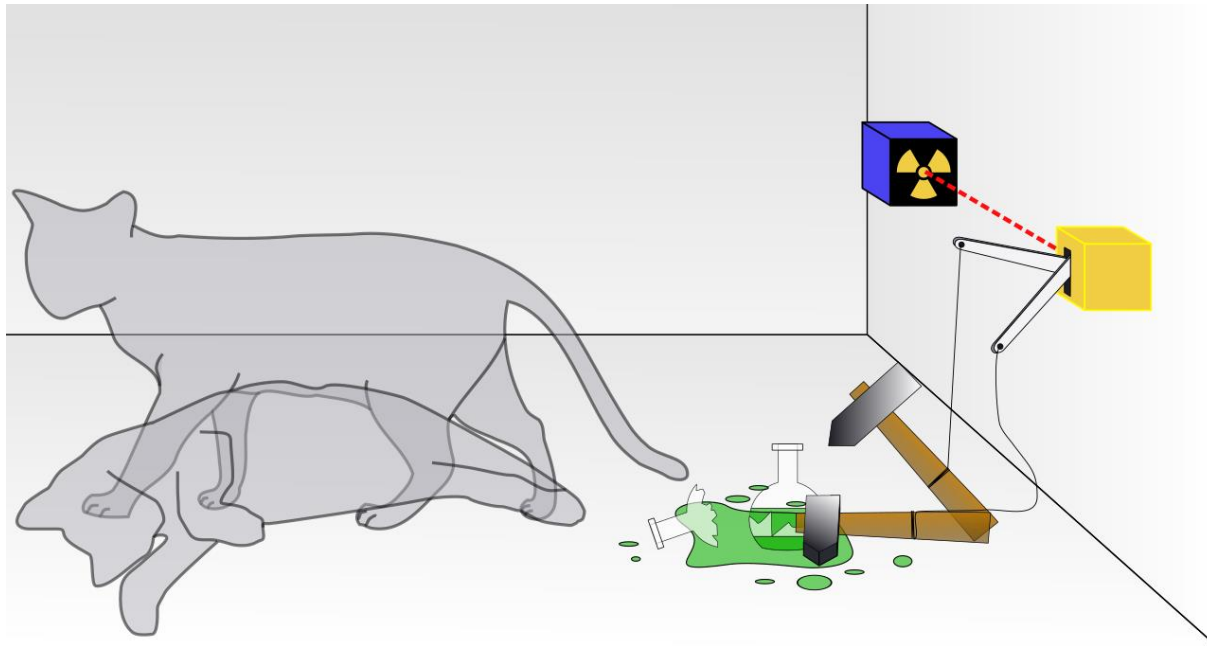




Resolution of elasto-plastic finite-elements problems by quantum annealing

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“On June 7, 2024, the United Nations proclaimed 2025 as the International Year of Quantum Science and Technology (IYQ)” [Indeed Quantum Science and Technology] “will be a key cross-cutting scientific field of the 21st century, having a tremendous impact on critical societal challenges highlighted by the U.N.'s 2030 Sustainable Development Goals, including climate, energy, food safety and security, and clean water”.

<https://quantum2025.org/en/>

Introduction to Quantum Computing

- Bits vs. Qubits:

- Superposition of states:

- A quantum bit can be 0 or 1 at the same time

- State vector of a qubit

- Computational basis $|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ & $|1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$

- Notations:
$$\begin{cases} |\phi\rangle = \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \alpha|0\rangle + \beta|1\rangle \\ \langle\phi| = (\alpha^* \quad \beta^*) \end{cases} \quad |\alpha|^2 + |\beta|^2 = 1$$

- Qubit represented on the surface of the Bloch Sphere

$$|\phi\rangle = e^{i\delta} \left(\cos\left(\frac{\theta}{2}\right) |0\rangle + e^{i\varphi} \sin\left(\frac{\theta}{2}\right) |1\rangle \right)$$

- Global phase $e^{i\delta}$ has no observable consequence
(NB relative phase has consequence)

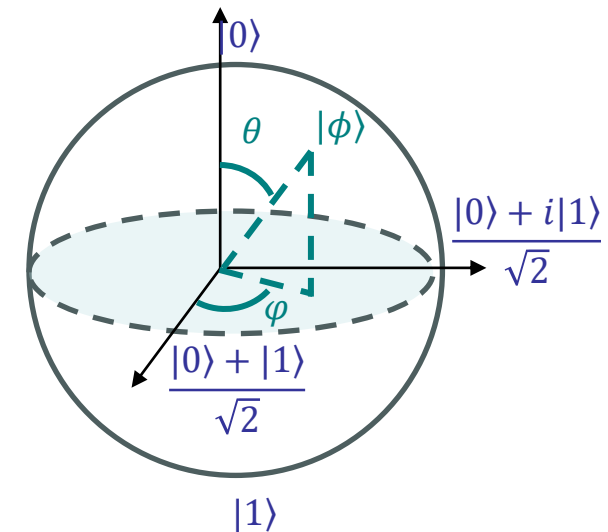
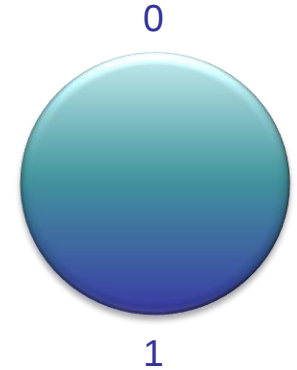
- At measurement (in the computational basis)

- Either $|0\rangle$ or $|1\rangle$ with respective probability $|\alpha|^2$ and $|\beta|^2$

Bit



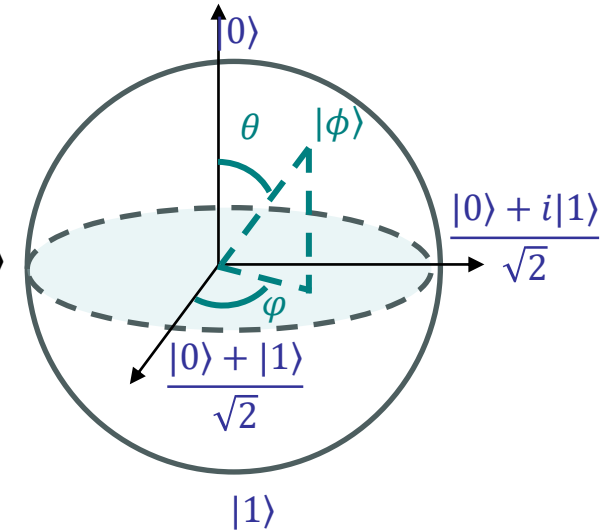
Qubit



- Multiple (connected) qubits:

- Product state of 2 1-qubit states:

$$\begin{cases} |\phi_0\rangle = \alpha_0|0\rangle + \beta_0|1\rangle \\ |\phi_1\rangle = \alpha_1|0\rangle + \beta_1|1\rangle \end{cases}$$



➡ $|\phi\rangle = |\phi_0\rangle \otimes |\phi_1\rangle = \alpha_0\alpha_1|00\rangle + \alpha_0\beta_1|01\rangle + \alpha_1\beta_0|10\rangle + \beta_0\beta_1|11\rangle$

- Most general 2-qubit state

$$|\phi\rangle = \alpha_{00}|00\rangle + \alpha_{01}|01\rangle + \alpha_{10}|10\rangle + \alpha_{11}|11\rangle$$

➡ Because of entanglement, a K -qubit state is more general
(it cannot always be written as the product of K 1-qubit states)

➡ There is not always K equivalent 1-qubit states to a K -qubit state, e.g.

$$|\phi\rangle = \frac{1}{\sqrt{2}}|00\rangle + 0|01\rangle + 0|10\rangle + \frac{1}{\sqrt{2}}|11\rangle$$

- A system of K coupled qubits

- Is a 2^K -state quantum-mechanical system
- Whose state can be represented by any normalised linear combination of 2^K basis states:

$$|\phi\rangle = \phi_0|0\rangle \otimes |0\rangle \dots \otimes |0\rangle + \phi_1|0\rangle \otimes |0\rangle \dots \otimes |1\rangle + \dots + \phi_{2^K-1}|1\rangle \dots \otimes |1\rangle \otimes |1\rangle$$

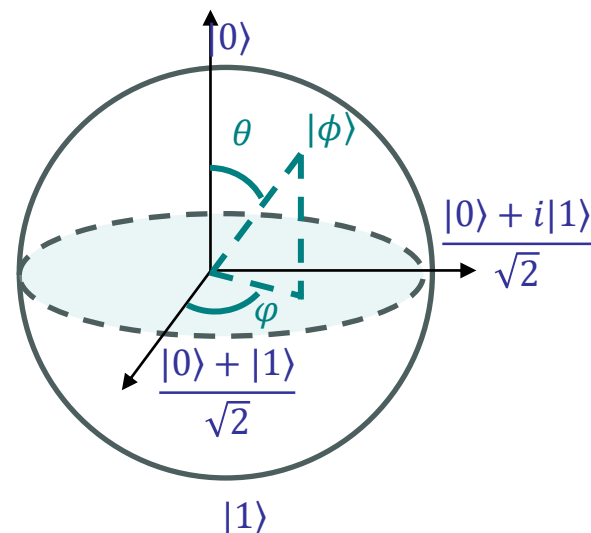
with $\sum_{i=0}^{2^K-1} |\phi_i|^2 = 1$



Because of superposition, potentially, a quantum computer with K qubits can take 2^K bitstrings of size K in parallel at the same time. A classical computer can only take 1 bitstring of size K

- Quantum computers:

- Trapped-ion quantum computer
 - Suspended ions in electromagnetic field
 - Ground state and excited states
 - Interactions controlled by laser
 - E.g. IonQ & Quantinuum
- Photonic quantum computers
 - State corresponds to direction of photon travel
- Superconducting quantum computers
 - Superconducting qubits as artificial atoms (ground state and excited state)
 - Superconducting capacitors and inductors are used to produce a resonant circuit
 - Operate at temperature of 10 mK
 - Qubit state controlled by external microwave signals
 - IBM, D-Wave
- Different platforms (2 different resolution methodologies)
 - IBM
 - 2022: 433-qubit Osprey'
 - 2023: 1121-qubit Condor
 - D-Wave
 - 5000+-qubit Advantage (35000 couplers)
 - Each qubit is only connected to a reduced number of other qubits



- Universal gate

- Gate on 1 qubit

- E.g. Hadamard $\mathbf{H}^d = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$ $|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ $|1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$


 $|0\rangle \xrightarrow{\mathbf{H}^d} \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$
 $|1\rangle \xrightarrow{\mathbf{H}^d} \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)$

- Gate on 2 qubits

- NB: $|01\rangle: \begin{pmatrix} 1 & \cdot \begin{pmatrix} 0 \\ 1 \end{pmatrix} \\ 0 & \cdot \begin{pmatrix} 0 \\ 1 \end{pmatrix} \end{pmatrix} = \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix}$
- E.g. controlled-not: $\mathbf{C}_{10} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$


 $\begin{array}{c} |x\rangle \\ |y\rangle \end{array} \xrightarrow{\mathbf{C}_{10}} \begin{array}{c} |x\rangle \\ |y \oplus x\rangle \end{array}$
 $x, y \in \{0,1\}$, the second qubit is flipped if and only if first is 1

