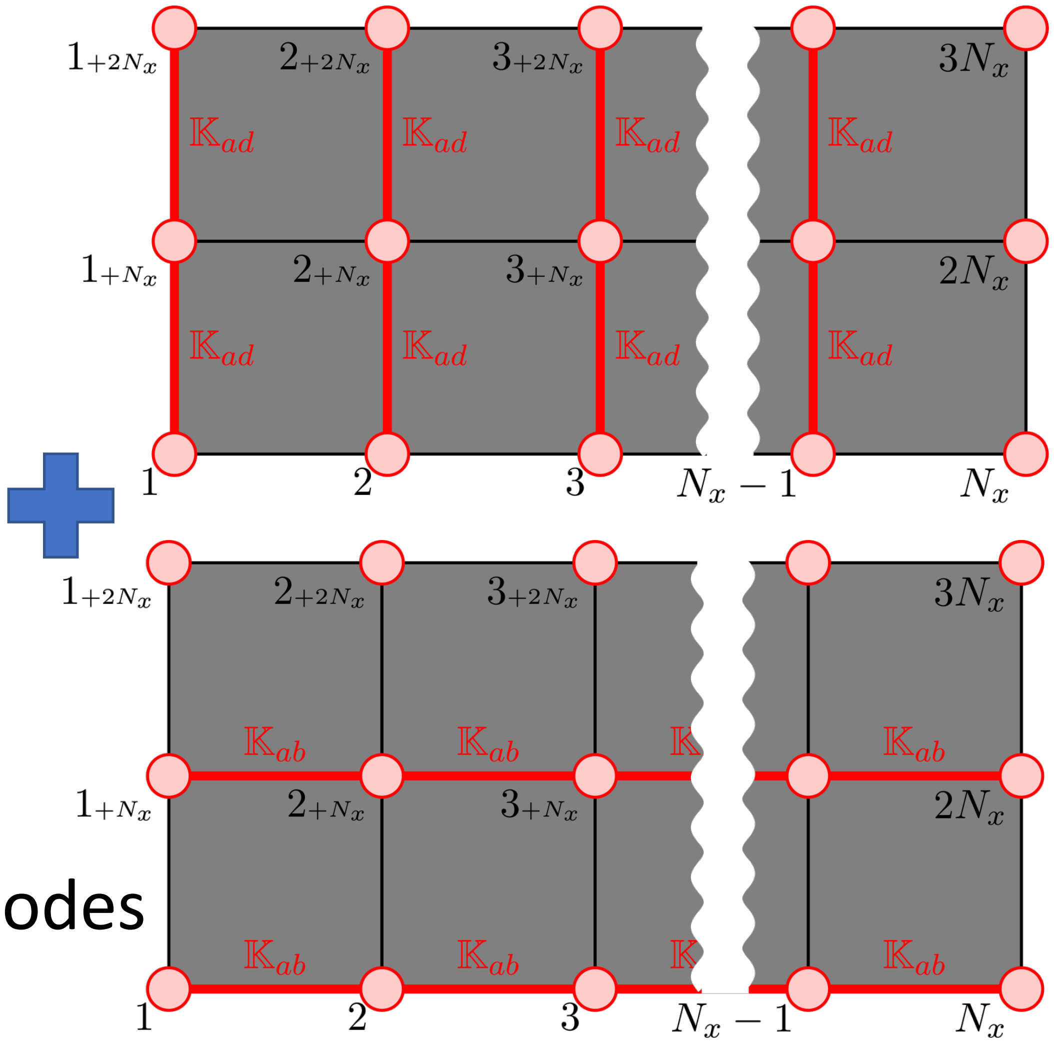
Efficient encoding of the problem

- VQA algorithm for structural mechanics

min (<u |K |u>/2 - <u|f>)





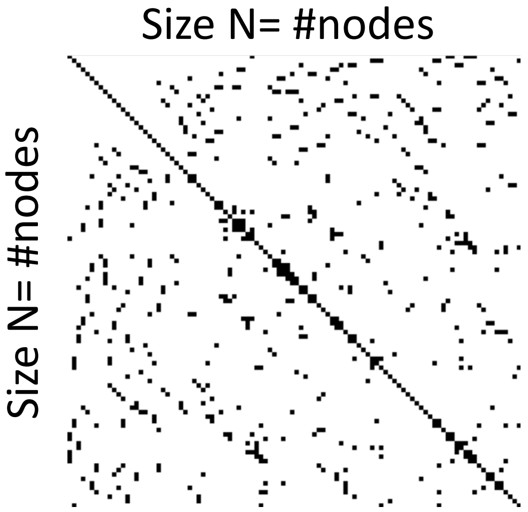


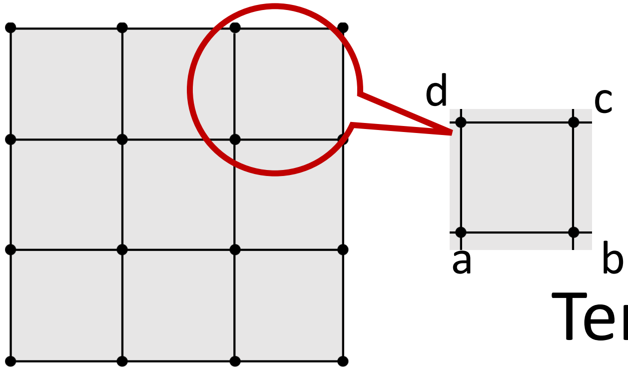
- The hermitian K encodes links between nodes

