Introduction to quantum computing and non-linear finite-element (re)formulation for quantum annealing

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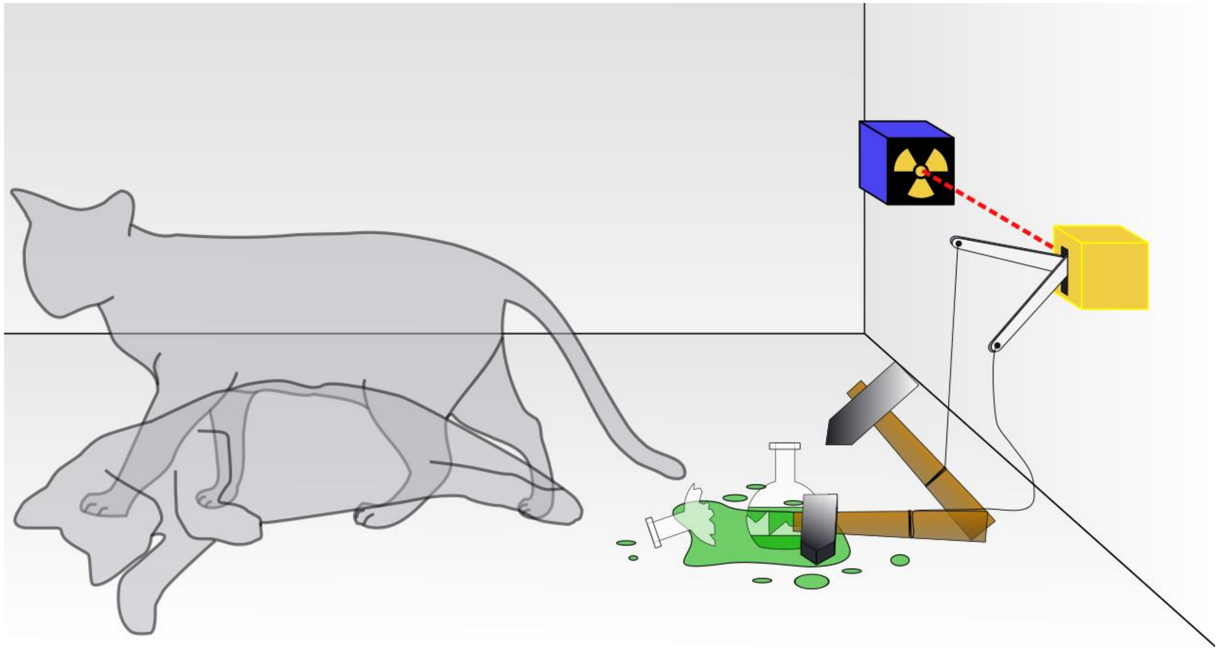

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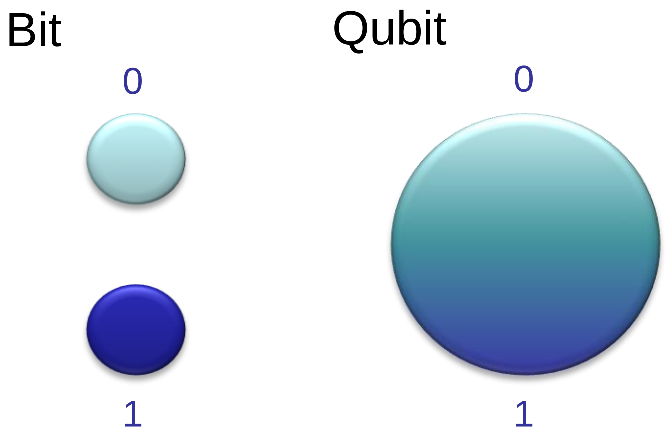
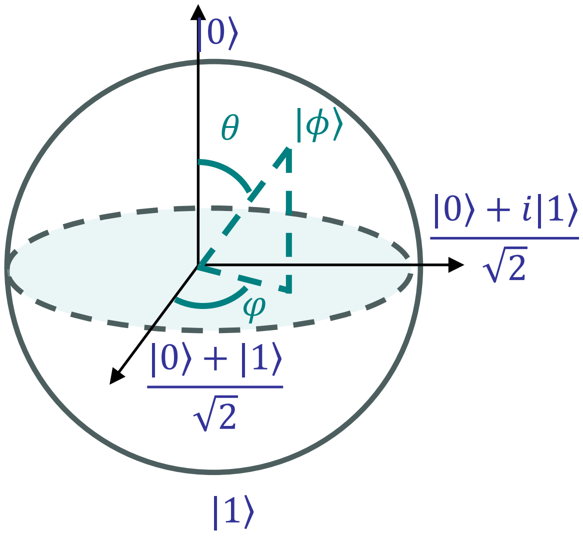
Introduction to Quantum Computing

- 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: $\begin{cases} |\phi\rangle = \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \alpha|0\rangle + \beta|1\rangle \\ \langle\phi| = (\alpha^* \quad \beta^*) \end{cases}$ $|\alpha|^2 + |\beta|^2 = 1$
    - Qubit represented on the surface of the Bloch Sphere

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

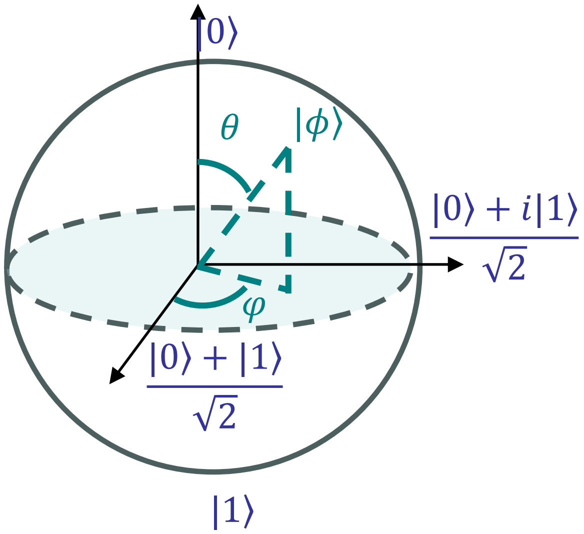


    - Global phase $\mathrm{e}^{i\delta}$ has no observable consequence

      (NB relative phase has consequence)
  - At measurement (in the computational basis)
    - Either $|0\rangle$ or $|1\rangle$ with respective probability $|\alpha|^2$ and $|\beta|^2$

Introduction to Quantum Computing

- Multiple (connected) qubits:
  - Product state of 2 1-qubit states: $\begin{cases} |\phi_0\rangle = \alpha_0|0\rangle + \beta_0|1\rangle \\ |\phi_1\rangle = \alpha_1|0\rangle + \beta_1|1\rangle \end{cases}$



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

  - Most general 2-qubit state

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

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.