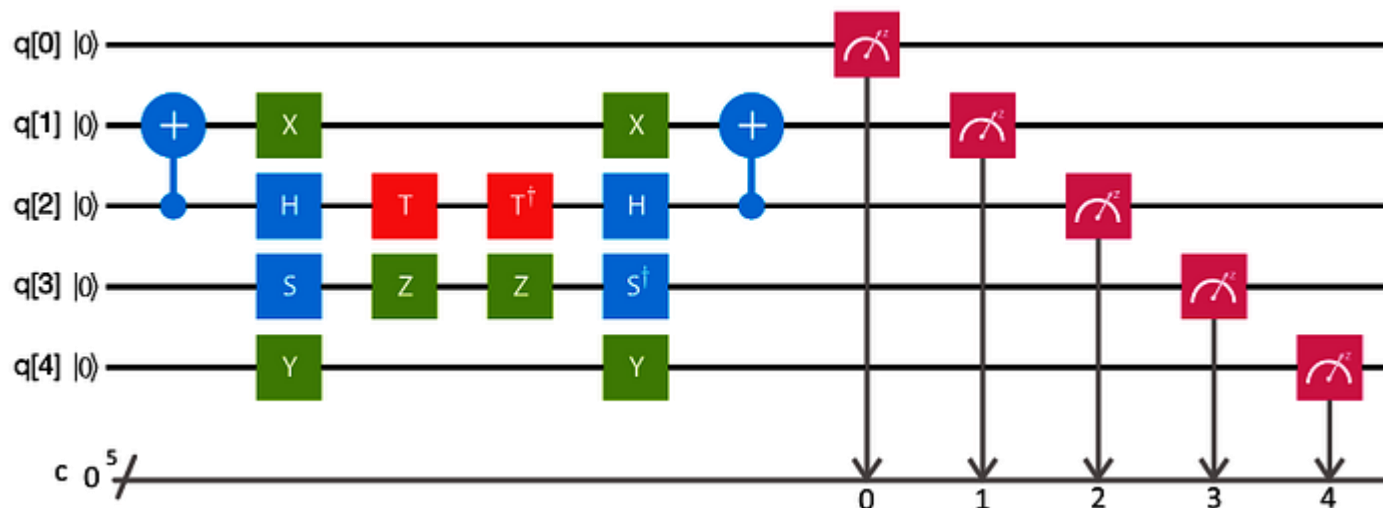
E.g. for $x = 1$ $y = 0$: $|\phi\rangle = 0|00\rangle + 0|01\rangle + 1|10\rangle + 0|11\rangle$

$$\begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix} \quad \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix} \quad \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix} \quad \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix}$$


 $|\phi'\rangle = \mathbf{C}_{10}|\phi\rangle = 0|00\rangle + 0|01\rangle + 0|10\rangle + 1|11\rangle$

- Gate on n qubits ...

- Universal gate
 - Circuit, e.g. on 5-qubits



- Gate-based QC
 - Universal approach (like classical computers operations are performed on qubits)
 - Highly sensitive to noise → difficulty in controlling error
 - Error controlled by using control qubits

- Quantum annealer

- Goal: finding the ground state of a Hamiltonian $\mathbf{H}$

$$|\phi_0\rangle = \arg \min_{|\phi\rangle} \langle \phi | \mathbf{H} | \phi \rangle$$

- Based on quantum adiabatic theorem:

- Considering a time-varying Hamiltonian $\mathbf{H}_{QA}(t)$ initially at ground state, if its time evolution is slow enough, it is likely to remain at the ground state

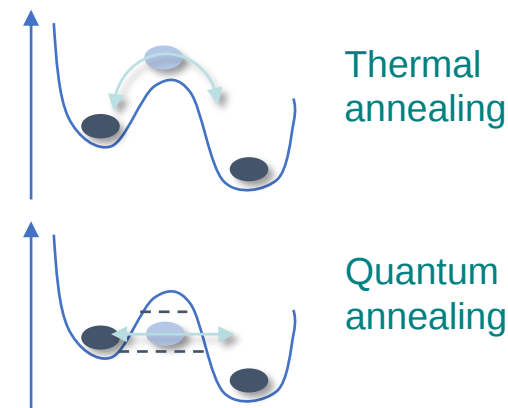
- Adiabatic quantum computing:

- Starts from the ground state of an easy to prepare Hamiltonian $\mathbf{H}_i$
- Evolves to the ground state of the Hamiltonian $\mathbf{H}$ which encodes the sought solution

$$\mathbf{H}_{QA}(t) = \frac{(t_a - t)}{t_a} \mathbf{H}_i + \frac{t}{t_a} \mathbf{H}$$

- Quantum annealing

- Exploits quantum effect such as quantum tunneling
- Less sensitive to noise than Gate-based QC
- Less versatile than Gate-based QC



- Ising Hamiltonian

- Goal: finding the ground state of a Hamiltonian $\mathbf{H}$

$$|\phi_0\rangle = \arg \min_{|\phi\rangle} \langle \phi | \mathbf{H} | \phi \rangle$$

- Some definitions

- Set of K qubits $V = \{0, \dots, K-1\}$
- Set of interactions between 2 qubits $E \subset \{(i, j) \mid i \in V, j \in V, i < j\}$
- Pauli- Z operator $\mathbf{Z} = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$ and identity $\mathbf{I} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$
- Pauli- Z operator applied on qubit i : $\mathbf{Z}_i = \underbrace{\mathbf{I} \otimes \dots \otimes \mathbf{I}}_0 \otimes \underbrace{\mathbf{Z}}_i \otimes \underbrace{\mathbf{I} \otimes \dots \otimes \mathbf{I}}_{K-1}$
- Pauli- Z operator applied on qubits i and j :

$$\mathbf{Z}_{ij} = \underbrace{\mathbf{I} \otimes \dots \otimes \mathbf{I}}_0 \otimes \underbrace{\mathbf{Z}}_i \otimes \underbrace{\mathbf{I} \otimes \dots \otimes \mathbf{I}}_j \otimes \underbrace{\mathbf{Z}}_j \otimes \underbrace{\mathbf{I} \otimes \dots \otimes \mathbf{I}}_{K-1}$$

- Ising Hamiltonian represented by an undirected graph (V, E) :

- $\mathbf{H} = \sum_{i \in V} h_i \mathbf{Z}_i + \sum_{(i, j) \in E} J_{ij} \mathbf{Z}_{ij}$

- Is a $2^K \times 2^K$ diagonal operator in the computational basis

- Quadratic Unconstrained Binary Optimization (QUBO)

- Goal: finding the ground state of a Hamiltonian $\mathbf{H}$

$$|\phi_0\rangle = \arg \min_{|\phi\rangle} \langle \phi | \mathbf{H} | \phi \rangle \quad \text{with} \quad \mathbf{H} = \sum_{i \in V} h_i \mathbf{Z}_i + \sum_{(i,j) \in E} J_{ij} \mathbf{Z}_{ij}$$

- In terms of spin variables

- Computational basis of $\mathbf{H}$ $|\phi\rangle = |b_0 b_1 \dots b_{K-1}\rangle$ with $b_i \in \{0, 1\}$

- We have successively

$$\mathbf{Z} = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \quad \Rightarrow \quad \mathbf{Z}|b_i\rangle = (-1)^{b_i}|b_i\rangle \quad |0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad |1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

$$\mathbf{Z}_i = \underbrace{\mathbf{I}}_0 \otimes \dots \otimes \mathbf{I} \otimes \underbrace{\mathbf{Z}}_i \otimes \mathbf{I} \otimes \dots \otimes \underbrace{\mathbf{I}}_{K-1} \quad \Rightarrow \quad \mathbf{Z}_i|\phi\rangle = (-1)^{b_i}|\phi\rangle$$

$$\mathbf{Z}_{ij} = \underbrace{\mathbf{I}}_0 \otimes \dots \otimes \mathbf{I} \otimes \underbrace{\mathbf{Z}}_i \otimes \mathbf{I} \otimes \dots \otimes \mathbf{I} \otimes \underbrace{\mathbf{Z}}_j \otimes \mathbf{I} \otimes \dots \otimes \underbrace{\mathbf{I}}_{K-1} \quad \Rightarrow \quad \mathbf{Z}_{ij}|\phi\rangle = (-1)^{b_i}(-1)^{b_j}|\phi\rangle$$

- Defining the vector of spin variables: $\mathbf{s} = [(-1)^{b_i} \forall i \in V]$

$$\Rightarrow \quad \text{The eigenvalue of } \mathbf{H} \text{ reads } \mathcal{F}_{\text{Ising}} = \sum_{i \in V} h_i s_i + \sum_{(i,j) \in E} J_{ij} s_i s_j = \mathbf{s}^T \mathbf{h} + \mathbf{s}^T \mathbf{J} \mathbf{s}$$

$$\text{with } \mathbf{h} = [h_i \forall i \in V] \quad \& \quad \mathbf{J} = [J_{ij} \forall (i,j) \in E]$$

$$\Rightarrow \quad |\phi_0\rangle = \arg \min_{\phi} \langle \phi | \mathbf{H} | \phi \rangle \quad \Leftrightarrow \quad \mathbf{s} = \arg \min_{\mathbf{s}'} \mathcal{F}_{\text{Ising}}(\mathbf{s}'; \mathbf{h}, \mathbf{J})$$

User programmable parameters

- Quadratic Unconstrained Binary Optimization (QUBO)

- Goal: finding the ground state of a Hamiltonian $\mathbf{H}$

$$|\phi_0\rangle = \arg \min_{|\phi\rangle} \langle \phi | \mathbf{H} | \phi \rangle \quad \text{with} \quad \mathbf{H} = \sum_{i \in V} h_i \mathbf{Z}_i + \sum_{(i,j) \in E} J_{ij} \mathbf{Z}_{ij}$$

- In terms of spin variables

- Computational basis of $\mathbf{H}$ $|\phi\rangle = |b_0 b_1 \dots b_{K-1}\rangle$ with $b_i \in \{0, 1\}$
- Vector of spin variables: $\mathbf{s} = [(-1)^{b_i} \forall i \in V]$

The eigenvalue of $\mathbf{H}$ reads $\mathcal{F}_{\text{Ising}} = \sum_{i \in V} h_i s_i + \sum_{(i,j) \in E} J_{ij} s_i s_j = \mathbf{s}^T \mathbf{h} + \mathbf{s}^T \mathbf{J} \mathbf{s}$

with $\mathbf{h} = [h_i \forall i \in V]$ & $\mathbf{J} = [J_{ij} \forall (i,j) \in E]$

$\Rightarrow |\phi_0\rangle = \arg \min_{\phi} \langle \phi | \mathbf{H} | \phi \rangle \quad \Leftrightarrow \quad \mathbf{s} = \arg \min_{\mathbf{s}'} \mathcal{F}_{\text{Ising}}(\mathbf{s}'; \mathbf{h}, \mathbf{J})$ User programmable parameters

- In terms of binary variables

- Vector of binary variables $\mathbf{b} = [b_i \forall i \in V]$
- Spin-binary variable transformation $s_i = 2b_i - 1 : \{0, 1\} \rightarrow \{-1, 1\}$ & property $b_i^2 = b_i$

$\Rightarrow \mathcal{F}_{\text{Ising}} = \sum_{i \in V} h_i s_i + \sum_{(i,j) \in E} J_{ij} s_i s_j \quad \Rightarrow \quad \mathcal{F}_{\text{QUBO}} = \sum_{(i,j) \in E \cup \{(i,i) \forall i \in V\}} A_{ij} b_i b_j = \mathbf{b}^T \mathbf{A} \mathbf{b}$

$\Rightarrow |\phi_0\rangle = \arg \min_{\phi} \langle \phi | \mathbf{H} | \phi \rangle \quad \Leftrightarrow \quad \mathbf{b} = \arg \min_{\mathbf{b}'} \mathcal{F}_{\text{QUBO}}(\mathbf{b}'; \mathbf{A})$ User programmable parameters

- Summary

- Goal: finding the ground state of a Hamiltonian $\mathbf{H}$

$$|\phi_0\rangle = \arg \min_{|\phi\rangle} \langle \phi | \mathbf{H} | \phi \rangle \quad \text{with} \quad \mathbf{H} = \sum_{i \in V} h_i \mathbf{Z}_i + \sum_{(i,j) \in E} J_{ij} \mathbf{Z}_{ij}$$

- Adiabatic annealing

- Starts from the ground state of an easy to prepare $\mathbf{H}_i$
- Evolves to the ground state of the Hamiltonian $\mathbf{H}$

$$\mathbf{H}_{\text{QA}}(t) = \frac{(t_a - t)}{t_a} \mathbf{H}_i + \frac{t}{t_a} \mathbf{H}$$



- Problem reformulated in terms of binary variables

- $\mathbf{b} = [b_i \forall i \in V]$ with $b_i \in \{0, 1\}$

- Eigenvalue $\mathcal{F}_{\text{QUBO}} = \mathbf{b}^T \mathbf{A} \mathbf{b}$

- QUBO optimization $\mathbf{b} = \arg \min_{\mathbf{b}'} \mathcal{F}_{\text{QUBO}}(\mathbf{b}'; \mathbf{A})$ User programmable parameters