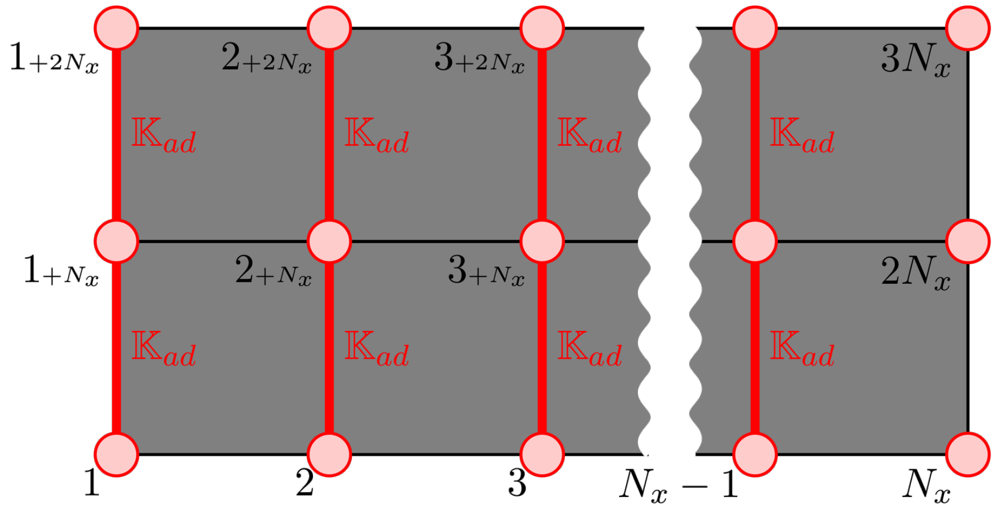
Efficient encoding of the problem

- VQA algorithm for structural mechanics

$$\min\left(\langle u|K|u\rangle/2 - \langle u|f\rangle\right)$$







Tensor product decomposition for vertical contributions :

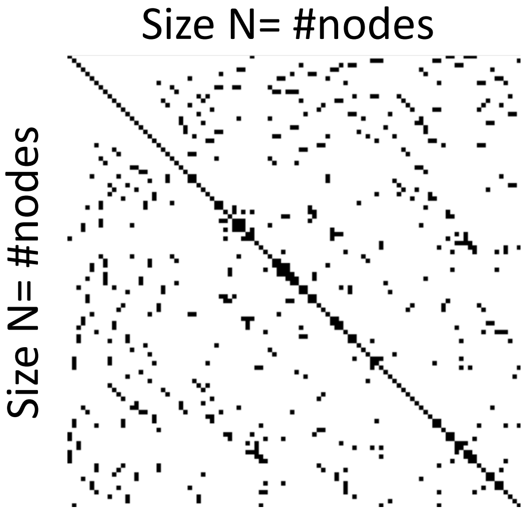
$$T_{N_y} \otimes D_{N_x} \otimes K_{ad}$$

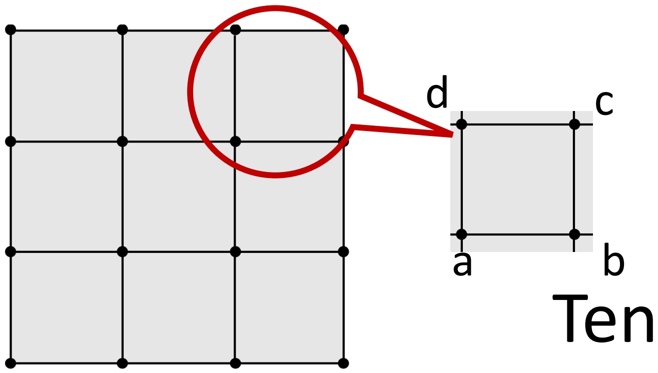
- The hermitian K encodes links between nodes

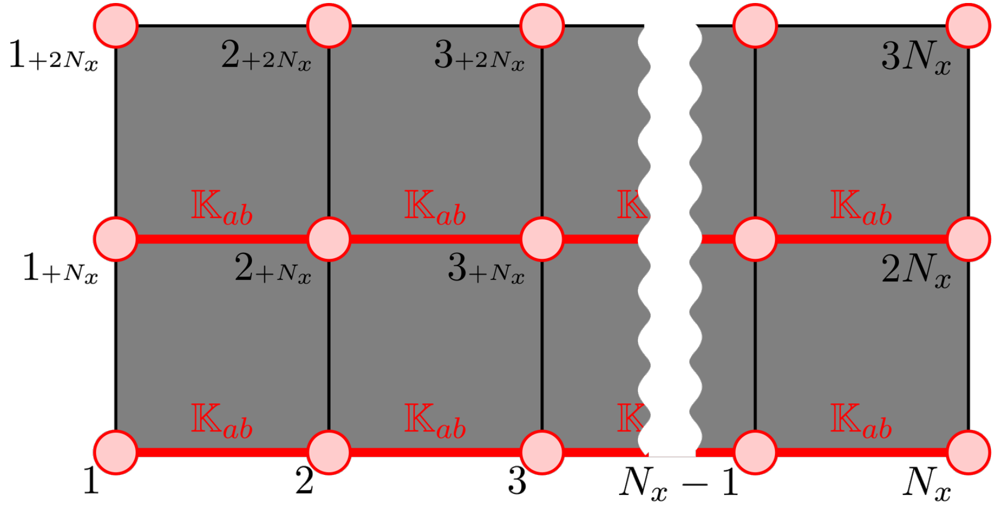
Efficient encoding of the problem

- VQA algorithm for structural mechanics

min (<u |K |u>/2 - <u|f>)







Tensor product decomposition for horizontal contributions :

$$D_{N_y} \otimes T_{N_x} \otimes K_{ab}$$

- The hermitian K encodes links between nodes

Efficient encoding of the problem

- Not decomposing into the Pauli basis, but into a larger set.
- This larger set still fits the chosen hardware.