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

  - 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:

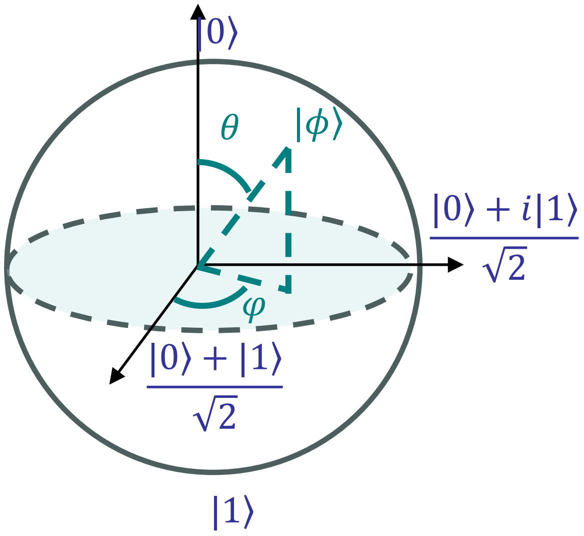
$$|\boldsymbol{\phi}\rangle = \phi_0|0\rangle \otimes |0\rangle \ldots \otimes |0\rangle + \phi_1|0\rangle \otimes |0\rangle \ldots \otimes |1\rangle + \cdots + \phi_{2^K-1}|1\rangle \ldots \otimes |1\rangle \otimes |1\rangle$$

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

Introduction to Quantum Computing

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

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

  - 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: $\mathbf{C}_{10} = \begin{bmatrix}1 & 0 & 0 & 0\\ 0 & 1 & 0 & 0\\ 0 & 0 & 0 & 1\\ 0 & 0 & 1 & 0\end{bmatrix}$

$$\begin{array}{lcl} |x\rangle — & \multirow{2}{*}{$\boxed{\mathbf{C}_{10}}$} & — |x\rangle \\ |y\rangle — & & — |y \oplus x\rangle \end{array}$$

$x, y \in \{0,1\}$, the second qubit is flipped if and only if first is 1

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

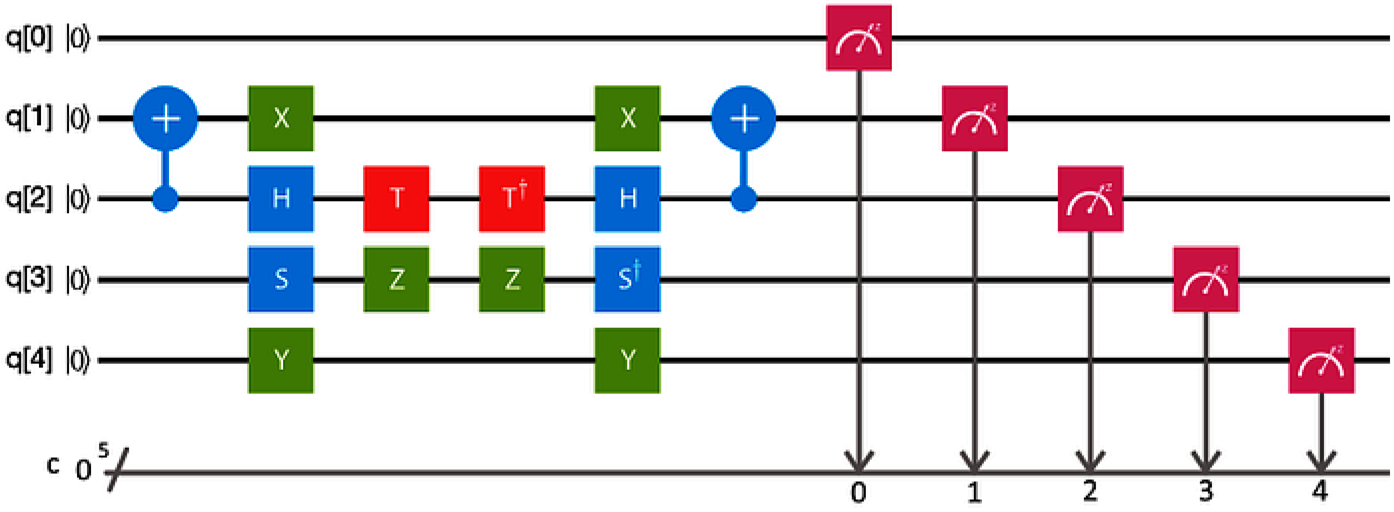
$$\begin{bmatrix}1\\0\\0\\0\end{bmatrix} \quad \begin{bmatrix}0\\1\\0\\0\end{bmatrix} \quad \begin{bmatrix}0\\0\\1\\0\end{bmatrix} \quad \begin{bmatrix}0\\0\\0\\1\end{bmatrix}$$

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

  - Gate on n qubits …

Introduction to Quantum Computing

- 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

Introduction to Quantum Computing

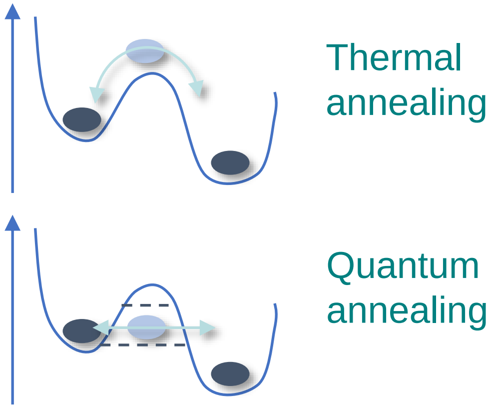
- Quantum annealer
  - Goal: finding the ground state of a Hamiltonian $\mathbf{H}$

$$|\boldsymbol{\phi}_0\rangle = \arg\min_{|\boldsymbol{\phi}\rangle} \langle\boldsymbol{\phi}|\mathbf{H}\,|\boldsymbol{\phi}\rangle$$

  - Based on quantum adiabatic theorem:
    - Considering a time-varying Hamiltonian $\mathbf{H}_{\mathbf{QA}}(t)$ 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

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

  - 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-based quantum annealing

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

$$|\boldsymbol{\phi}_0\rangle = \arg\min_{|\boldsymbol{\phi}\rangle} \langle\boldsymbol{\phi}|\mathbf{H}\,|\boldsymbol{\phi}\rangle$$