- In practice

- Provide the QUBO matrix $\mathbf{A}$
- Set the annealing time t_a (typically 20 μs)
- One annealing returns a sample of $\mathbf{b}$
- A single run may not provide the global minimum due to environmental noises, hardware imperfections, pre- and post-processing errors  requires several reads

- Set of PDEs to be solved

- Strong form  Weak form:

$$\nabla \cdot \boldsymbol{\sigma}(\mathbf{x}) + \mathbf{b}_0(\mathbf{x}) = \mathbf{0} \quad \xrightarrow{\text{blue arrow}} \quad \int_V \boldsymbol{\sigma}(\mathbf{x}) : \nabla \otimes^s \delta \mathbf{u}(\mathbf{x}) dV = \int_V \mathbf{b}_0 \cdot \delta \mathbf{u} dV + \int_{\partial_{NV}} \mathbf{n} \cdot \boldsymbol{\sigma} \cdot \delta \mathbf{u} d\partial V$$

- Constitutive model:

$$\boldsymbol{\sigma}(\mathbf{x}, t) = \boldsymbol{\sigma}(\nabla \otimes^s \mathbf{u}(\mathbf{x}, t); \mathbf{q}(\mathbf{x}, t)) \quad \text{with evolution law} \quad \mathcal{Q}(\boldsymbol{\sigma}(\mathbf{x}, t), \mathbf{q}(\nabla \otimes^s \mathbf{u}(\mathbf{x}, \tau); \tau \leq t)) = \mathbf{0}$$

- Finite element formulation

- Displacement field at quadrature point Ξ from nodal displacements vector $\mathbf{U}$

$$\mathbf{u}(\Xi) = N_a(\Xi) \mathbf{U}_a \quad \xrightarrow{\text{blue arrow}} \quad \boldsymbol{\varepsilon}(\Xi) = \nabla \otimes^s \mathbf{u}(\Xi) = \mathbf{B}_a(\Xi) \mathbf{U}_a$$

- Resulting non-linear system of equations on time interval $[t_n, t_{n+1}]$

$$\int_V \boldsymbol{\sigma}(\mathbf{x}) : \nabla \otimes^s \delta \mathbf{u}(\mathbf{x}, t) dV = \int_V \mathbf{b}_0 \cdot \delta \mathbf{u} dV + \int_{\partial_{NV}} \mathbf{n} \cdot \boldsymbol{\sigma} \cdot \delta \mathbf{u} d\partial V$$

$$\xrightarrow{\text{blue arrow}} \delta \mathbf{U}_b^T \cdot \sum_{\Xi} \mathbf{B}_b^T(\Xi) \boldsymbol{\sigma}(\Xi) \omega^{\Xi} = \delta \mathbf{U}_b^T \cdot \sum_{\Xi} N_b(\Xi) \mathbf{b}_0(\Xi) \omega^{\Xi}$$

Omitting surface tractions

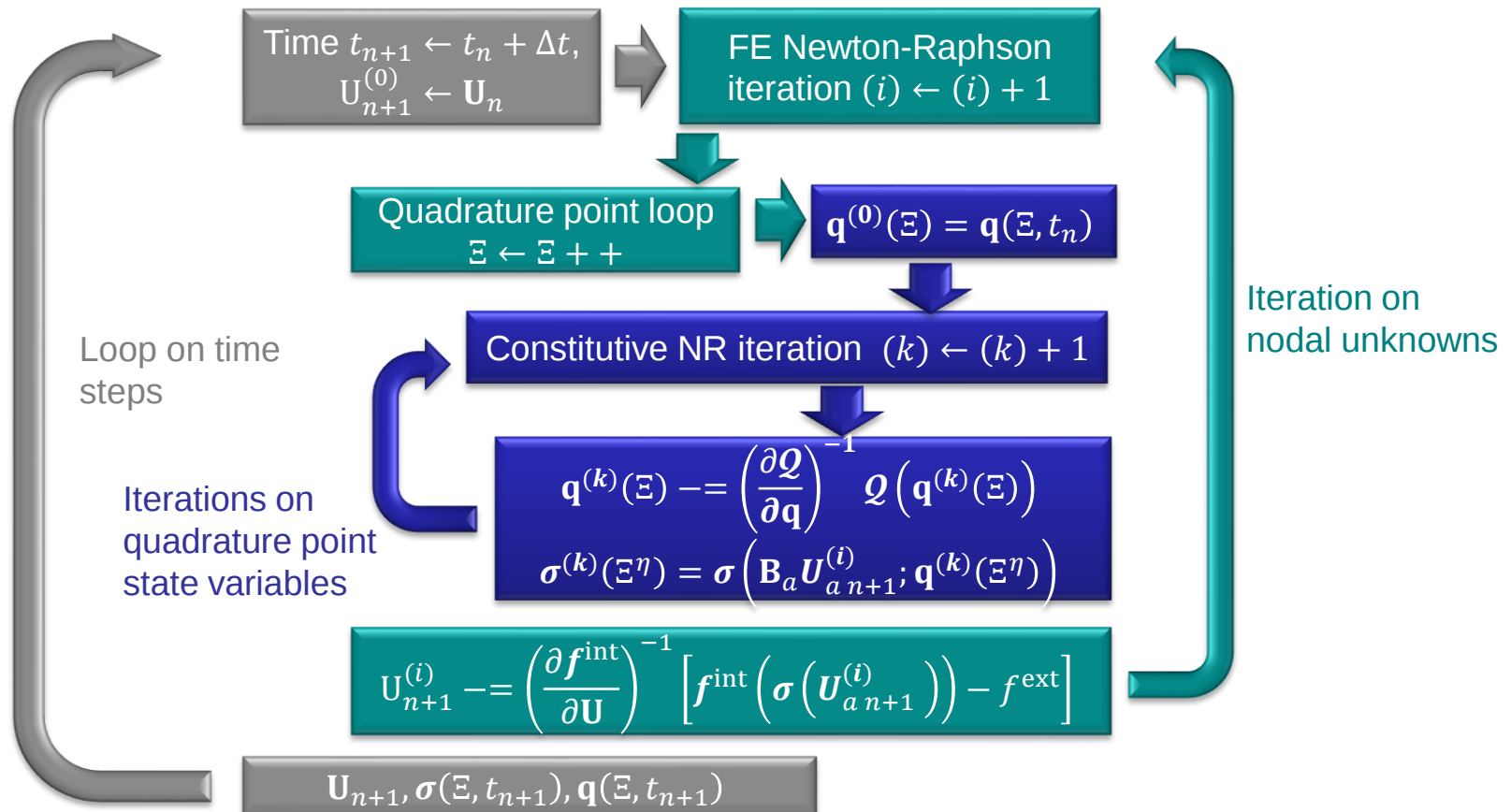
$$\xrightarrow{\text{blue arrow}} \mathbf{f}_b^{\text{int}} = \sum_{\Xi} \mathbf{B}_b^T(\Xi) \boldsymbol{\sigma}(\Xi) \omega^{\Xi} = \sum_{\Xi} N_b(\Xi) \mathbf{b}_0(\Xi) \omega^{\Xi} = \mathbf{f}_b^{\text{ext}}$$

$$\text{with} \quad \left\{ \begin{array}{l} \boldsymbol{\sigma}(\Xi, t_{n+1}) = \boldsymbol{\sigma}(\mathbf{B}_a(\Xi) \mathbf{U}_{a, n+1}; \mathbf{q}(\Xi, t_{n+1})) \\ \mathcal{Q}(\boldsymbol{\sigma}(\Xi, t_{n+1}), \mathbf{q}(\Xi, t_{n+1}), \mathbf{q}(\Xi, t_n)) = \mathbf{0} \end{array} \right.$$

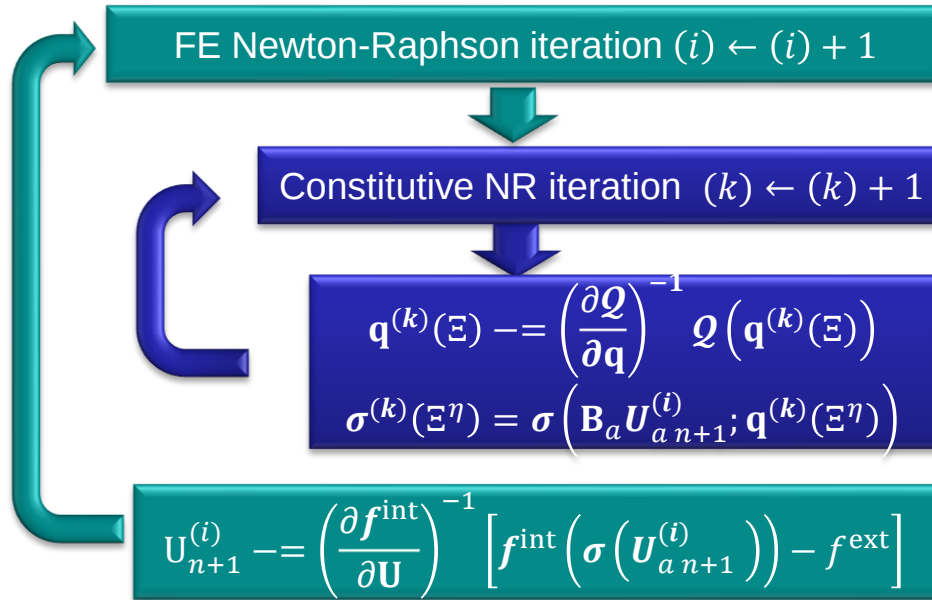
- Finite element formulation

- Resulting non-linear system of equations on time interval $[t_n, t_{n+1}]$

$$\begin{cases} \mathbf{f}_b^{\text{int}} = \sum_{\Xi} \mathbf{B}_b^T(\Xi) \boldsymbol{\sigma}(\Xi) \omega^\Xi = \sum_{\Xi} N_b(\Xi) \mathbf{b}_0(\Xi) \omega^\Xi = \mathbf{f}_b^{\text{ext}} \\ \boldsymbol{\sigma}(\Xi, t_{n+1}) = \boldsymbol{\sigma}(\mathbf{B}_a(\Xi) \mathbf{U}_{a, n+1}; \mathbf{q}(\Xi, t_{n+1})) \quad \& \quad \mathcal{Q}(\boldsymbol{\sigma}(\Xi, t_{n+1}), \mathbf{q}(\Xi, t_{n+1}), \mathbf{q}(\Xi, t_n)) = \mathbf{0} \end{cases}$$



- Consider classical finite element resolution on Quantum Computers?



- What can be solved on a Quantum Computer?
 - Optimization problems can be solved (Actually Quantum Annealers look for a ground state)
 - Some operations can be achieved efficiently on classical computers like assembly
- Do we need the same resolution structure?
 - Do we need intricate NR loops?
 - Do we even need to use the discretized form of the weak form?

$$\int_V \boldsymbol{\sigma}(x) : \nabla \otimes^s \boldsymbol{\delta u}(x) dV = \int_V \mathbf{b}_0 \cdot \boldsymbol{\delta u} dV \quad \Rightarrow \quad \mathbf{f}_b^{\text{int}} = \sum_{\Xi} \mathbf{B}_b^T(\Xi) \boldsymbol{\sigma}(\Xi) \omega^\Xi = \mathbf{f}_b^{\text{ext}}$$

• Linear finite element resolution on Quantum Computers?