$$\mathbb{K} = polynomial(\mathbb{G}_{2x2}) \otimes^{\log N_x \log N_y}$$

$$\mathbb{G}_{2x2} \equiv \{p_\pm; \sigma_\pm; I_2\} \qquad I_2 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

$$p_+ = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \quad p_- = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$$

$$\sigma_+ = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \quad \sigma_- = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$$

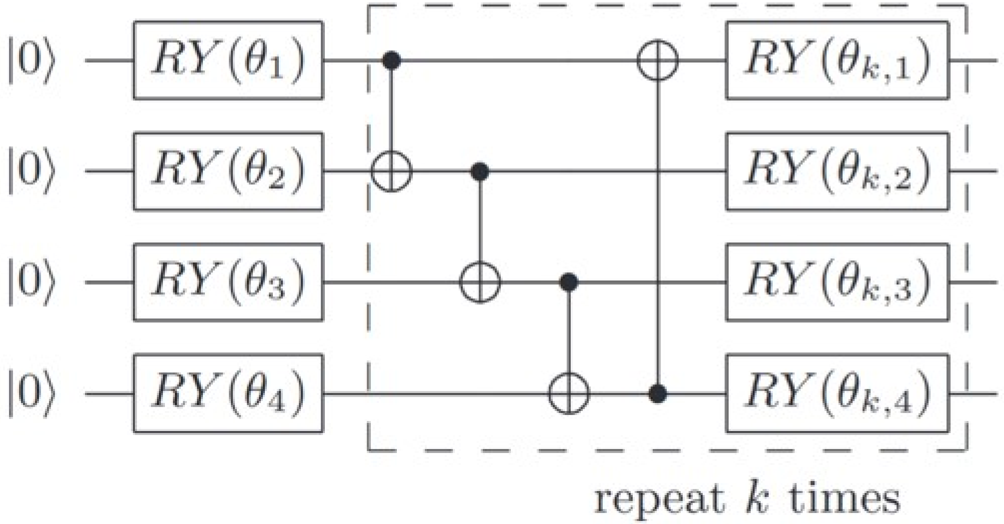
$$\mathbb{T}_{N_y} \otimes \mathbb{D}_{N_x} \otimes \mathbb{K}_{ad}$$

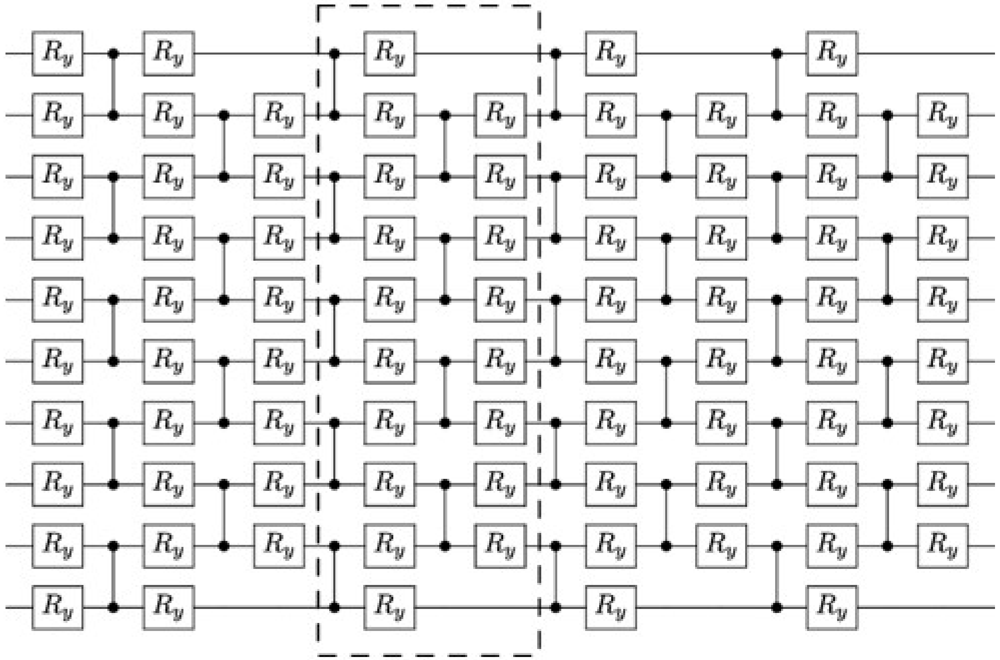
$$\mathbb{D}_{N_y} \otimes \mathbb{T}_{N_x} \otimes \mathbb{K}_{ab}$$