  - Some definitions
    - Set of K qubits $V = \{0, \ldots K-1\}$
    - 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: $\mathbf{Z}_i = \underbrace{\mathbf{I}}_{0} \otimes \cdots \otimes \mathbf{I} \otimes \underbrace{\mathbf{Z}}_{i} \otimes \mathbf{I} \otimes \cdots \otimes \underbrace{\mathbf{I}}_{K-1}$
    - Pauli- Z operator applied on qubits i and j:

$$\mathbf{Z}_{ij} = \underbrace{\mathbf{I}}_{0} \otimes \cdots \otimes \mathbf{I} \otimes \underbrace{\mathbf{Z}}_{i} \otimes \mathbf{I} \otimes \cdots \otimes \mathbf{I} \otimes \underbrace{\mathbf{Z}}_{j} \otimes \mathbf{I} \otimes \cdots \otimes \underbrace{\mathbf{I}}_{K-1}$$

  - 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

Ising Hamiltonian-based quantum annealing

- Quadratic Unconstrained Binary Optimization (QUBO)
  - Goal: finding the ground state of a Hamiltonian $\mathbf{H}$

$$|\boldsymbol{\phi}_0\rangle = \arg\min_{|\boldsymbol{\phi}\rangle} \langle \boldsymbol{\phi}|\mathbf{H}\,|\boldsymbol{\phi}\rangle \qquad \text{with} \quad \mathbf{H} = \sum_{i\in V} h_i \mathbf{Z}_i + \sum_{(i,j)\in E} J_{ij}\mathbf{Z}_{ij}$$

  - In terms of spin variables
    - Computational basis of $\mathbf{H}$ $\quad |\boldsymbol{\phi}\rangle = |b_0\, b_1\, \dots b_{K-1}\rangle$ with $\quad b_i \in \{0,1\}$
    - We have successively

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

$$\mathbf{Z}_i = \underbrace{\mathbf{I}}_{0} \otimes \cdots \otimes \mathbf{I} \otimes \underbrace{\mathbf{Z}}_{i} \otimes \mathbf{I} \otimes \cdots \otimes \underbrace{\mathbf{I}}_{K-1} \quad \Rightarrow \quad \mathbf{Z}_i|\boldsymbol{\phi}\rangle = (-1)^{b_i}|\boldsymbol{\phi}\rangle$$

$$\mathbf{Z}_{ij} = \underbrace{\mathbf{I}}_{0} \otimes \cdots \otimes \mathbf{I} \otimes \underbrace{\mathbf{Z}}_{i} \otimes \mathbf{I} \otimes \cdots \otimes \mathbf{I} \otimes \underbrace{\mathbf{Z}}_{j} \otimes \mathbf{I} \otimes \cdots \otimes \underbrace{\mathbf{I}}_{K-1} \quad \Rightarrow \quad \mathbf{Z}_{ij}|\boldsymbol{\phi}\rangle = (-1)^{b_i}(-1)^{b_j}|\boldsymbol{\phi}\rangle$$

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

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

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

User programmable parameters

$$\Rightarrow \quad |\boldsymbol{\phi}_0\rangle = \arg\min_{\boldsymbol{\phi}} \langle \boldsymbol{\phi}|\mathbf{H}\,|\boldsymbol{\phi}\rangle \quad \Leftrightarrow \quad \mathbf{s} = \arg\min_{\mathbf{s}'} \mathcal{F}_{\text{Ising}}(\mathbf{s}'; \boxed{\mathbf{h},\mathbf{J}})$$

Ising Hamiltonian-based quantum annealing

- Quadratic Unconstrained Binary Optimization (QUBO)
  - Goal: finding the ground state of a Hamiltonian $\mathbf{H}$

$$|\boldsymbol{\phi}_0\rangle = \arg\min_{|\boldsymbol{\phi}\rangle} \langle\boldsymbol{\phi}|\mathbf{H}\,|\boldsymbol{\phi}\rangle \qquad \text{with} \quad \mathbf{H} = \sum_{i\in V} h_i \mathbf{Z}_i + \sum_{(i,j)\in E} J_{ij}\mathbf{Z}_{ij}$$

  - In terms of spin variables
    - Computational basis of $\mathbf{H}$ $\quad |\boldsymbol{\phi}\rangle = |b_0\ b_1\ \dots b_{K-1}\rangle$ $\quad$ with $\quad b_i \in \{0,1\}$
    - 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 $\quad \mathbf{h} = [h_i\ \ \forall i \in V]$ $\quad$ & $\mathbf{J} = \left[J_{ij}\ \ \forall (i,j) \in E\right]$

User programmable parameters

$$\Rightarrow\ |\boldsymbol{\phi}_0\rangle = \arg\min_{\boldsymbol{\phi}} \langle\boldsymbol{\phi}|\mathbf{H}\,|\boldsymbol{\phi}\rangle \quad \Leftrightarrow \quad \mathbf{s} = \arg\min_{\mathbf{s}'} \mathcal{F}_{\text{Ising}}(\mathbf{s}';\mathbf{h},\mathbf{J})$$

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

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

$$\Rightarrow\ |\boldsymbol{\phi}_0\rangle = \arg\min_{\boldsymbol{\phi}} \langle\boldsymbol{\phi}|\mathbf{H}\,|\boldsymbol{\phi}\rangle \quad \Leftrightarrow \quad \mathbf{b} = \arg\min_{\mathbf{b}'} \mathcal{F}_{\text{QUBO}}(\mathbf{b}';\mathbf{A})$$

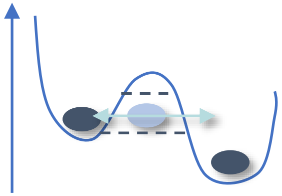
User programmable parameters

Ising Hamiltonian-based quantum annealing

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

    $$|\boldsymbol{\phi}_0\rangle = \arg\min_{|\boldsymbol{\phi}\rangle} \langle\boldsymbol{\phi}|\mathbf{H}\,|\boldsymbol{\phi}\rangle \qquad \text{with} \quad \mathbf{H} = \sum_{i\in V} h_i \mathbf{Z}_i + \sum_{(i,j)\in E} J_{ij}\mathbf{Z}_{ij}$$

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



Quantum annealing

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

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

User programmable parameters

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

Quantum computing & finite elements

- Set of PDEs to be solved
  - Strong form $\Rightarrow$ Weak form:

$$\boldsymbol{\nabla}\cdot\boldsymbol{\sigma}(\boldsymbol{x})+\boldsymbol{b_0}(\boldsymbol{x})=\mathbf{0} \quad\Rightarrow\quad \int_V \boldsymbol{\sigma}(\boldsymbol{x}):\nabla\otimes^s \boldsymbol{\delta u}(\boldsymbol{x})dV = \int_V \boldsymbol{b}_0\cdot\boldsymbol{\delta u}dV + \int_{\partial_N V}\boldsymbol{n}\cdot\boldsymbol{\sigma}\cdot\boldsymbol{\delta u}d\partial V$$

  - Constitutive model:

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

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

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

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

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

$$\Rightarrow\quad \boldsymbol{\delta U}_{\boldsymbol{b}}^{\mathrm{T}}\cdot\sum_{\Xi}\mathbf{B}_b^{\mathrm{T}}(\Xi)\,\boldsymbol{\sigma}\big((\Xi)\big)\omega^{\Xi}=\boldsymbol{\delta U}_{\boldsymbol{b}}^{\mathrm{T}}\cdot\sum_{\Xi}N_b(\Xi)\,\boldsymbol{b}_0(\Xi)\omega^{\Xi}$$

Omitting surface tractions

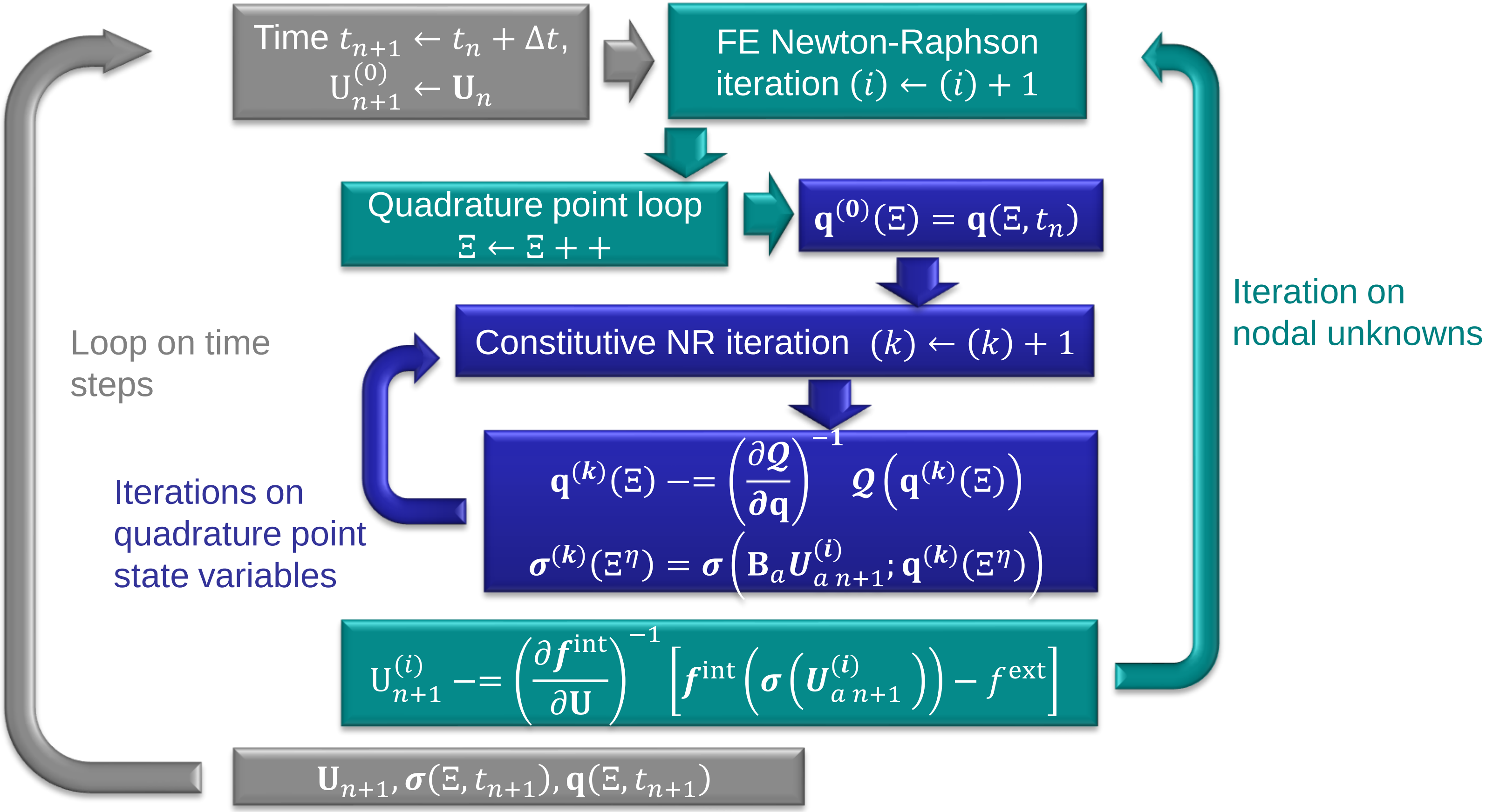
$$\Rightarrow\quad \boldsymbol{f}_b^{\mathrm{int}}=\sum_{\Xi}\mathbf{B}_b^{\mathrm{T}}(\Xi)\,\boldsymbol{\sigma}(\Xi)\omega^{\Xi}=\sum_{\Xi}N_b(\Xi)\,\boldsymbol{b}_0(\Xi)\omega^{\Xi}=\boldsymbol{f}_b^{\mathrm{ext}}$$

$$\text{with}\quad \left\{\begin{array}{l}\boldsymbol{\sigma}(\Xi,t_{n+1})=\boldsymbol{\sigma}\big(\mathbf{B}_a(\Xi)\boldsymbol{U}_{a\,n+1};\mathbf{q}(\Xi,t_{\boldsymbol{n+1}})\big)\\[2ex] \boldsymbol{Q}\big(\boldsymbol{\sigma}(\Xi,t_{n+1}),\mathbf{q}(\Xi,t_{n+1}),\mathbf{q}(\Xi,t_n)\big)=\mathbf{0}\end{array}\right.$$

Quantum computing & finite elements

- Finite element formulation
  - Resulting non-linear system of equations on time interval $[t_n \; t_{n+1}]$

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



Time $t_{n+1} \leftarrow t_n + \Delta t$, $\mathrm{U}_{n+1}^{(0)} \leftarrow \mathbf{U}_n$

FE Newton-Raphson iteration $(i) \leftarrow (i) + 1$

Quadrature point loop $\Xi \leftarrow \Xi + +$

$\mathbf{q}^{(0)}(\Xi) = \mathbf{q}(\Xi, t_n)$

Constitutive NR iteration $(k) \leftarrow (k) + 1$

$$\mathbf{q}^{(k)}(\Xi) -= \left(\frac{\partial \boldsymbol{Q}}{\partial \mathbf{q}}\right)^{-1} \boldsymbol{Q}\left(\mathbf{q}^{(k)}(\Xi)\right)$$

$$\boldsymbol{\sigma}^{(k)}(\Xi^{\eta}) = \boldsymbol{\sigma}\left(\mathrm{B}_a \boldsymbol{U}_{a\,n+1}^{(i)}; \mathbf{q}^{(k)}(\Xi^{\eta})\right)$$

$$\mathrm{U}_{n+1}^{(i)} -= \left(\frac{\partial \boldsymbol{f}^{\text{int}}}{\partial \mathbf{U}}\right)^{-1} \left[\boldsymbol{f}^{\text{int}}\left(\boldsymbol{\sigma}\left(\boldsymbol{U}_{a\,n+1}^{(i)}\right)\right) - f^{\text{ext}}\right]$$