– Assuming linear elasticity

• Existence of a free energy $\Psi = \frac{1}{2} \boldsymbol{\varepsilon}(x) : \mathbb{C}(x) : \boldsymbol{\varepsilon}(x)$ with $\boldsymbol{\varepsilon}(x) = \nabla \otimes^s \mathbf{u}(x)$

• Stress results from $\boldsymbol{\sigma}(x) = \frac{\partial \Psi}{\partial \boldsymbol{\varepsilon}} = \mathbb{C}(x) : \boldsymbol{\varepsilon}(x) = \mathbb{C}(x) : (\nabla \otimes^s \mathbf{u}(x))$

– Finite element form:

• At quadrature point using nodal shape function derivatives: $\boldsymbol{\sigma}(\Xi) = \mathbb{C}(\Xi) \mathbf{B}_a(\Xi) \mathbf{U}_a$

• FE equations $\mathbf{f}_b^{\text{int}} = \sum_{\Xi} \mathbf{B}_b^T(\Xi) \boldsymbol{\sigma}(\Xi) \omega^{\Xi} = \mathbf{f}_b^{\text{ext}}$

$$\Rightarrow \sum_{\Xi} \mathbf{B}_b^T(\Xi) \mathbb{C}(x) \mathbf{B}_a \omega^{\Xi} \mathbf{U}_a = \mathbf{K}_{ab} \mathbf{U}_a = \mathbf{f}_b^{\text{ext}}$$

• Defining the internal energy and work of external forces

$$\Phi = \frac{1}{2} \mathbf{U}_b \mathbf{K}_{ab} \mathbf{U}_a - W^{\text{ext}} \quad \text{with} \quad W^{\text{ext}} = \mathbf{f}_b^{\text{ext}} \mathbf{U}_b$$



The solution of the FE equations minimizes the energy

$$\mathbf{U} = \arg \min_{\mathbf{U}'} \left(\frac{1}{2} \mathbf{U}'^T \mathbf{K} \mathbf{U}' - \mathbf{f}^{\text{ext}T} \mathbf{U}' \right)$$

– We are looking for the ground state of a Hamiltonian

$$\mathbf{H} = \sum_{i \in V} h_i \mathbf{Z}_i + \sum_{(i,j) \in E} J_{ij} \mathbf{Z}_{ij}$$

- Non-linear finite element resolution on Quantum Computers?

- Weak form: $\int_V \boldsymbol{\sigma}(\mathbf{x}) : \nabla \otimes^s \boldsymbol{\delta u}(\mathbf{x}) dV = \int_V \mathbf{b}_0 \cdot \boldsymbol{\delta u} dV$

- Assuming non-linear elasticity

- Existence of a free energy $\Psi(\boldsymbol{\varepsilon}(\mathbf{x}))$ with $\boldsymbol{\varepsilon}(\mathbf{x}) = \nabla \otimes^s \mathbf{u}(\mathbf{x})$

- Stress results from $\boldsymbol{\sigma}(\mathbf{x}) = \frac{\partial \Psi}{\partial \boldsymbol{\varepsilon}}$

 The weak form becomes $\int_V \frac{\partial \Psi(\mathbf{x})}{\partial \boldsymbol{\varepsilon}} : \boldsymbol{\delta \varepsilon}(\mathbf{x}) dV = \int_V \mathbf{b}_0 \cdot \boldsymbol{\delta u} dV$

- Introduction of a functional

- $\Phi(\mathbf{u}(V)) = \int_V \Psi(\nabla \otimes^s \mathbf{u}(\mathbf{x})) dV - W^{\text{ext}}(\mathbf{u}(V))$ & $W^{\text{ext}} = \int_V \mathbf{b}_0 \cdot \mathbf{u}(\mathbf{x}) dV$

- The weak form results from nulling the Gâteaux derivative

$$\Phi'(\mathbf{u}(V); \boldsymbol{\delta u}(V)) = \int_V \boldsymbol{\sigma}(\mathbf{x}) : \nabla \otimes^s \boldsymbol{\delta u}(\mathbf{x}) dV - \int_V \mathbf{b}_0 \cdot \boldsymbol{\delta u} dV = 0$$

 The solution of the weak form minimizes the energy: $\mathbf{u}(V) = \arg \min_{\mathbf{u}'(V)} \Phi(\mathbf{u}'(V))$

- We are looking for the solution of a minimization problem

- The potential is convex
 - But it is not quadratic
 - Quid inelastic materials?

• Non-linear finite element resolution on Quantum Computers?

– Inelastic materials

- Existence of a Helmholtz free energy $\Psi(\boldsymbol{\varepsilon}(x), \mathbf{q}(x))$ with $\left\{ \begin{array}{l} \text{internal variables } \mathbf{q}(x) \\ \boldsymbol{\varepsilon}(x) = \nabla \otimes^s \mathbf{u}(x) \end{array} \right.$

– Dissipation $\mathcal{D}$ and Clausius-Duhem inequality

- $\mathcal{D} = \boldsymbol{\sigma} : \dot{\boldsymbol{\varepsilon}} - \dot{\Psi} \geq 0$ with $\dot{\Psi} = \frac{\partial \Psi}{\partial \boldsymbol{\varepsilon}} : \dot{\boldsymbol{\varepsilon}} + \frac{\partial \Psi}{\partial \mathbf{q}} \cdot \dot{\mathbf{q}}$

- Equality holds in case of a reversible transformation

$$\Rightarrow \boldsymbol{\sigma} = \frac{\partial \Psi}{\partial \boldsymbol{\varepsilon}} \Rightarrow \text{for an irreversible process: } \mathcal{D} = \mathbf{Y} \cdot \dot{\mathbf{q}} \geq 0 \quad \text{with} \quad \mathbf{Y} = -\frac{\partial \Psi}{\partial \mathbf{q}}$$

– Postulate the existence of a pseudo-potential $\theta(\dot{\mathbf{q}})$ and its convex dual $\theta^*(\mathbf{Y})$

- $\theta(\dot{\mathbf{q}}) = \max_{\mathbf{Y}} [\mathbf{Y} \cdot \dot{\mathbf{q}} - \theta^*(\mathbf{Y})] \Rightarrow \dot{\mathbf{q}} = \frac{\partial \theta^*(\mathbf{Y})}{\partial \mathbf{Y}} \quad \& \quad \mathbf{Y} = \frac{\partial \theta(\dot{\mathbf{q}})}{\partial \dot{\mathbf{q}}}$

– Power functional $\mathcal{E}$

- New independent variables $(\dot{\boldsymbol{\varepsilon}}, \dot{\mathbf{q}})$

- $\mathcal{E}(\dot{\boldsymbol{\varepsilon}}, \dot{\mathbf{q}}) = \dot{\Psi} + \theta(\dot{\mathbf{q}}) = \frac{\partial \Psi}{\partial \boldsymbol{\varepsilon}} : \dot{\boldsymbol{\varepsilon}} - \mathbf{Y} \cdot \dot{\mathbf{q}} + \theta(\dot{\mathbf{q}})$

$$\Rightarrow \frac{\partial \mathcal{E}}{\partial \dot{\mathbf{q}}} = -\mathbf{Y} + \frac{\partial \theta(\dot{\mathbf{q}})}{\partial \dot{\mathbf{q}}} = \mathbf{0} \Rightarrow \mathcal{E} \text{ has to be minimized with respect to internal state}$$

- Effective power functional* $\mathcal{E}^{\text{eff}}(\dot{\boldsymbol{\varepsilon}}) = \min_{\dot{\mathbf{q}}} \mathcal{E}(\dot{\boldsymbol{\varepsilon}}, \dot{\mathbf{q}})$ with $\boldsymbol{\sigma} = \frac{\partial \Psi}{\partial \boldsymbol{\varepsilon}} = \frac{\partial \mathcal{E}^{\text{eff}}}{\partial \dot{\boldsymbol{\varepsilon}}}$

– The constitutive model is also a minimization problem

*Radovitzky, R. Ortiz M, CMAME 1999
Ortiz, M., Stainier, L., CMAME 1999

• Non-linear finite element resolution on Quantum Computers?

– In elasticity we had

- $\mathbf{u}(V) = \arg \min_{\mathbf{u}'(V)} \Phi(\mathbf{u}'(V))$ with $\Phi(\mathbf{u}(V)) = \int_V \Psi(\nabla \otimes^s \mathbf{u}(x)) dV - W^{\text{ext}}(\mathbf{u}(x))$

– Double minimization problem in inelasticity

- Power functional $\mathcal{E}$

$$\mathcal{E}(\dot{\boldsymbol{\varepsilon}}, \dot{\mathbf{q}}) = \frac{\partial \Psi}{\partial \boldsymbol{\varepsilon}} : \dot{\boldsymbol{\varepsilon}} - \mathbf{Y} \cdot \dot{\mathbf{q}} + \Theta(\dot{\mathbf{q}}) \quad \& \quad \mathcal{E}^{\text{eff}}(\dot{\boldsymbol{\varepsilon}}) = \min_{\dot{\mathbf{q}}} \mathcal{E}(\dot{\boldsymbol{\varepsilon}}, \dot{\mathbf{q}}) \quad \Rightarrow \quad \boldsymbol{\sigma} = \frac{\partial \mathcal{E}^{\text{eff}}}{\partial \dot{\boldsymbol{\varepsilon}}}$$

- Volume power functional

$$\Phi(\dot{\mathbf{u}}(V), \dot{\mathbf{q}}(V)) = \int_V \mathcal{E}(\nabla \otimes^s \dot{\mathbf{u}}, \dot{\mathbf{q}}) - \dot{W}^{\text{ext}}(\dot{\mathbf{u}}(V))$$

- Incremental volume energy functional on time interval $[t_n, t_{n+1}]^*$

$$\Delta \Phi(\mathbf{u}_{n+1}, \mathbf{q}_{n+1}) = \int_V \Delta \mathcal{E}(\nabla \otimes^s \mathbf{u}_{n+1}, \mathbf{q}_{n+1}) - \Delta W^{\text{ext}}(\mathbf{u}_{n+1})$$

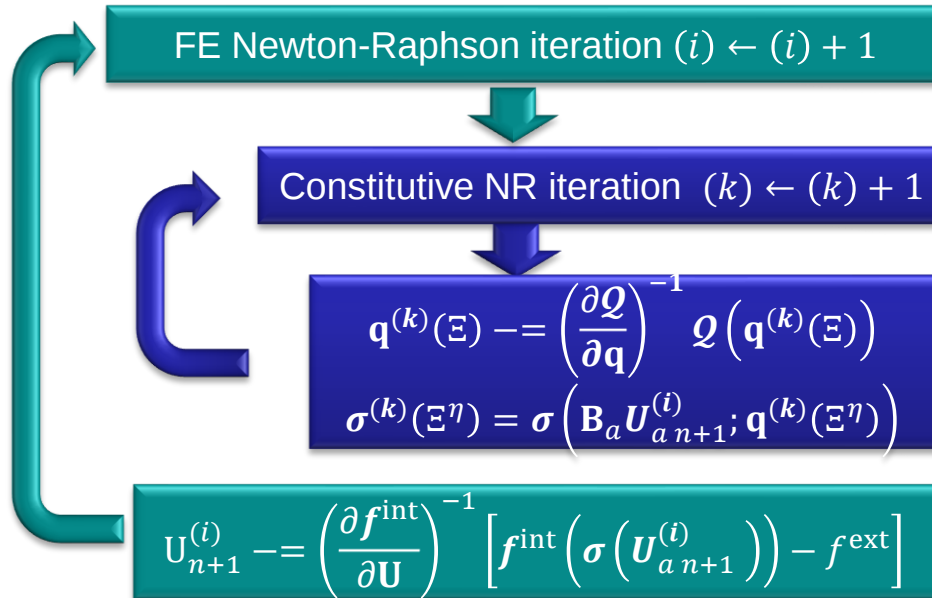
$$\text{with } \Delta \mathcal{E}(\nabla \otimes^s \mathbf{u}_{n+1}, \mathbf{q}_{n+1}) = \int_{t_n}^{t_{n+1}} \mathcal{E}(\nabla \otimes^s \dot{\mathbf{u}}, \dot{\mathbf{q}}) \quad \& \quad \Delta \mathcal{E}^{\text{eff}}(\boldsymbol{\varepsilon}) = \min_{\mathbf{q}} \Delta \mathcal{E}(\boldsymbol{\varepsilon}, \mathbf{q}) \quad , \quad \boldsymbol{\sigma} = \frac{\partial \Delta \mathcal{E}^{\text{eff}}}{\partial \boldsymbol{\varepsilon}}$$

- The problem solution reads

$$\left\{ \begin{array}{l} \mathbf{q}_{n+1} = \arg \min_{\mathbf{q}'} \Delta \Phi(\mathbf{u}_{n+1}, \mathbf{q}') \\ \Delta \Phi^{\text{eff}}(\mathbf{u}_{n+1}) = \min_{\mathbf{q}'} \Delta \Phi(\mathbf{u}_{n+1}, \mathbf{q}') = \int_V \Delta \mathcal{E}^{\text{eff}}(\nabla \otimes^s \mathbf{u}_{n+1}) - \Delta W^{\text{ext}} \\ \mathbf{u}_{n+1} = \arg \min_{\mathbf{u}' \text{ admissible}} \Delta \Phi^{\text{eff}}(\mathbf{u}') \end{array} \right.$$

*Ortiz, M., Stainier, L., CMAME 1999

- Classical finite element resolution



- Finite element as a double-minimization problem

Loop until convergence

$$\mathbf{q}_{n+1} = \arg \min_{\mathbf{q}' \text{ constrained}} \Delta \Phi(\mathbf{u}_{n+1}, \mathbf{q}');$$

$$\Delta \Phi^{\text{eff}} = \min_{\mathbf{q}' \text{ constrained}} \Delta \Phi(\mathbf{u}_{n+1}, \mathbf{q}')$$

$$\mathbf{u}_{n+1} = \arg \min_{\mathbf{u}' \text{ admissible}} \Delta \Phi^{\text{eff}}(\mathbf{u}')$$

- Quantum annealers: ground state of an Ising-Hamiltonian
 - No need for Jacobians
 - No problem of convergence
- But how to make the optimisation problem solvable by quantum annealing?