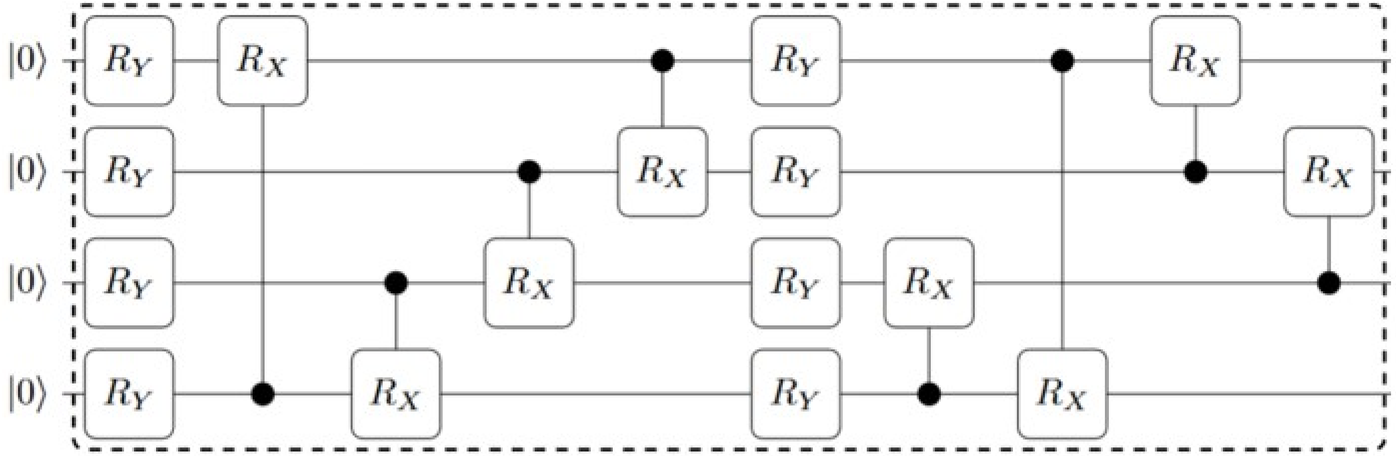
Recovering the solution

Ansätze: quantum parametrization

$$|u\rangle = U^{\otimes layer}\,|0\cdots 00\rangle$$

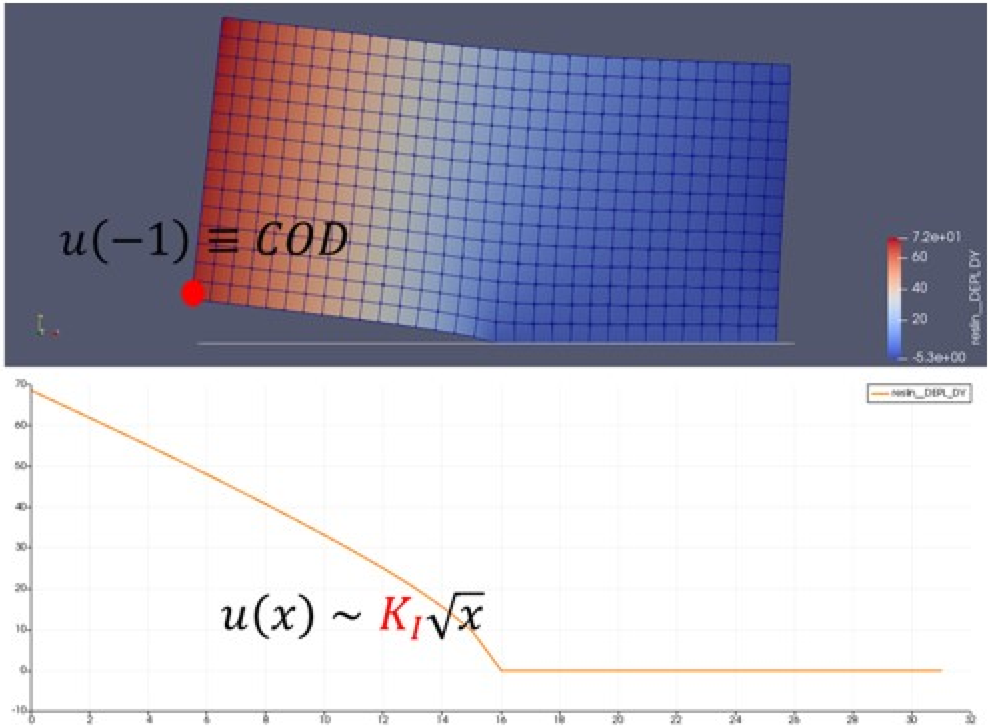


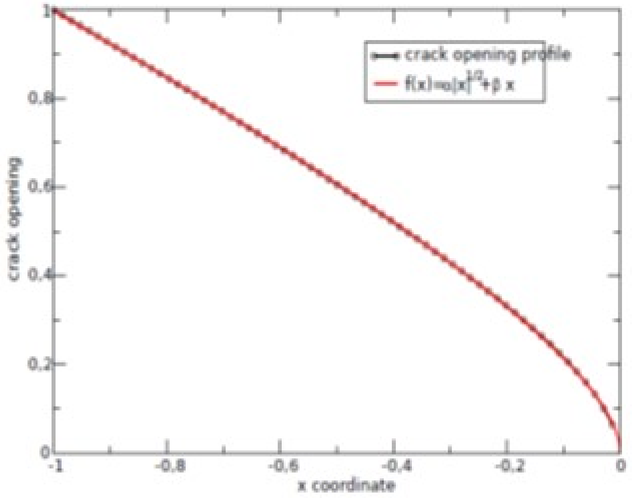