$\mathbf{U}_{n+1}, \boldsymbol{\sigma}(\Xi, t_{n+1}), \mathbf{q}(\Xi, t_{n+1})$

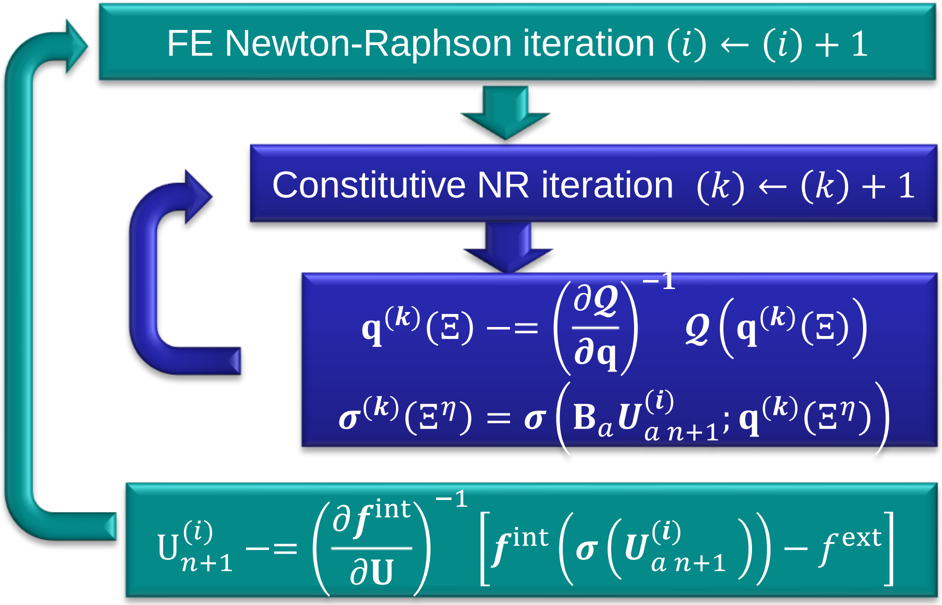
Loop on time steps

Iterations on quadrature point state variables

Iteration on nodal unknowns

Quantum computing & finite elements

- Consider classical finite element resolution on Quantum Computers?



FE Newton-Raphson iteration $(i) \leftarrow (i) + 1$

Constitutive NR iteration $(k) \leftarrow (k) + 1$

$$\mathbf{q}^{(k)}(\Xi) -= \left(\frac{\partial \mathcal{Q}}{\partial \mathbf{q}}\right)^{-1} \mathcal{Q}\left(\mathbf{q}^{(k)}(\Xi)\right)$$

$$\boldsymbol{\sigma}^{(k)}(\Xi^{\eta}) = \boldsymbol{\sigma}\left(\mathbf{B}_a \boldsymbol{U}_{a\,n+1}^{(i)}; \mathbf{q}^{(k)}(\Xi^{\eta})\right)$$

$$\mathrm{U}_{n+1}^{(i)} -= \left(\frac{\partial \boldsymbol{f}^{\mathrm{int}}}{\partial \mathbf{U}}\right)^{-1} \left[\boldsymbol{f}^{\mathrm{int}}\left(\boldsymbol{\sigma}\left(\boldsymbol{U}_{a\,n+1}^{(i)}\right)\right) - f^{\mathrm{ext}}\right]$$

  - 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 intricated NR loops?
    - Do we even need to use the discretized form of the weak form?

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

Quantum computing & finite elements

- 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 $\boldsymbol{\varepsilon}(x) = \nabla \otimes^{s} \boldsymbol{u}(\boldsymbol{x})$
    - Stress results from $\boldsymbol{\sigma}(\boldsymbol{x}) = \frac{\partial \Psi}{\partial \boldsymbol{\varepsilon}} = \mathbb{C}(x):\boldsymbol{\varepsilon}(x) = \mathbb{C}(x):\left(\nabla \otimes^{s} \boldsymbol{u}(\boldsymbol{x})\right)$
  - Finite element form:
    - At quadrature point using nodal shape function derivatives: $\boldsymbol{\sigma}(\Xi) = \boldsymbol{C}(\Xi)\mathbf{B}_a(\Xi)\boldsymbol{U}_a$
    - FE equations $\boldsymbol{f}_b^{\text{int}} = \sum_{\Xi} \mathbf{B}_b^{\text{T}}(\Xi)\, \boldsymbol{\sigma}(\Xi)\omega^{\Xi} = \boldsymbol{f}_b^{\text{ext}}$

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

    - Defining the internal energy and work of external forces

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

⇨ The solution of the FE equations minimizes the energy

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

  - We are looking for the ground state of a Hamiltonian

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

Quantum computing & finite elements

- Non-linear finite element resolution on Quantum Computers?
  - Weak form: $\int_V \boldsymbol{\sigma}(\boldsymbol{x}) : \nabla \otimes^s \boldsymbol{\delta u}(\boldsymbol{x}) dV = \int_V \boldsymbol{b}_0 \cdot \boldsymbol{\delta u} dV$
  - Assuming non-linear elasticity
    - Existence of a free energy $\Psi\left(\boldsymbol{\varepsilon}(x)\right)$ with $\boldsymbol{\varepsilon}(x) = \nabla \otimes^s \boldsymbol{u}(\boldsymbol{x})$
    - Stress results from $\boldsymbol{\sigma}(\boldsymbol{x}) = \frac{\partial \Psi}{\partial \boldsymbol{\varepsilon}}$

    The weak form becomes $\int_V \frac{\partial \Psi(\boldsymbol{x})}{\partial \boldsymbol{\varepsilon}} : \boldsymbol{\delta\varepsilon}(\boldsymbol{x}) dV = \int_V \boldsymbol{b}_0 \cdot \boldsymbol{\delta u} dV$
  - Introduction of a functional
    - $\Phi\left(\boldsymbol{u}(V)\right) = \int_V \Psi\left(\nabla \otimes^s \boldsymbol{u}(\boldsymbol{x})\right) dV - W^{\text{ext}}\left(\boldsymbol{u}(V)\right)$ & $W^{\text{ext}} = \int_V \boldsymbol{b}_0 \cdot \boldsymbol{u}(\boldsymbol{x}) dV$
    - The weak form results from nulling the Gâteaux derivative

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

    The solution of the weak form minimizes the energy: $\boldsymbol{u}(V) = \arg\min_{\boldsymbol{u}'(V)} \Phi\left(\boldsymbol{u}'(V)\right)$
  - We are looking for the solution of a minimization problem
    - The potential is convex
    - But it is not quadratic
    - Quid inelastic materials?