Double-minimization process solved by Quantum annealing

- Finite element as a double-minimization problem

- Finite element problem

Loop until convergence

$$\mathbf{q}_{n+1} = \arg \min_{\mathbf{q}' \text{ constrained}} \Delta\Phi(\mathbf{u}_{n+1}, \mathbf{q}');$$

$$\Delta\Phi^{\text{eff}} = \min_{\mathbf{q}' \text{ constrained}} \Delta\Phi(\mathbf{u}_{n+1}, \mathbf{q}')$$

$$\mathbf{u}_{n+1} = \arg \min_{\mathbf{u}' \text{ admissible}} \Delta\Phi^{\text{eff}}(\mathbf{u}')$$

- Ising Hamiltonian for Quantum annealing

- Goal: finding the ground state of a Hamiltonian $\mathbf{H}$:
$$\mathbf{H} = \sum_{i \in V} h_i \mathbf{Z}_i + \sum_{(i,j) \in E} J_{ij} \mathbf{Z}_{ij}$$

➡ $|\phi_0\rangle = \arg \min_{|\phi\rangle} \langle \phi | \mathbf{H} | \phi \rangle$

- Problem reformulated in terms of binary variables $\mathbf{b} = [b_i \forall i \in V]$ with $b_i \in \{0, 1\}$

- QUBO optimisation problem
$$\mathcal{F}_{\text{QUBO}} = \sum_{(i,j) \in EU \cup \{(i,i) \forall i \in V\}} A_{ij} b_i b_j = \mathbf{b}^T \mathbf{A} \mathbf{b}$$

➡ $\mathbf{b} = \arg \min_{\mathbf{b}'} \mathcal{F}_{\text{QUBO}}(\mathbf{b}'; \mathbf{A})$ User programmable parameters

- Steps to follow

- Transform the constrained minimization problem into an unconstrained one
- Transform the general unconstrained optimization problem into a series of quadratic ones
- Transform each continuous quadratic optimization problem into a binarized one
- Apply to the double-minimization framework

Double-minimization process solved by Quantum annealing

- Transform the constrained minimization problem into an unconstrained one
 - Constrained multivariate minimization problem
 - $\min_{\mathbf{w}} f(\mathbf{w})$ with $\mathbf{w}^{\min} \leq \mathbf{w} \leq \mathbf{w}^{\max}$
 - Under constraints $h(\mathbf{w}) = 0$ & $l(\mathbf{w}) \leq 0$
 - Augmented minimization problem
 - $f_{\text{aug}}(\mathbf{v}) = f_{\text{aug}}(\mathbf{w}, \lambda) = f(\mathbf{w}) + c^h(h(\mathbf{w}))^2 + c^l(l(\mathbf{w}) + \lambda)^2$ with $\mathbf{v} = \{\mathbf{w}, \lambda \geq 0\}$
 - Unconstrained minimization problem
 - $\min_{\mathbf{v}} f_{\text{aug}}(\mathbf{v})$ with $\mathbf{v}^{\min} \leq \mathbf{v} \leq \mathbf{v}^{\max}$
 - Bounds will be enforced during the binarization process
 - Definition of the double-unconstrained minimization problem

Loop until convergence

$$\mathbf{q}_{n+1} = \arg \min_{\mathbf{q}' \text{ constrained}} \Delta\Phi(\mathbf{u}_{n+1}, \mathbf{q}');$$

$$\Delta\Phi^{\text{eff}} = \min_{\mathbf{q}' \text{ constrained}} \Delta\Phi(\mathbf{u}_{n+1}, \mathbf{q}')$$

$$\mathbf{u}_{n+1} = \arg \min_{\mathbf{u}' \text{ admissible}} \Delta\Phi^{\text{eff}}(\mathbf{u}')$$



Loop until convergence

$$\mathbf{q}_{n+1}, \lambda = \arg \min_{\{\mathbf{q}', \lambda'\}} \Delta\Phi_{\text{aug}}(\mathbf{u}_{n+1}, \mathbf{q}', \lambda');$$

$$\Delta\Phi^{\text{eff}} = \min_{\{\mathbf{q}', \lambda'\}} \Delta\Phi_{\text{aug}}(\mathbf{u}_{n+1}, \mathbf{q}', \lambda')$$

$$\mathbf{u}_{n+1} = \arg \min_{\mathbf{u}' \text{ admissible}} \Delta\Phi^{\text{eff}}(\mathbf{u}')$$

Double-minimization process solved by Quantum annealing

- Transform the optimization problem into a series of quadratic ones

- Unconstrained optimization problem

- $\min_{\mathbf{v}} f_{\text{aug}}(\mathbf{v})$ with $\mathbf{v}^{\min} \leq \mathbf{v} \leq \mathbf{v}^{\max}$

- Taylor's expansion

- $f_{\text{aug}}(\mathbf{v} + \mathbf{z}) \simeq f_{\text{aug}}(\mathbf{v}) + \mathbf{z}^T f_{\text{aug},\mathbf{v}} + \frac{1}{2} \mathbf{z}^T f_{\text{aug},\mathbf{v}\mathbf{v}} \mathbf{z}$

$$\left\{ \begin{array}{l} f_{\text{aug},\mathbf{v}}{}_i = \left. \frac{\partial f_{\text{aug}}}{\partial v_i} \right|_{\mathbf{v}} \\ f_{\text{aug},\mathbf{v}\mathbf{v}}{}_{ij} = \left. \frac{\partial^2 f_{\text{aug}}}{\partial v_i \partial v_j} \right|_{\mathbf{v}} \end{array} \right.$$

- New series of optimization problems

- Iterate on $\mathbf{z}$ with: $\mathbf{z} = \arg \min_{\mathbf{z}'} QF(\mathbf{z}'; f_{\text{aug},\mathbf{v}}, f_{\text{aug},\mathbf{v}\mathbf{v}})$

- Application to the double minimisation problem

Loop until convergence

$$\mathbf{q}_{n+1}, \lambda = \arg \min_{\{\mathbf{q}', \lambda'\}} \Delta \Phi_{\text{aug}}(\mathbf{u}_{n+1}, \mathbf{q}', \lambda');$$

$$\Delta \Phi^{\text{eff}} = \min_{\{\mathbf{q}', \lambda'\}} \Delta \Phi_{\text{aug}}(\mathbf{u}_{n+1}, \mathbf{q}', \lambda')$$

$$\mathbf{u}_{n+1} = \arg \min_{\mathbf{u}' \text{ admissible}} \Delta \Phi^{\text{eff}}(\mathbf{u}')$$



Loop until convergence

Loop on $\mathbf{u}_{n+1} \leftarrow \mathbf{u}_{n+1} + \Delta \mathbf{u}$

$$\Delta \mathbf{u} = \arg \min_{\Delta \mathbf{u}' \text{ admissible}} \Delta \mathbf{u}'^T \Delta \Phi_{,\mathbf{u}}^{\text{eff}} + \frac{1}{2} \Delta \mathbf{u}'^T \Delta \Phi_{,\mathbf{u}\mathbf{u}}^{\text{eff}} \Delta \mathbf{u}'$$

Loop on $\mathbf{q}_{n+1} \leftarrow \mathbf{q}_{n+1} + \Delta \mathbf{q}, \lambda \leftarrow \lambda + \Delta \lambda$

$$\Delta \mathbf{q}, \Delta \lambda = \arg \min_{\{\Delta \mathbf{q}', \Delta \lambda'\}} [\Delta \mathbf{q}'^T \Delta \lambda'] \Delta \Phi_{\text{aug},\{\mathbf{q} \lambda\}} + \frac{1}{2} [\Delta \mathbf{q}'^T \Delta \lambda'] \Delta \Phi_{\text{aug},\{\mathbf{q} \lambda\}\{\mathbf{q} \lambda\}} [\Delta \mathbf{q}'^T \Delta \lambda']^T$$

$$\Delta \Phi^{\text{eff}} = \Delta \Phi_{\text{aug}}(\mathbf{u}_{n+1}, \mathbf{q}_{n+1}, \lambda)$$

Double-minimization process solved by Quantum annealing

- Transform each continuous quadratic optimization problem into a binarized one

- Optimization problems to be solved

- $\mathbf{z} = \arg \min_{\mathbf{z}'} \text{QF}(\mathbf{z}', f_{\text{aug},\mathbf{v}}, f_{\text{aug},\mathbf{v}\mathbf{v}})$ & $\text{QF}(\mathbf{z}; f_{\text{aug},\mathbf{v}}, f_{\text{aug},\mathbf{v}\mathbf{v}}) = \mathbf{z}^T f_{\text{aug},\mathbf{v}} + \frac{1}{2} \mathbf{z}^T f_{\text{aug},\mathbf{v}\mathbf{v}} \mathbf{z}$
- With bounds: $\mathbf{v}_{\min} \leq \mathbf{v} + \mathbf{z} \leq \mathbf{v}_{\max}$
- These are Ising Hamiltonians to be minimized, but not of the QUBO type

- QUBO

- $\mathbf{b} = [b_i \forall i \in V]$ with $b_i \in \{0, 1\}$
- Eigen value $\mathcal{F}_{\text{QUBO}} = \mathbf{b}^T \mathbf{A} \mathbf{b}$
- QUBO optimization $\mathbf{b} = \arg \min_{\mathbf{b}'} \mathcal{F}_{\text{QUBO}}(\mathbf{b}'; \mathbf{A})$ User programmable parameters

- Binary-decimal conversion of a scalar field

- Definition of a L -bit string under the form $\mathbf{b}_1 = [b_0 \dots b_{L-1}]^T$ with $b_i \in \{0, 1\}$
- Conversion $b_{L-1} \dots b_0 \equiv \sum_{j=0}^{L-1} b_j 2^j = \boldsymbol{\beta}^T \mathbf{b}_1$ with $\boldsymbol{\beta} = [2^0 \ 2^1 \ \dots \ 2^{L-1}]^T$
- Introduce the bounds $z \in [z^{\min}, z^{\max}]$

 $z = z^{\min} + \epsilon_1 \boldsymbol{\beta}^T \mathbf{b}_1$ with the scaling $\epsilon_1 = \frac{z^{\max} - z^{\min}}{2^L - 1}$

- One scalar is represented (in a discrete way) by L qubits

- Binary-decimal conversion of a vector field

- Vector of size N represented by $N \times L$ qubits
- $\mathbf{z} = \mathbf{z}^{\min} + [\epsilon_i \boldsymbol{\beta}^T \mathbf{b}_i \text{ for } i = 0..N-1]$  $\mathbf{z} = \mathbf{a} + \mathbf{D}(\boldsymbol{\epsilon}) \mathbf{b}$

Double-minimization process solved by Quantum annealing

- Transform each continuous quadratic optimization problem into a binarized one

- Optimization problems to be solved

- $\mathbf{z} = \arg \min_{\mathbf{z}'} \text{QF}(\mathbf{z}', f_{\text{aug},v}, f_{\text{aug},vv})$ & $\text{QF}(\mathbf{z}; f_{\text{aug},v}, f_{\text{aug},vv}) = \mathbf{z}^T f_{\text{aug},v} + \frac{1}{2} \mathbf{z}^T f_{\text{aug},vv} \mathbf{z}$