Crack propagation: relevant observables

Application for pre-cracked plate: two scalar observables

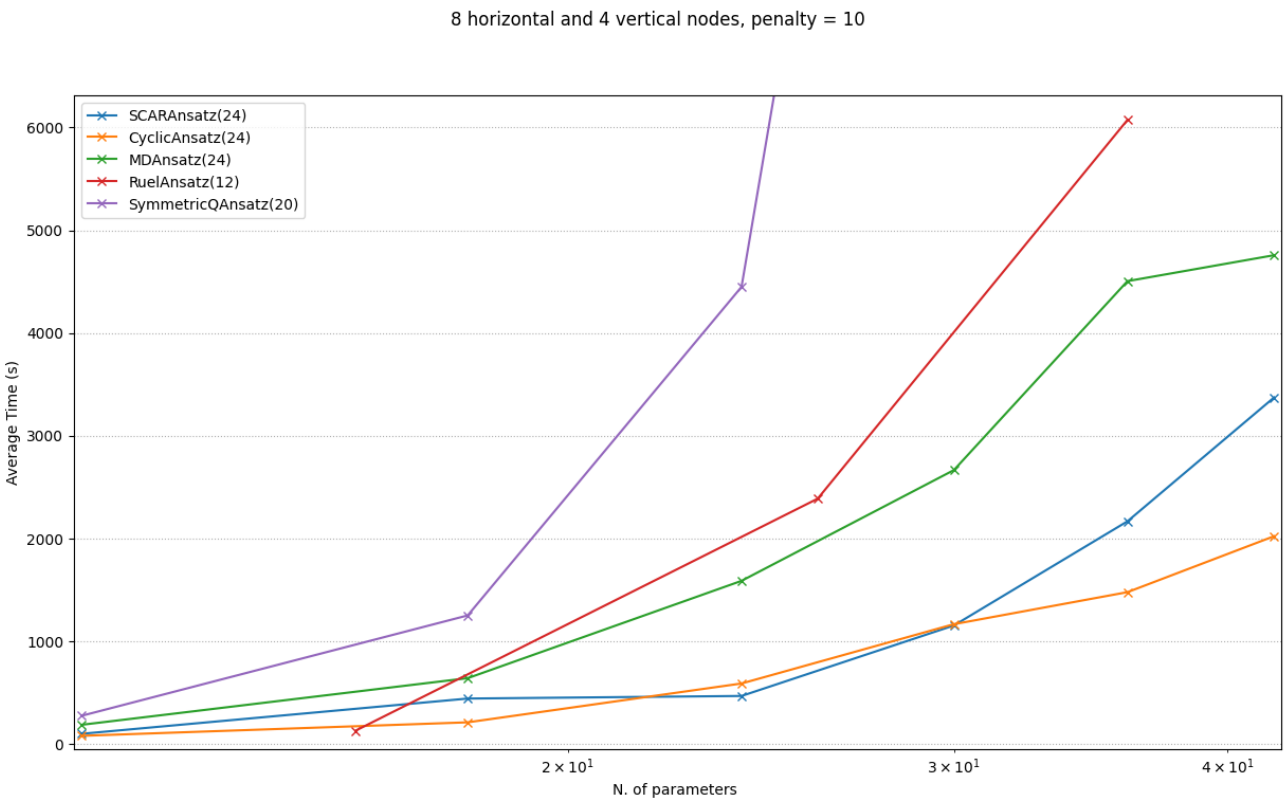


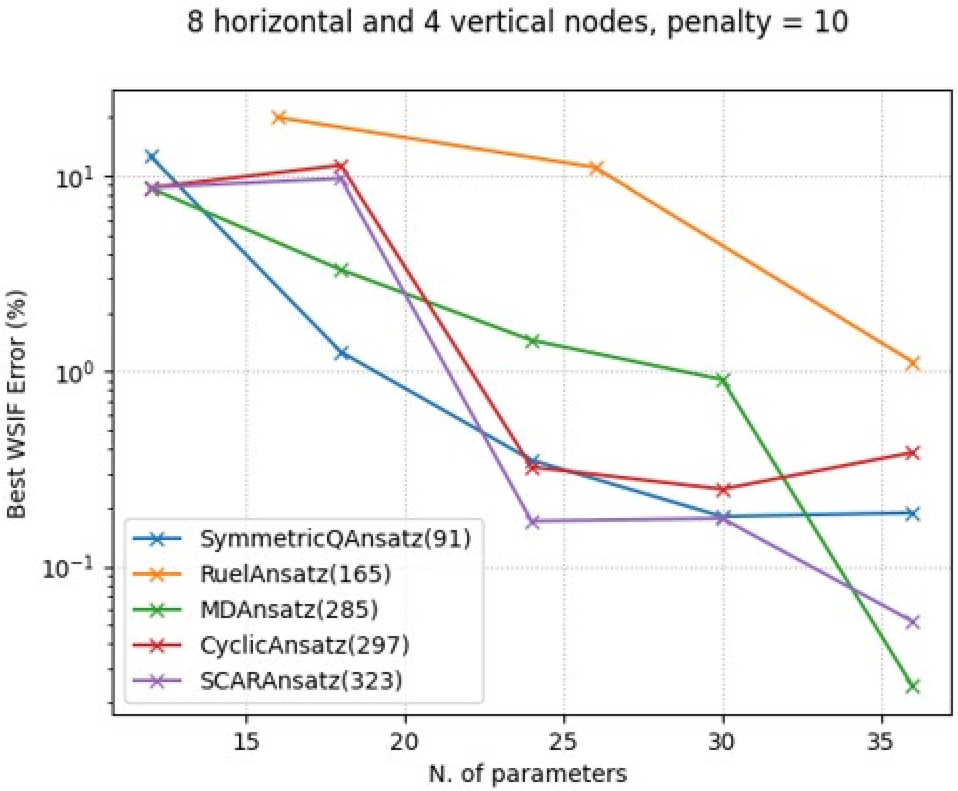


- Crack opening displacement (COD)
- Stress intensity factor K_I (SIF)