Quantum computing & finite elements

- Non-linear finite element resolution on Quantum Computers?
  - Inelastic materials
    - Existence of a Helmholtz free energy $\Psi(\boldsymbol{\varepsilon}(x), \mathbf{q}(x))$ with $\begin{cases} \text{internal variables } \mathbf{q}(x) \\ \boldsymbol{\varepsilon}(x) = \nabla \otimes^{s} \boldsymbol{u}(\boldsymbol{x}) \end{cases}$
  - 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

      ⇒ $\boldsymbol{\sigma} = \frac{\partial \Psi}{\partial \boldsymbol{\varepsilon}}$ ⇒ for an irreversible process: $\mathcal{D} = \mathbf{Y} \cdot \dot{\mathbf{q}} \geq 0$ with $\mathbf{Y} = -\frac{\partial \Psi}{\partial \mathbf{q}}$
  - Postulate the existence of a pseudo-potential $\Theta(\dot{\mathbf{q}})$ and its convex dual $\Theta^{*}(\mathbf{Y})$
    - $\Theta(\dot{\mathbf{q}}) = \max_{\mathbf{Y}} [\mathbf{Y} \cdot \dot{\mathbf{q}} - \Theta^{*}(\mathbf{Y})]$ ⇒ $\dot{\mathbf{q}} = \frac{\partial \Theta^{*}(\mathbf{Y})}{\partial \mathbf{Y}}$ & $\mathbf{Y} = \frac{\partial \Theta(\dot{\mathbf{q}})}{\partial \dot{\mathbf{q}}}$
  - Power functional $\mathcal{E}$
    - New independent variables $(\dot{\boldsymbol{\varepsilon}}, \dot{\mathbf{q}})$
    - $\mathcal{E}(\dot{\boldsymbol{\varepsilon}}, \dot{\mathbf{q}}) = \dot{\Psi} + \Theta(\dot{\mathbf{q}}) = \frac{\partial \Psi}{\partial \boldsymbol{\varepsilon}} : \dot{\boldsymbol{\varepsilon}} - \mathbf{Y} \cdot \dot{\mathbf{q}} + \Theta(\dot{\mathbf{q}})$

      ⇒ $\frac{\partial \mathcal{E}}{\partial \dot{\mathbf{q}}} = -\mathbf{Y} + \frac{\partial \Theta(\dot{\mathbf{q}})}{\partial \dot{\mathbf{q}}} = \mathbf{0}$ ⇒ $\mathcal{E}$ has to be minimized with respect to internal state
    - Effective power functional* $\mathcal{E}^{\mathrm{eff}}(\dot{\boldsymbol{\varepsilon}}) = \min_{\dot{\mathbf{q}}} \mathcal{E}(\dot{\boldsymbol{\varepsilon}}, \dot{\mathbf{q}})$ with $\boldsymbol{\sigma} = \frac{\partial \Psi}{\partial \boldsymbol{\varepsilon}} = \frac{\partial \mathcal{E}^{\mathrm{eff}}}{\partial \dot{\boldsymbol{\varepsilon}}}$
  - The constitutive model is also a minimization problem

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

Quantum computing & finite elements

- Non-linear finite element resolution on Quantum Computers?
  - In elasticity we had
    - $\boldsymbol{u}(V) = \arg\min_{\boldsymbol{u}'(V)} \Phi\big(\boldsymbol{u}'(V)\big)$ with $\Phi\big(\boldsymbol{u}(V)\big) = \int_V \Psi\big(\nabla \otimes^s \boldsymbol{u}(\boldsymbol{x})\big) dV - W^{\text{ext}}\big(\boldsymbol{u}(\boldsymbol{x})\big)$
  - Double minimization problem in inelasticity
    - Power functional $\mathcal{E}$

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

    - Volume power functional

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

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

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

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

    - The problem solution reads

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

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

Quantum computing & finite elements

- Example: J2-elasto-plasticity
  - Helmholtz free energy
    - $\Psi(\boldsymbol{\varepsilon},\mathbf{q}) = \frac{1}{2}\left(\boldsymbol{\varepsilon}-\boldsymbol{\varepsilon}^{\mathrm{pl}}\right):\mathbb{C}^{\mathrm{el}}:\left(\boldsymbol{\varepsilon}-\boldsymbol{\varepsilon}^{\mathrm{pl}}\right)$ with $\boldsymbol{\Delta\varepsilon}^{\mathrm{pl}} = \Delta\gamma\mathbf{N}$

    Internal variables $\mathbf{q} = \{\mathbf{N},\Delta\gamma\}$ under constraints $\mathbf{N}:\mathbf{N} = \frac{3}{2}$, $\mathrm{tr}(\mathbf{N}) = 0$ & $\Delta\gamma \geq 0$
  - Dissipation pseudo-potential
    - $\Theta(\dot{\mathbf{q}}) = \begin{cases} \left(\sigma_y^0 + R(\gamma)\right)\dot{\gamma} & \text{if } \dot{\gamma} \geq 0 \\ \infty & \text{otherwise} \end{cases}$ $\Theta^*(\mathbf{Y}) = \begin{cases} 0 & \text{if } \sigma_{\mathrm{eq}} - \sigma_y^0 - R \leq 0 \\ \infty & \text{otherwise} \end{cases}$
  - Increment of the energy functional
    - $\mathcal{E}(\dot{\boldsymbol{\varepsilon}},\dot{\mathbf{q}}) = \dot{\Psi} + \Theta(\dot{\mathbf{q}})$

$$\Delta\mathcal{E}(\boldsymbol{\varepsilon}_{n+1},\mathbf{q}) = \frac{1}{2}\left(\boldsymbol{\varepsilon}_{n+1} - \Delta\gamma\mathbf{N} - \boldsymbol{\varepsilon}_n^{\mathrm{pl}}\right):\mathbb{C}^{\mathrm{el}}:\left(\boldsymbol{\varepsilon}_{n+1} - \Delta\gamma\mathbf{N} - \boldsymbol{\varepsilon}_n^{\mathrm{pl}}\right) + \int_{\gamma_n}^{\gamma_{n+1}} \left(\sigma_y^0 + R(\gamma')\right) d\gamma' \\ -\frac{1}{2}\left(\boldsymbol{\varepsilon}_n - \boldsymbol{\varepsilon}_n^{\mathrm{pl}}\right):\mathbb{C}^{\mathrm{el}}:\left(\boldsymbol{\varepsilon}_n - \boldsymbol{\varepsilon}_n^{\mathrm{pl}}\right)$$