- With bounds: $\mathbf{v}_{\min} \leq \mathbf{v} + \mathbf{z} \leq \mathbf{v}_{\max}$

- Binarization of $\mathbf{z} \in \mathbb{R}^N$ into $N \times L$ qubits

- $\mathbf{z} = \mathbf{a} + \mathbf{D}(\epsilon)\mathbf{b}$ with the bounds defining $\mathbf{a} = \mathbf{z}^{\min}$ & the scales $\epsilon = \frac{\mathbf{z}^{\max} - \mathbf{z}^{\min}}{2^L - 1}$



$$\text{QF}(\mathbf{z}; f_{\text{aug},v}, f_{\text{aug},vv}) = \frac{1}{2} \mathbf{b}^T \mathbf{D}^T f_{\text{aug},vv} \mathbf{D} \mathbf{b} + \mathbf{b}^T \mathbf{D}^T (f_{\text{aug},v} + f_{\text{aug},vv} \mathbf{a}) + \frac{1}{2} \mathbf{a}^T (f_{\text{aug},vv} \mathbf{a} + f_{\text{aug},v})$$

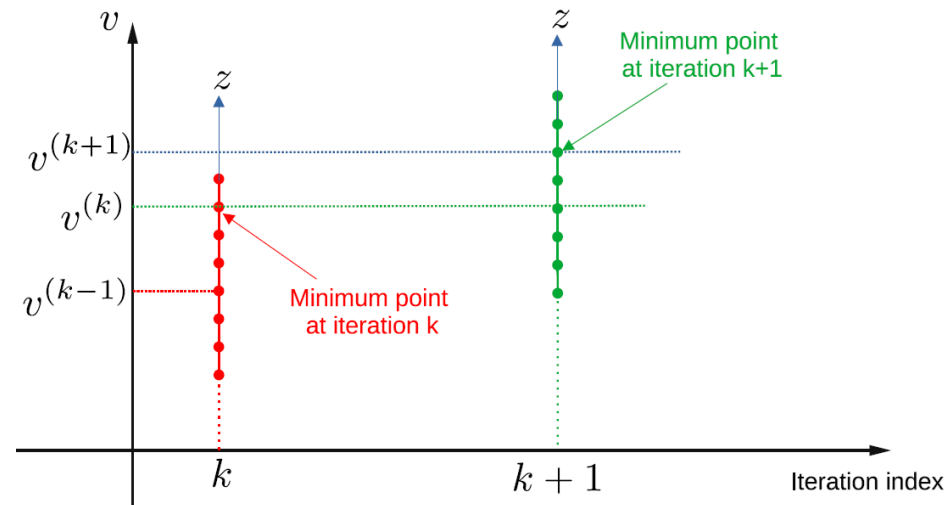
$$\mathcal{F}_{\text{QUBO}}(\mathbf{b}; \mathbf{A})$$

- Minimization

- Bound $\mathbf{a} = \mathbf{z}^{\min}$ and

- Scale $\epsilon = \frac{\mathbf{z}^{\max} - \mathbf{z}^{\min}}{2^L - 1}$

- Updated when building the QUBO



Double-minimization process solved by Quantum annealing

- Application to the double-minimization problem

Loop until convergence

Loop on $\mathbf{u}_{n+1} \leftarrow \mathbf{u}_{n+1} + \Delta \mathbf{u}$

$$\Delta \mathbf{u} = \arg \min_{\Delta \mathbf{u}' \text{ admissible}} \Delta \mathbf{u}'^T \Delta \Phi_{\mathbf{u}}^{\text{eff}} + \frac{1}{2} \Delta \mathbf{u}'^T \Delta \Phi_{\mathbf{u}\mathbf{u}}^{\text{eff}} \Delta \mathbf{u}'$$

Loop on $\mathbf{q}_{n+1} \leftarrow \mathbf{q}_{n+1} + \Delta \mathbf{q}, \lambda \leftarrow \lambda + \Delta \lambda$

$$\Delta \mathbf{q}, \Delta \lambda = \arg \min_{\{\Delta \mathbf{q}', \Delta \lambda'\}} [\Delta \mathbf{q}'^T \Delta \lambda'] \Delta \Phi_{\text{aug}, \{\mathbf{q} \lambda\}} + \frac{1}{2} [\Delta \mathbf{q}'^T \Delta \lambda'] \Delta \Phi_{\text{aug}, \{\mathbf{q} \lambda\} \{\mathbf{q} \lambda\}} [\Delta \mathbf{q}'^T \Delta \lambda']^T$$

$$\Delta \Phi^{\text{eff}} = \Delta \Phi_{\text{aug}}(\mathbf{u}_{n+1}, \mathbf{q}_{n+1}, \lambda)$$



Loop until convergence

Loop on $\mathbf{u}_{n+1} \leftarrow \mathbf{u}_{n+1} + \Delta \mathbf{u}$

$$f(\Delta \mathbf{u}) = \Delta \mathbf{u}^T \Delta \Phi_{\mathbf{u}}^{\text{eff}} + \frac{1}{2} \Delta \mathbf{u}^T \Delta \Phi_{\mathbf{u}\mathbf{u}}^{\text{eff}} \Delta \mathbf{u}$$

Update $\mathbf{a}_{\mathbf{u}}, \mathbf{D}(\epsilon_{\mathbf{u}})$

$$\mathbf{b}_{\mathbf{u}} = \arg \min_{\mathbf{b}'_{\mathbf{u}}} \left(\frac{1}{2} \mathbf{b}'_{\mathbf{u}}^T \mathbf{D}^T \Delta \Phi_{\mathbf{u}\mathbf{u}}^{\text{eff}} \mathbf{D} \mathbf{b}'_{\mathbf{u}} + \mathbf{b}'_{\mathbf{u}}^T \mathbf{D}^T (\Delta \Phi_{\mathbf{u}}^{\text{eff}} + \Delta \Phi_{\mathbf{u}\mathbf{u}}^{\text{eff}} \mathbf{a}_{\mathbf{u}}) \right)$$

Loop on $\mathbf{q}_{n+1} \leftarrow \mathbf{q}_{n+1} + \Delta \mathbf{q}, \lambda \leftarrow \lambda + \Delta \lambda$

$$f(\Delta \mathbf{q}, \Delta \lambda) = [\Delta \mathbf{q}^T \Delta \lambda] \Delta \Phi_{\text{aug}, \{\mathbf{q} \lambda\}} + \frac{1}{2} [\Delta \mathbf{q}^T \Delta \lambda] \Delta \Phi_{\text{aug}, \{\mathbf{q} \lambda\} \{\mathbf{q} \lambda\}} [\Delta \mathbf{q}^T \Delta \lambda]^T$$

Update $\mathbf{a}_{\mathbf{q}}, \mathbf{D}(\epsilon_{\mathbf{q}})$

$$\mathbf{b}_{\mathbf{q}} = \arg \min_{\mathbf{b}'_{\mathbf{q}}} \left(\frac{1}{2} \mathbf{b}'_{\mathbf{q}}^T \mathbf{D}^T \Delta \Phi_{\text{aug}, \{\mathbf{q} \lambda\} \{\mathbf{q} \lambda\}} \mathbf{D} \mathbf{b}'_{\mathbf{q}} + \mathbf{b}'_{\mathbf{q}}^T \mathbf{D}^T (\Delta \Phi_{\text{aug}, \{\mathbf{q} \lambda\}} + \Delta \Phi_{\text{aug}, \{\mathbf{q} \lambda\} \{\mathbf{q} \lambda\}} \mathbf{a}_{\mathbf{q}}) \right)$$

$$\Delta \Phi^{\text{eff}} = \Delta \Phi_{\text{aug}}(\mathbf{u}_{n+1}, \mathbf{q}_{n+1}, \lambda)$$

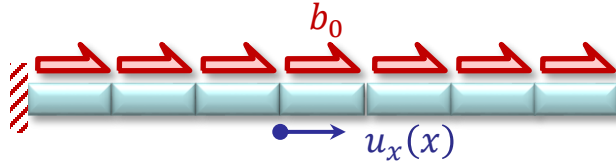
Quantum annealing



Quantum annealing



- Uniaxial-strain test



- Elastic case

- Simple minimization conducted on the displacement field

- Consider different numbers N of elements

- Consider different binarizations L of each nodal displacement: $b_{L-1} \dots b_0 \equiv \sum_{j=0}^{L-1} b_j 2^j = \boldsymbol{\beta}^T \mathbf{b}_i$

- Resolution by quantum annealing on DWave Advantage QPU

Loop on $\mathbf{u}_{n+1} \leftarrow \mathbf{u}_{n+1} + \Delta \mathbf{u}$

$$f(\Delta \mathbf{u}) = \Delta \mathbf{u}^T \Delta \Phi_{,u}^{\text{eff}} + \frac{1}{2} \Delta \mathbf{u}^T \Delta \Phi_{,uu}^{\text{eff}} \Delta \mathbf{u}$$

Update $\mathbf{a}_u, \mathbf{D}(\epsilon_u)$

$$\mathbf{b}_u = \arg \min_{\mathbf{b}'_u} \left(\frac{1}{2} \mathbf{b}'_u{}^T \mathbf{D}^T \Delta \Phi_{,uu}^{\text{eff}} \mathbf{D} \mathbf{b}'_u + \mathbf{b}'_u{}^T \mathbf{D}^T (\Delta \Phi_{,u}^{\text{eff}} + \Delta \Phi_{,uu}^{\text{eff}} \mathbf{a}_u) \right)$$

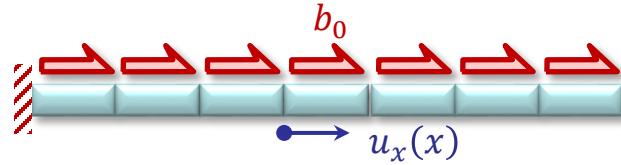
$$\mathbf{b}'_u{}^T \mathbf{A} \mathbf{b}'_u$$

Quantum
annealing

```
from dwave.system import DWaveSampler, EmbeddingComposite
sampler = EmbeddingComposite(DWaveSampler())
sampleset = sampler.sample_qubo(A, num_reads=100, annealing_time=20)
b = sampleset.first.sample
```