Benchmarking real Ansätze

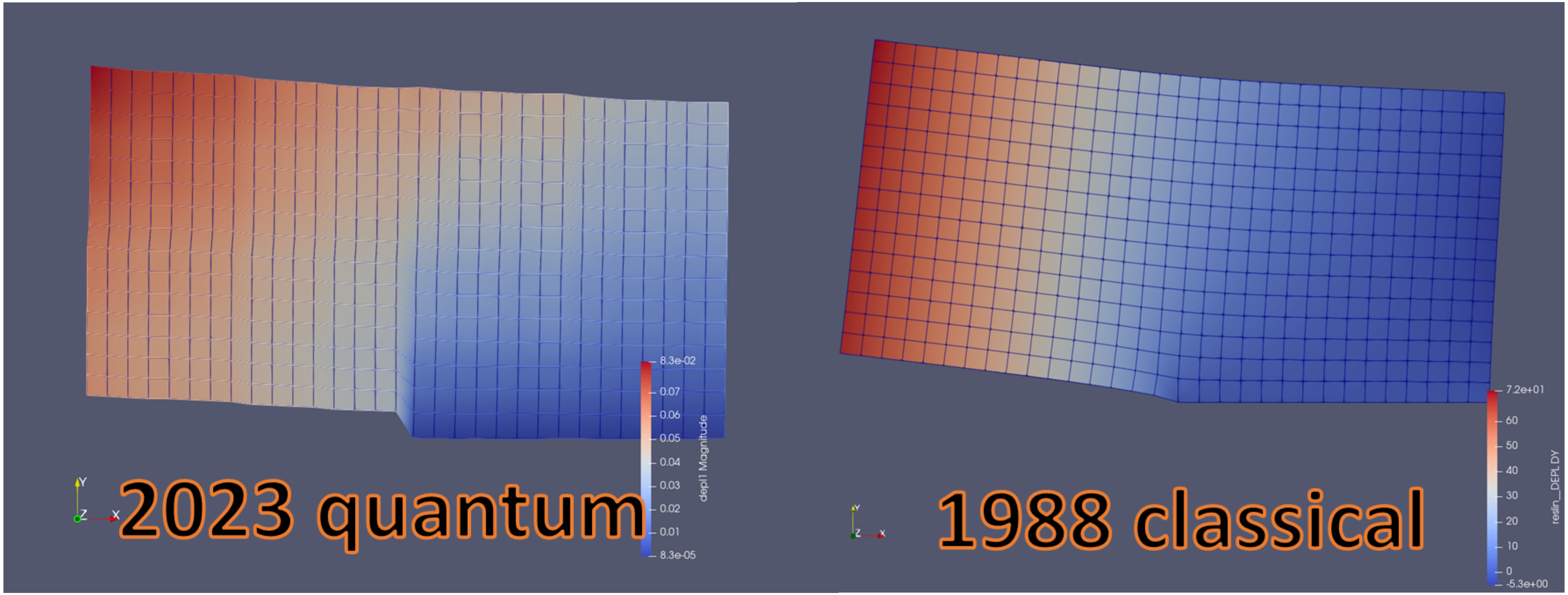
Application for pre-cracked plate: convergence of SIF observable





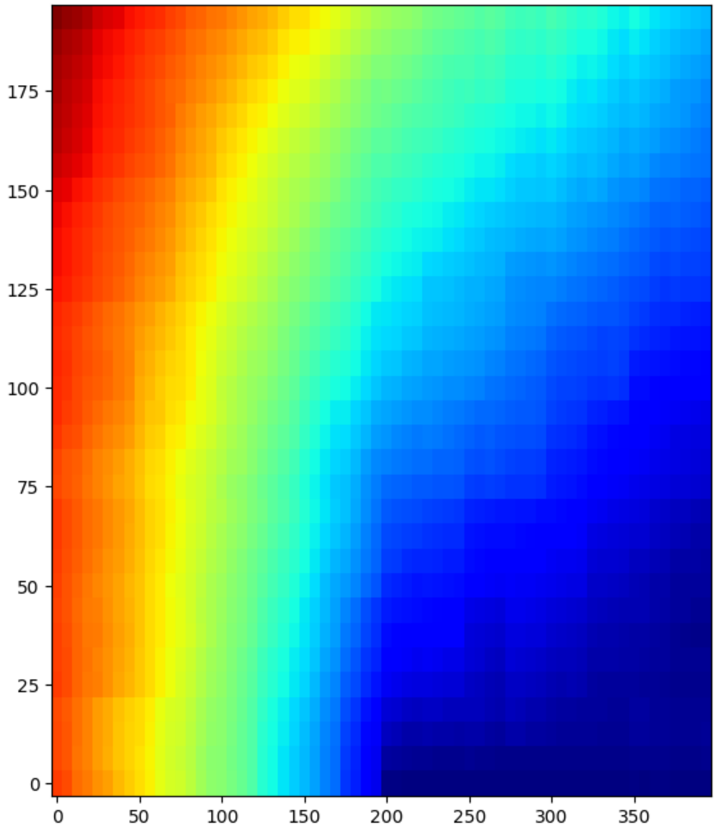
Simulations: classical versus quantum

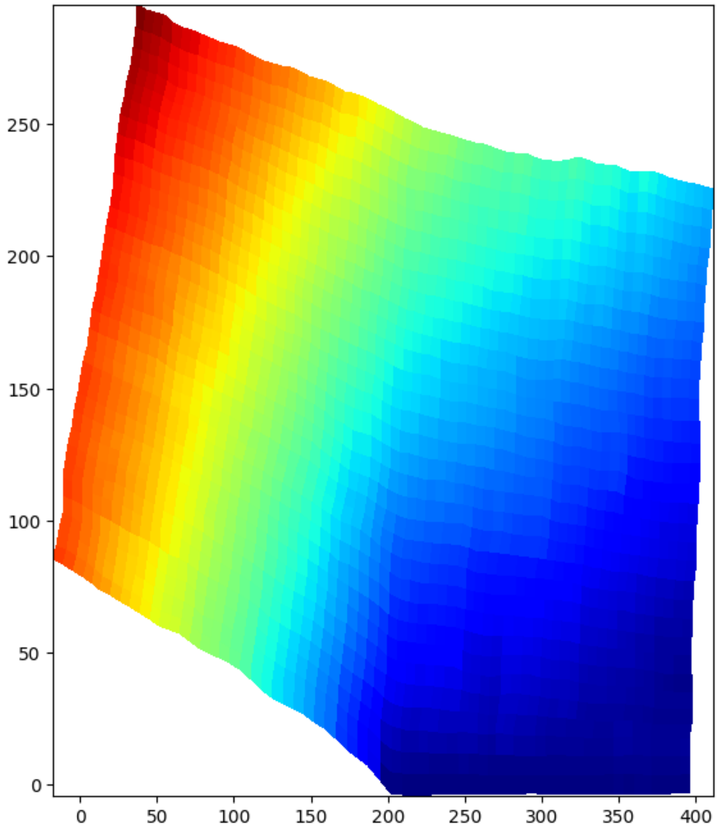
Application for pre-cracked plate: simulated quantum ‘tomography’