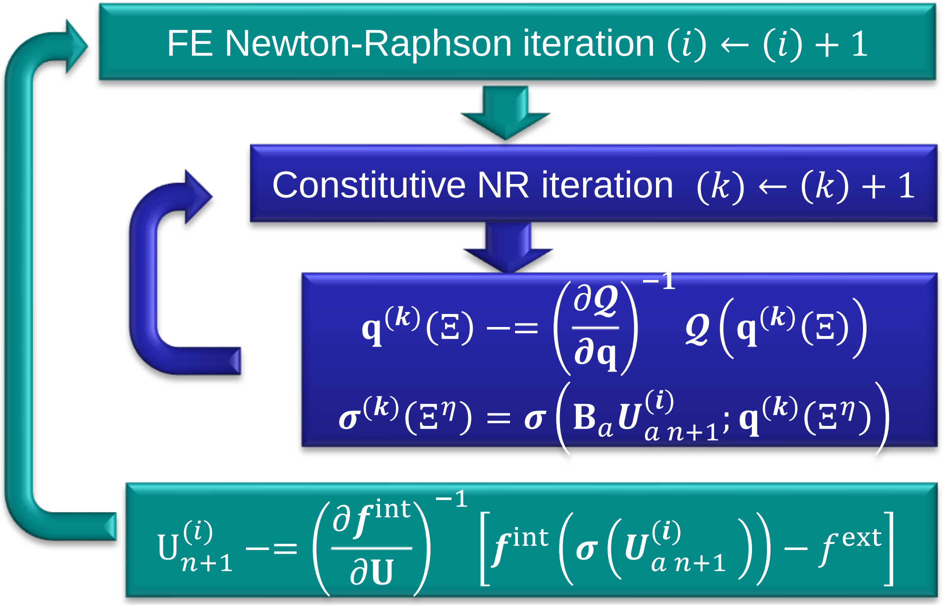
$\Delta\mathcal{E}^{\mathrm{eff}}(\boldsymbol{\varepsilon}) = \min_{\mathbf{q}} \Delta\mathcal{E}(\boldsymbol{\varepsilon},\mathbf{q})$ with constraints $\mathbf{N}:\mathbf{N} = \frac{3}{2}$, $\mathrm{tr}(\mathbf{N}) = 0$ & $\Delta\gamma \geq 0$

  - The problem is stated as a double constrained minimization problem

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

Quantum computing & finite elements

- Classical finite element resolution



FE Newton-Raphson iteration $(i) \leftarrow (i) + 1$

Constitutive NR iteration $(k) \leftarrow (k) + 1$

$$\mathbf{q}^{(k)}(\Xi) -= \left(\frac{\partial \mathcal{Q}}{\partial \mathbf{q}}\right)^{-1} \mathcal{Q}\left(\mathbf{q}^{(k)}(\Xi)\right)$$

$$\boldsymbol{\sigma}^{(k)}(\Xi^{\eta}) = \boldsymbol{\sigma}\left(\mathbf{B}_a \boldsymbol{U}_{a\,n+1}^{(i)}; \mathbf{q}^{(k)}(\Xi^{\eta})\right)$$

$$\mathrm{U}_{n+1}^{(i)} -= \left(\frac{\partial \boldsymbol{f}^{\mathrm{int}}}{\partial \mathbf{U}}\right)^{-1} \left[\boldsymbol{f}^{\mathrm{int}}\left(\boldsymbol{\sigma}\left(\boldsymbol{U}_{a\,n+1}^{(i)}\right)\right) - f^{\mathrm{ext}}\right]$$

- Finite element as a double-minimization problem

Loop until convergence

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

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

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

  - 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

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

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

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

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

$$|\boldsymbol{\phi}_0\rangle = \arg\min_{|\boldsymbol{\phi}\rangle} \langle\boldsymbol{\phi}|\mathbf{H}\,|\boldsymbol{\phi}\rangle$$

    - Problem reformulated in terms of binary variables $\mathbf{b} = [b_i\ \forall i \in V]$ with $b_i \in \{0,1\}$
    - QUBO optimisation problem $\mathcal{F}_{\text{QUBO}} = \sum_{(i,j)\in E\cup\{(i,i)\forall i\in V\}} A_{ij} b_i b_j = \mathbf{b}^T\mathbf{A}\mathbf{b}$

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

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
    - $f_{\text{aug}}(\mathbf{v}) = f_{\text{aug}}(\mathbf{w}, \lambda) = f(\mathbf{w}) + c^h\big(h(\mathbf{w})\big)^2 + c^l(l(\mathbf{w}) + \lambda)^2$ with $\mathbf{v} = \{\boldsymbol{w}, \lambda \geq 0\}$
  - 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

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

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

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

Loop until convergence

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

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

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

Double-minimization process solved by Quantum annealing

- Transform the constrained minimization problem into an unconstrained one
  - E.g. J2-plasticity
    - $$\Delta\mathcal{E} = \frac{1}{2}\left(\boldsymbol{\varepsilon}_{n+1} - \Delta\gamma\mathbf{N} - \boldsymbol{\varepsilon}_n^{\mathrm{pl}}\right):\mathbb{C}^{\mathbf{el}}:\left(\boldsymbol{\varepsilon}_{n+1} - \Delta\gamma\mathbf{N} - \boldsymbol{\varepsilon}_n^{\mathrm{pl}}\right) + \int_{\gamma_n}^{\gamma_{n+1}}\left(\sigma_y^0 + R(\gamma')\right)d\gamma' \\ - \frac{1}{2}\left(\boldsymbol{\varepsilon}_n - \boldsymbol{\varepsilon}_n^{\mathrm{pl}}\right):\mathbb{C}^{\mathbf{el}}:\left(\boldsymbol{\varepsilon}_n - \boldsymbol{\varepsilon}_n^{\mathrm{pl}}\right)$$
    - Under constraints $\mathbf{N}:\mathbf{N} = \frac{3}{2}$, $\mathrm{tr}(\mathbf{N}) = 0$ & $\Delta\gamma \geq 0$
    - Change of variables

$$\begin{cases} \mathbf{N}:\mathbf{N} = \boldsymbol{\alpha}^T\mathbf{M}\boldsymbol{\alpha} = \frac{3}{2} \\ \boldsymbol{\alpha} = [\alpha_0 \ldots \alpha_4]^{\mathrm{T}}, -\sqrt{\frac{3}{2}} \leq \alpha_i \leq -\sqrt{\frac{3}{2}}, \end{cases} , \quad \mathbf{N} = \begin{bmatrix} \alpha_0 & \alpha_2/\sqrt{2} & \alpha_2/\sqrt{2} \\ & \alpha_1 & \alpha_4/\sqrt{2} \\ \mathrm{SYM} & & -\alpha_0 - \alpha_1 \end{bmatrix} \quad \& \quad \mathbf{M} = \mathbf{cst}$$