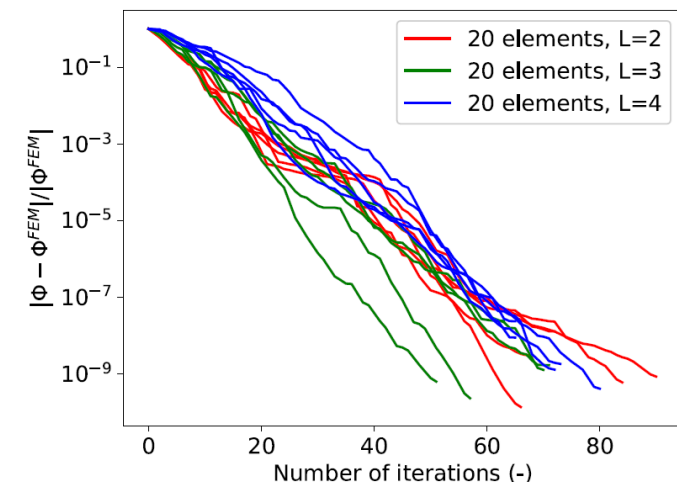
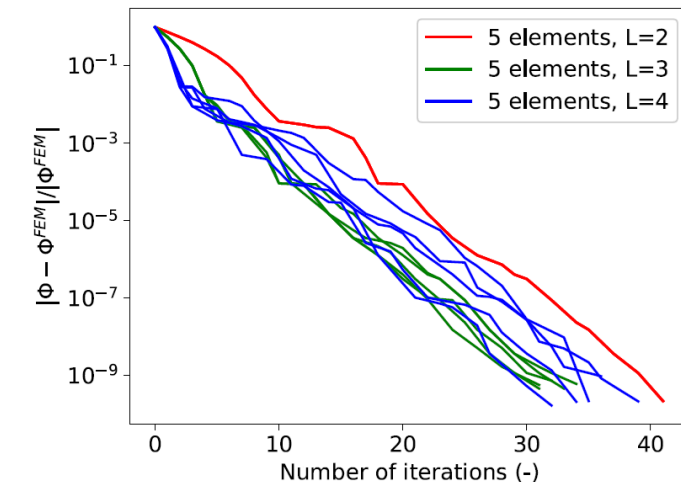
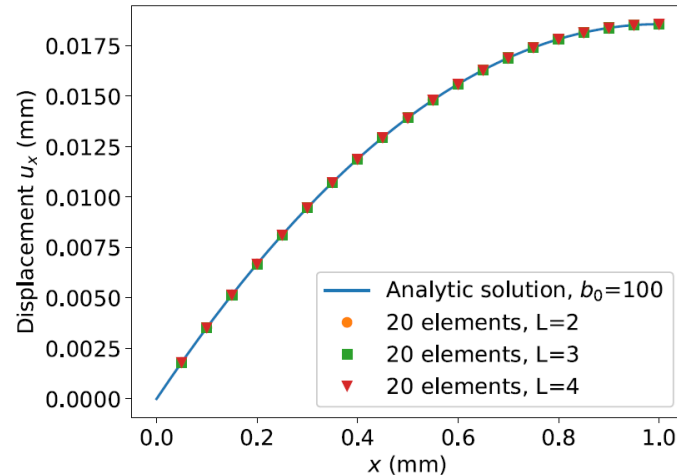
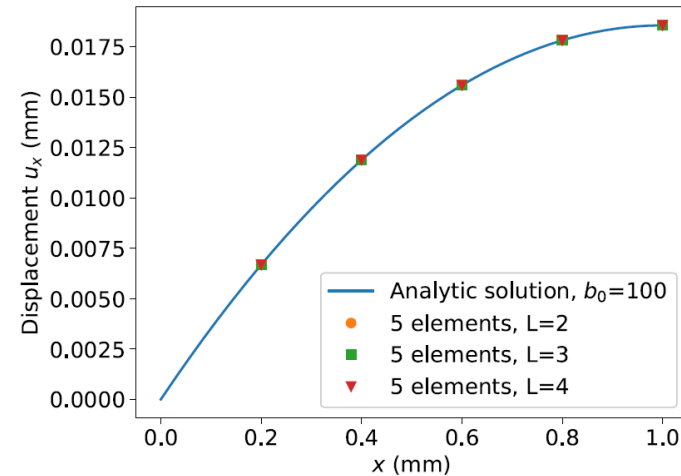
Application on 1D problems

- Uniaxial-strain test
- Elastic case



$$b_{L-1} \dots b_0 \equiv \sum_{j=0}^{L-1} b_j 2^j = \boldsymbol{\beta}^T \mathbf{b}_i$$

- Error analysis for 5 realizations for different total numbers of qubits

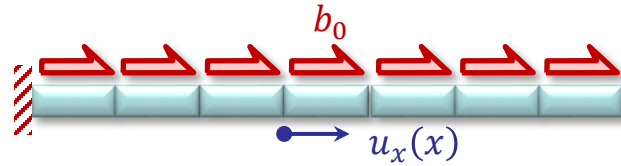


With increasing total number $N \times L$ of qubits

- Discrepancy between realizations increases
- Required number of iterations increases

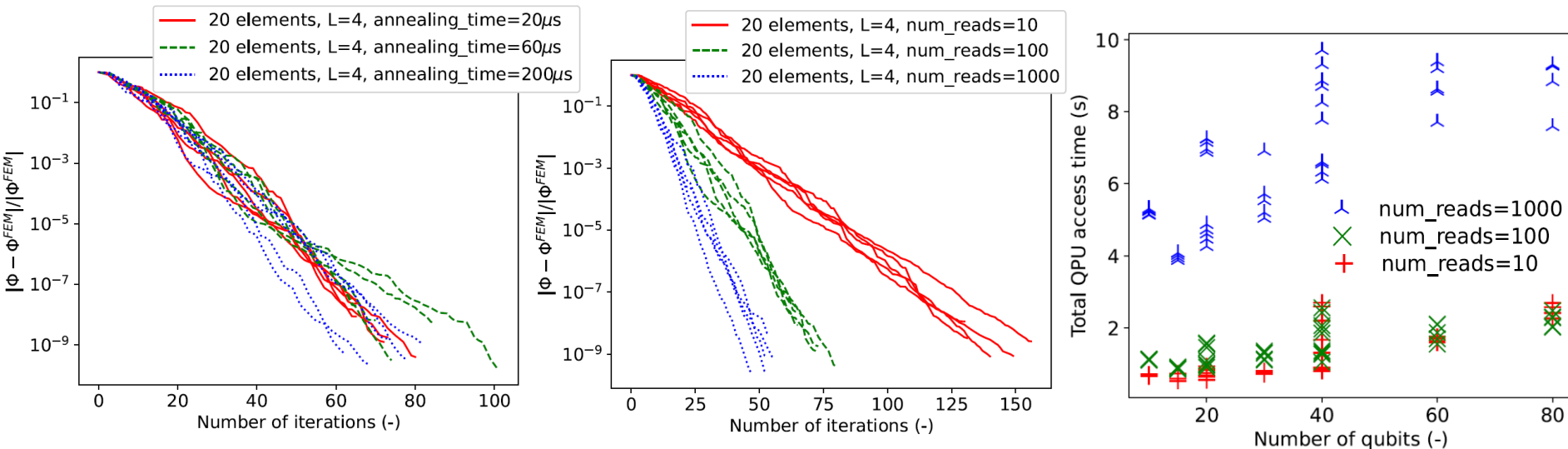
Application on 1D problems

- Uniaxial-strain test
- Elastic case



$$b_{L-1} \dots b_0 \equiv \sum_{j=0}^{L-1} b_j 2^j = \boldsymbol{\beta}^T \mathbf{b}_i$$

- Effect of annealing time and number of reads

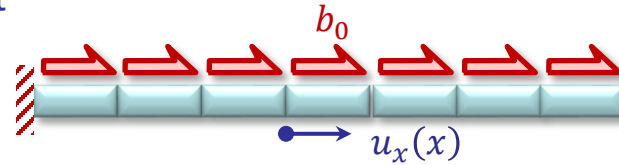


With increasing number of reads

- Required number of iterations decreases
- But not necessarily the quantum processing unit (QPU) access time

Application on 1D problems

- Uniaxial-strain test



- Elasto-plastic case

- Double minimization

- Binarizations L of each nodal displacement and internal variable: $b_{L-1} \dots b_0 \equiv \sum_{j=0}^{L-1} b_j 2^j = \boldsymbol{\beta}^T \mathbf{b}_i$

- Resolution by quantum annealing on DWave Advantage QPU

Loop until convergence

Loop on $\mathbf{u}_{n+1} \leftarrow \mathbf{u}_{n+1} + \Delta \mathbf{u}$

$$f(\Delta \mathbf{u}) = \Delta \mathbf{u}^T \Delta \Phi_{,\mathbf{u}}^{\text{eff}} + \frac{1}{2} \Delta \mathbf{u}^T \Delta \Phi_{,\mathbf{u}\mathbf{u}}^{\text{eff}} \Delta \mathbf{u}$$

Update $\mathbf{a}_{\mathbf{u}}, \mathbf{D}(\epsilon_{\mathbf{u}})$

$$\mathbf{b}_{\mathbf{u}} = \arg \min_{\mathbf{b}'_{\mathbf{u}}} \left(\frac{1}{2} \mathbf{b}'_{\mathbf{u}}{}^T \mathbf{D}^T \Delta \Phi_{,\mathbf{u}\mathbf{u}}^{\text{eff}} \mathbf{D} \mathbf{b}'_{\mathbf{u}} + \mathbf{b}'_{\mathbf{u}}{}^T \mathbf{D}^T (\Delta \Phi_{,\mathbf{u}}^{\text{eff}} + \Delta \Phi_{,\mathbf{u}\mathbf{u}}^{\text{eff}} \mathbf{a}_{\mathbf{u}}) \right)$$

Loop on $\mathbf{q}_{n+1} \leftarrow \mathbf{q}_{n+1} + \Delta \mathbf{q}, \lambda \leftarrow \lambda + \Delta \lambda$

$$f(\Delta \mathbf{q}, \Delta \lambda) = [\Delta \mathbf{q}^T \Delta \lambda] \Delta \Phi_{\text{aug},\{\mathbf{q} \lambda\}} + \frac{1}{2} [\Delta \mathbf{q}^T \Delta \lambda] \Delta \Phi_{\text{aug},\{\mathbf{q} \lambda\}\{\mathbf{q} \lambda\}} [\Delta \mathbf{q}^T \Delta \lambda]^T$$

Update $\mathbf{a}_{\mathbf{q}}, \mathbf{D}(\epsilon_{\mathbf{q}})$

$$\mathbf{b}_{\mathbf{q}} = \arg \min_{\mathbf{b}'_{\mathbf{q}}} \left(\frac{1}{2} \mathbf{b}'_{\mathbf{q}}{}^T \mathbf{D}^T \Delta \Phi_{\text{aug},\{\mathbf{q} \lambda\}\{\mathbf{q} \lambda\}} \mathbf{D} \mathbf{b}'_{\mathbf{q}} + \mathbf{b}'_{\mathbf{q}}{}^T \mathbf{D}^T (\Phi_{\text{aug},\{\mathbf{q} \lambda\}} + \Delta \Phi_{\text{aug},\{\mathbf{q} \lambda\}\{\mathbf{q} \lambda\}} \mathbf{a}_{\mathbf{q}}) \right)$$

$$\Delta \Phi^{\text{eff}} = \Delta \Phi_{\text{aug}}(\mathbf{u}_{n+1}, \mathbf{q}_{n+1}, \lambda)$$