Simulations: classical versus quantum

Application for pre-cracked plate: simulated quantum ‘tomography’

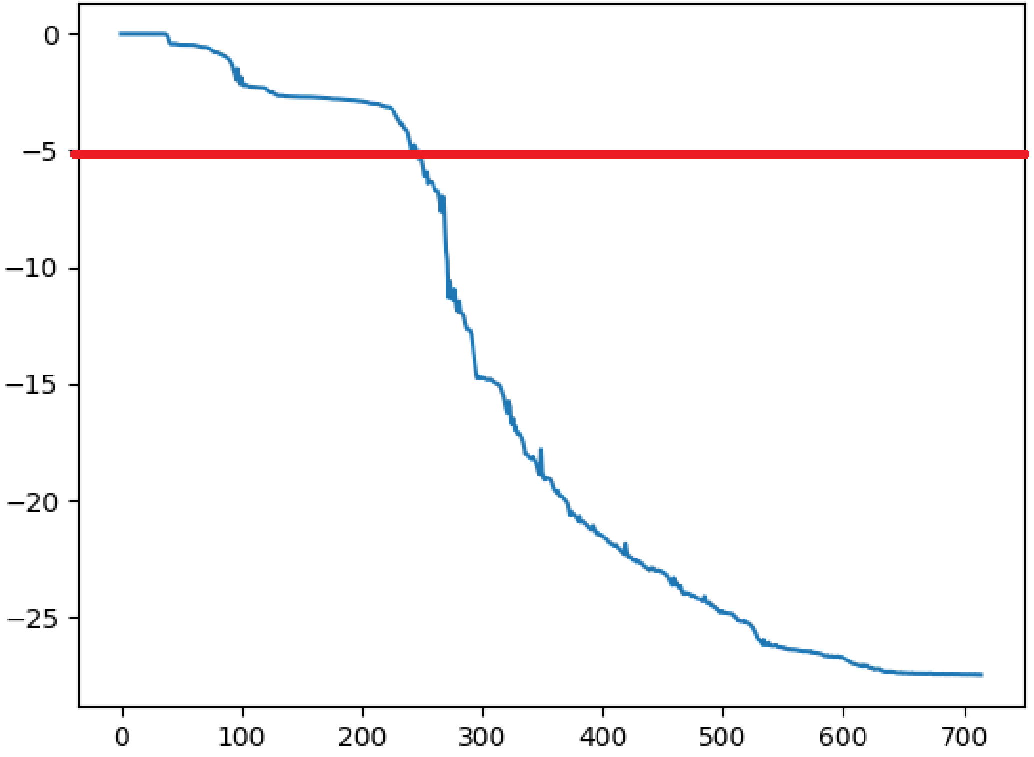




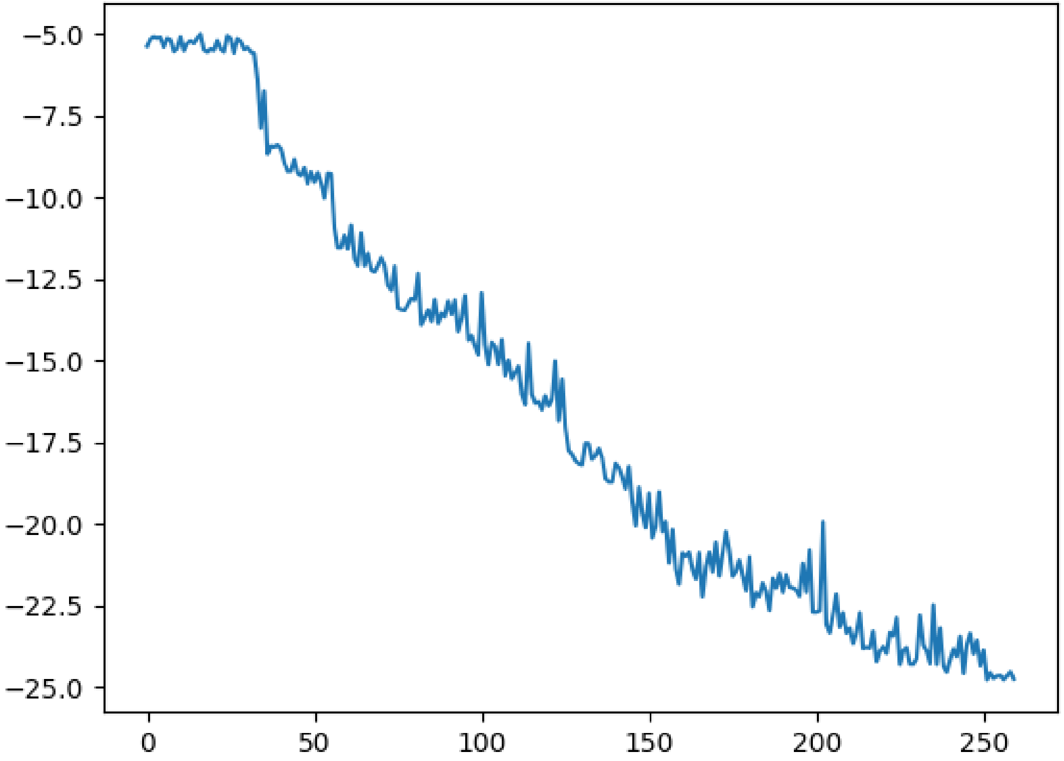
Quantum Simulations

Example for 4 qubits :

Noiseless gradient descent



Noisy gradient descent



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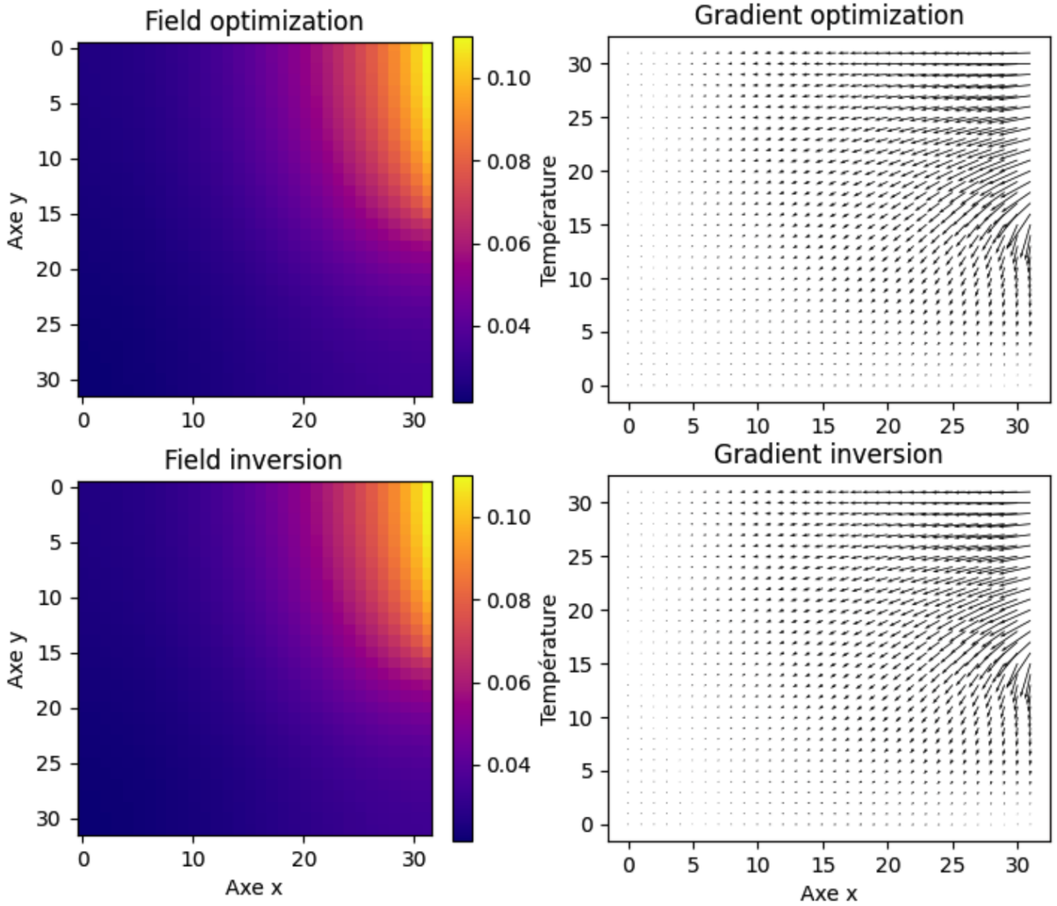
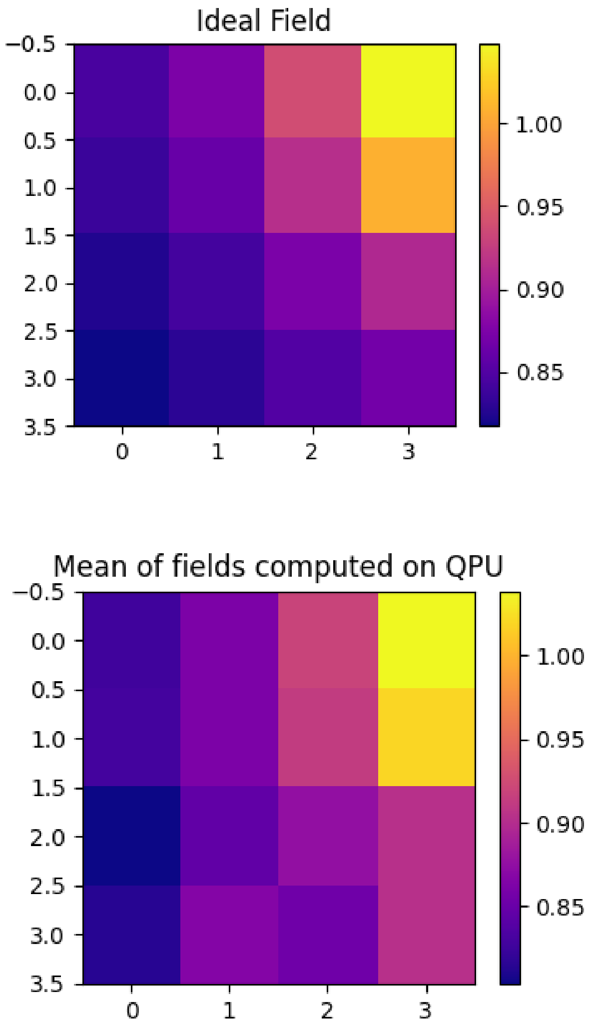
Application to thermodynamics

- Application on QPU and large-scale simulations





Further improvements & applications

- Analyzing noise effects and hardware dependency
- Hardware-efficient 2D heat conduction
- Demonstration and formalization of quantum advantage
- Complex 2D geometries (block-wise)
- 3D case, polar case, more complex FEM geometries
- Find a mechanical case corresponding to a HHL implementation

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Thanks for listening !