Double minimization iterations

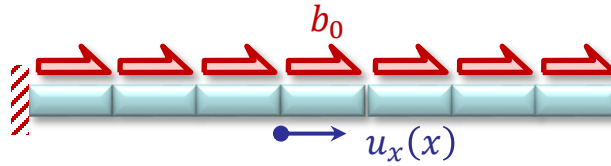
Local iterations

Quantum annealing

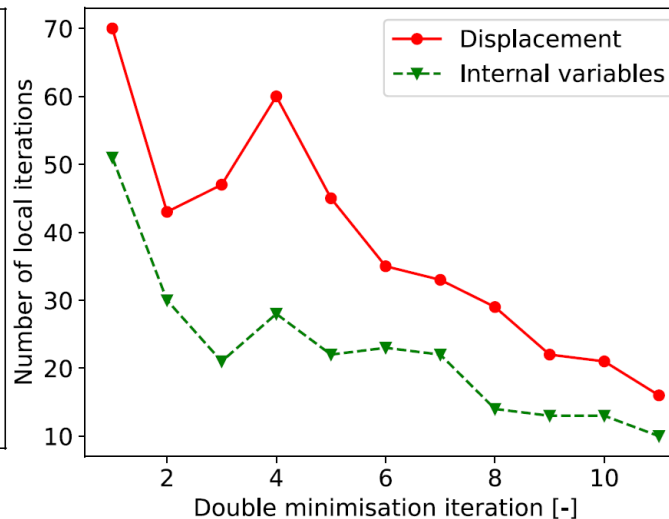
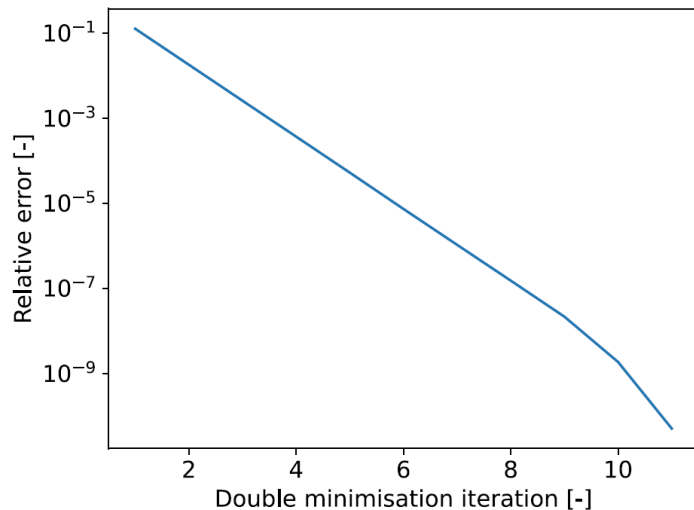
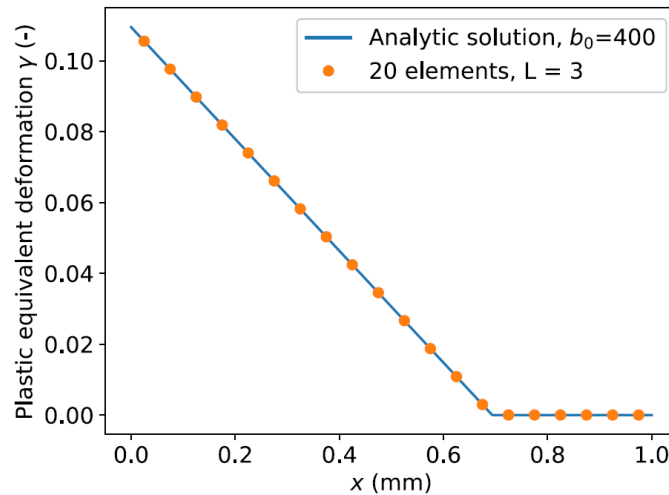
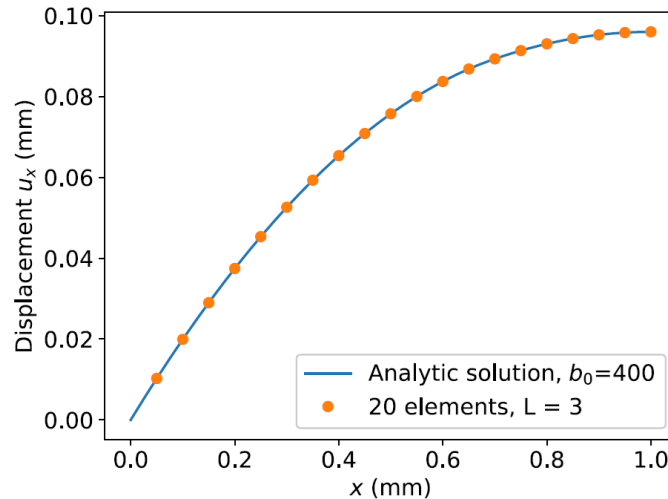
Quantum annealing

Application on 1D problems

- Uniaxial-strain test
- Elasto-plastic case



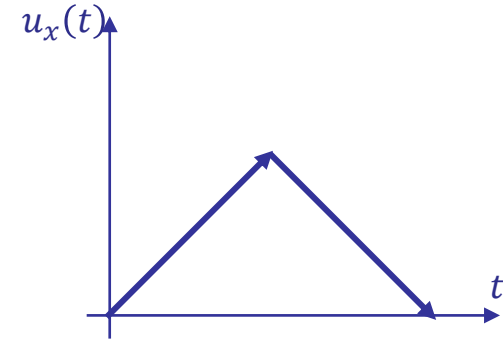
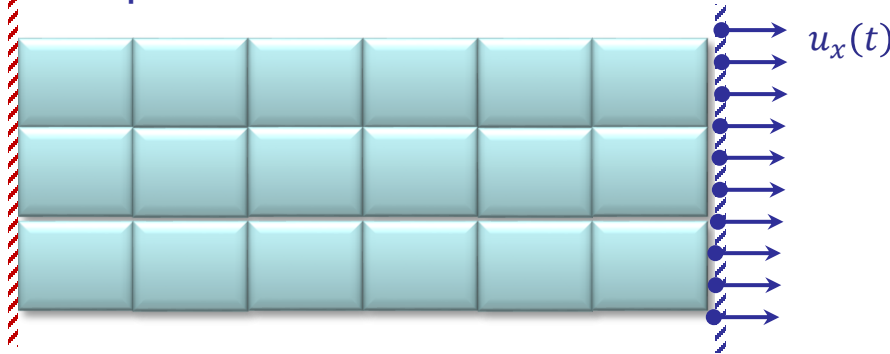
– Effect of double-minimization & local iterations



The number of local iterations decreases as the double minimisation iterations proceed

Application on 2D problems

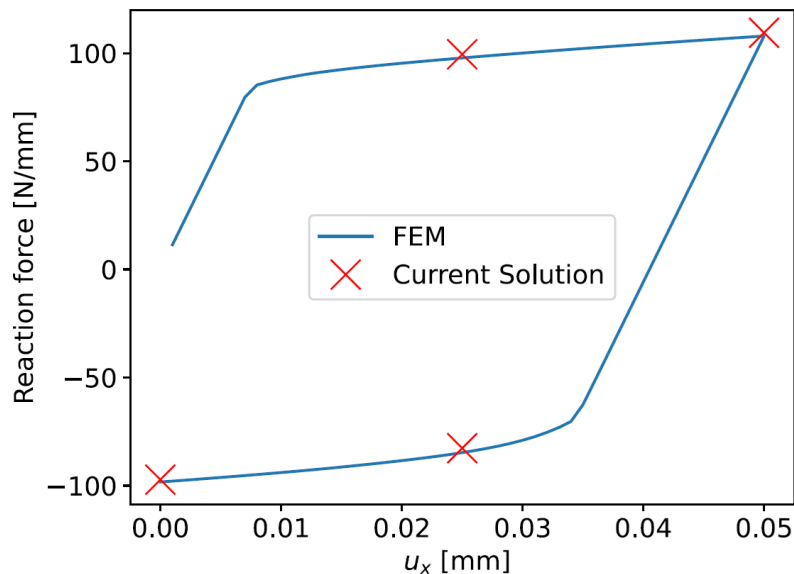
- 2D-elasto-plastic case



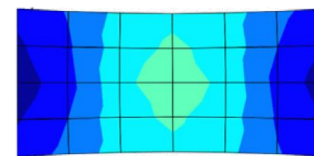
- Double minimization

- Binarizations L of each nodal displacement and internal variable: $b_{L-1} \dots b_0 \equiv \sum_{j=0}^{L-1} b_j 2^j = \boldsymbol{\beta}^T \mathbf{b}_i$

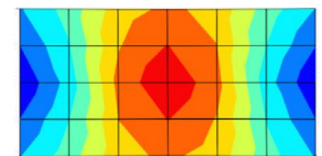
- Resolution by quantum annealing on DWave Advantage QPU



Current solution

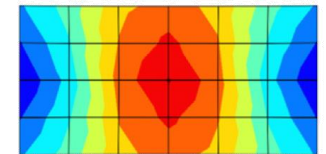
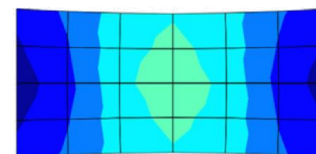


$t = 1$ s



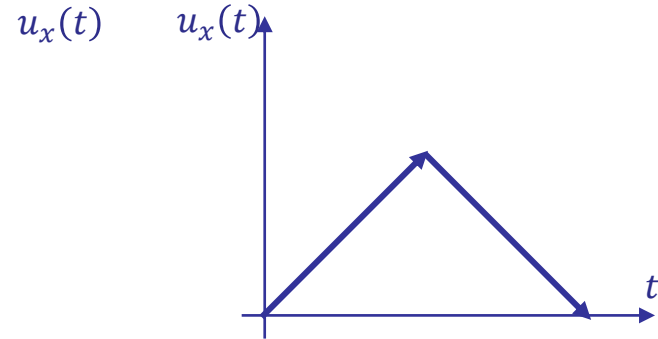
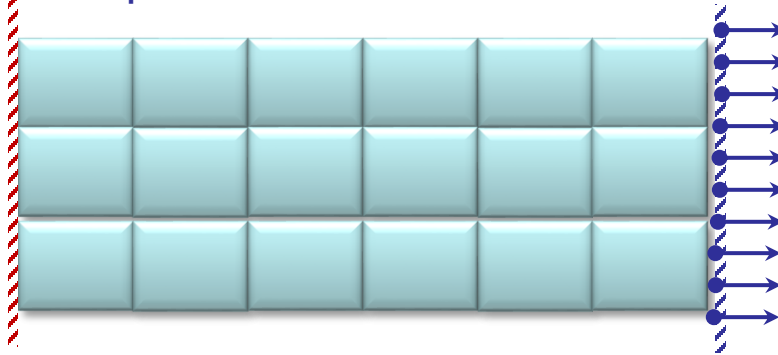
Equivalent plastic strain
0.01 0.15

FEM

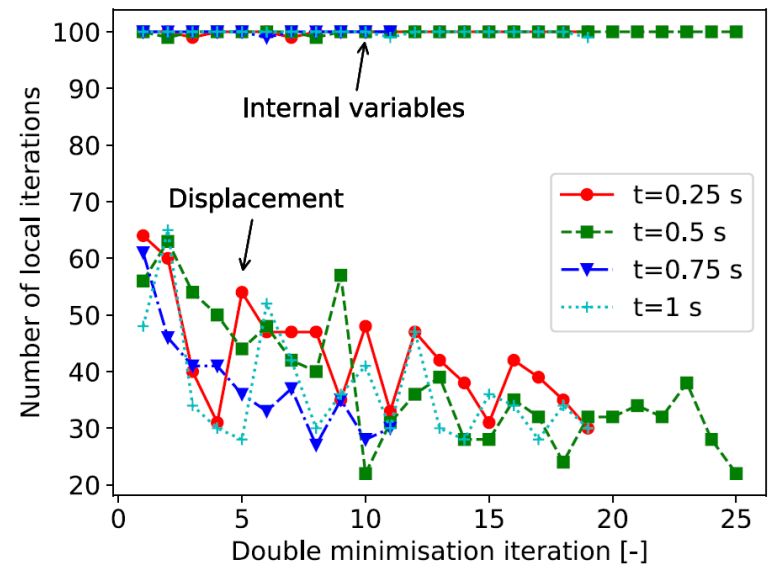
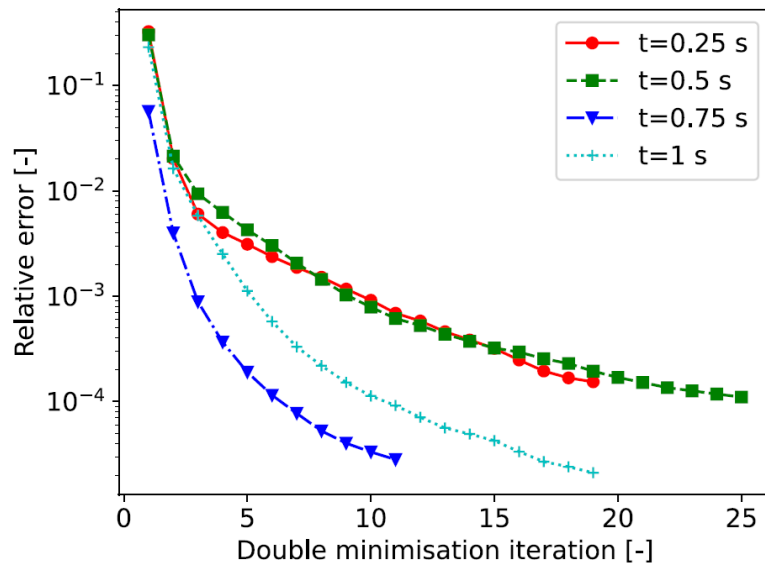


Application on 2D problems

- 2D-elasto-plastic case



– Effect of double-minimization & local iterations



- Application of QC to FEM
 - FE resolution needs to be rethought
 - It will probably stay advantageous to solve part of the problem on classical computers
- Quantum annealing
 - Real annealers can now be used
 - Efficient to solve optimization problem.... FEM is actually a minimization problem
 - Main current limitation is the number of connected qubits
- Publication
 - V. D. Nguyen, L. Wu, F. Remacle, L. Noels. A quantum annealing-sequential quadratic programming assisted finite element simulation for non-linear and history-dependent mechanical problems. *European Journal of Mechanics – A/solids* 105, 105254
[10.1016/j.euromechsol.2024.105254](https://doi.org/10.1016/j.euromechsol.2024.105254)
- Data and code on
 - Doi: [10.5281/zenodo.10451584](https://doi.org/10.5281/zenodo.10451584)