    - Definition of the double unconstrained minimization problem

Loop until convergence

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

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

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

Loop until convergence

$$\{\Delta\gamma, \boldsymbol{\alpha}\} = \arg \min_{\{\Delta\gamma', \boldsymbol{\alpha}'\}} \left[\int_V \Delta\mathcal{E}\left(\boldsymbol{u}_{n+1}, \Delta\gamma', \boldsymbol{\alpha}'\right) + c^h\left(\alpha^T\mathrm{M}\alpha - \frac{3}{2}\right)^2 dV\right]$$

$$\Delta\Phi^{\mathrm{eff}} = \min_{\{\Delta\gamma', \boldsymbol{\alpha}'\}} \Delta\Phi_{\mathrm{aug}}(\boldsymbol{u}_{n+1}, \Delta\gamma', \boldsymbol{\alpha}')$$

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

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 $\mathbf{v}^{\min} \le \mathbf{v} \le \mathbf{v}^{\max}$
  - Taylor's expansion
    - $f_{\text{aug}}(\mathbf{v}+\mathbf{z}) \simeq f_{\text{aug}}(\mathbf{v}) + \overbrace{\mathbf{z}^{\text{T}} f_{\text{aug},\mathbf{v}} + \frac{1}{2}\mathbf{z}^{\text{T}} f_{\text{aug},\mathbf{vv}}\,\mathbf{z}}^{\text{QF}\left(\mathbf{z};\, f_{\text{aug},\mathbf{v}},\, f_{\text{aug},\mathbf{vv}}\right)}$
  - New series of optimization problems
    - Iterate on $\mathbf{z}$ with: $\mathbf{z} = \arg\min_{\mathbf{z}'} \text{QF}(\mathbf{z}';\, f_{\text{aug},\mathbf{v}},\, f_{\text{aug},\mathbf{vv}})$
  - Application to the double minimisation problem

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

Loop until convergence

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

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

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

Loop until convergence

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

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

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

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

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

Double-minimization process solved by Quantum annealing

- Transform the optimization problem into a series of quadratic ones
  - E.g. J2-plasticity
    - Minimization with respect to the internal variables (at constant displacement field)
      - $$\Delta\Phi_{\text{aug}}(\boldsymbol{u}_{n+1},\Delta\gamma,\boldsymbol{\alpha}) = \int_V \Delta\mathcal{E}(\boldsymbol{u}_{n+1},\Delta\gamma',\boldsymbol{\alpha}) + c^h\left(\boldsymbol{\alpha}^T\mathrm{M}\boldsymbol{\alpha} - \frac{3}{2}\right)^2 dV - \Delta W^{\text{ext}}(\boldsymbol{u}_{n+1})$$

        with $$\Delta\mathcal{E} = \frac{1}{2}\left(\boldsymbol{\varepsilon}_{n+1} - \Delta\gamma\mathbf{N} - \boldsymbol{\varepsilon}_n^{\text{pl}}\right):\mathbb{C}^{\text{el}}:\left(\boldsymbol{\varepsilon}_{n+1} - \Delta\gamma\mathbf{N} - \boldsymbol{\varepsilon}_n^{\text{pl}}\right) + \int_{\gamma_n}^{\gamma_{n+1}}\left(\sigma_y^0 + R(\gamma')\right)d\gamma' - \frac{1}{2}\left(\boldsymbol{\varepsilon}_n - \boldsymbol{\varepsilon}_n^{\text{pl}}\right):\mathbb{C}^{\text{el}}:\left(\boldsymbol{\varepsilon}_n - \boldsymbol{\varepsilon}_n^{\text{pl}}\right)$$

$$\Delta\Phi_{\text{aug},\boldsymbol{\alpha}} = \sum_{\Xi}\left(\Delta\mathcal{E}_{,\mathbf{N}}:\frac{\partial\mathbf{N}}{\partial\boldsymbol{\alpha}} + 2c^h\mathbf{M}\boldsymbol{\alpha}\left(\boldsymbol{\alpha}^T\mathrm{M}\boldsymbol{\alpha} - \frac{3}{2}\right)\right)\omega^{\Xi} \quad \& \quad \Delta\Phi_{\text{aug},\Delta\gamma} = \sum_{\Xi}\Delta\mathcal{E}_{,\boldsymbol{\Delta\gamma}}\omega^{\Xi}$$

$$\Delta\Phi_{\text{aug},\boldsymbol{\alpha\alpha}},\ \Delta\Phi_{\text{aug},\boldsymbol{\alpha}\Delta\gamma},\ \Delta\Phi_{\text{aug},\Delta\gamma\boldsymbol{\alpha}},\ \Delta\Phi_{\text{aug},\Delta\gamma\Delta\gamma}$$

- Minimization with respect to $\boldsymbol{u}_{n+1}$ (at constant internal variables)
  - $$\Delta\Phi^{\text{eff}}(\boldsymbol{u}_{n+1}) = \int_V \Delta\mathcal{E}^{\text{eff}}(\boldsymbol{u}_{n+1})\,dV - \Delta W^{\text{ext}}(\boldsymbol{u}_{n+1})$$ with $$\boldsymbol{\sigma} = \frac{\partial\Delta\mathcal{E}^{\text{eff}}}{\partial\boldsymbol{\varepsilon}}$$

$$\begin{cases} \Delta\Phi^{\text{eff}}_{,\mathbf{u}}(\boldsymbol{u}_{n+1}) = \sum_{\Xi}\mathbf{B}^{\mathrm{T}}(\Xi)\,\boldsymbol{\sigma}(\Xi)\omega^{\Xi} - \mathbf{f}^{\text{ext}} \\ \Delta\Phi^{\text{eff}}_{,\mathbf{uu}}(\boldsymbol{u}_{n+1}) = \sum_{\Xi}\mathbf{B}^{\mathrm{T}}(\Xi)\boxed{\mathbb{C}^{\text{el}}(\Xi)}\mathbf{B}(\Xi)\omega^{\Xi} - \mathbf{f}^{\text{ext}} \end{cases}$$

Constant material tensor

  - Only assembly operations required → Performed on classical computers

Double-minimization process solved by Quantum annealing

- Transform each continuous quadratic optimization problem into a binarized one
  - Optimization problems to be solved
    - $\mathbf{z} = \arg\min_{\mathbf{z}'} \mathrm{QF}(\mathbf{z}', f_{\mathrm{aug},\mathbf{v}}, f_{\mathrm{aug},\mathbf{vv}})$ & $\mathrm{QF}(\mathbf{z}; f_{\mathrm{aug},\mathbf{v}}, f_{\mathrm{aug},\mathbf{vv}}) = \mathbf{z}^{\mathrm{T}} f_{\mathrm{aug},\mathbf{v}} + \frac{\mathbf{1}}{\mathbf{2}} \mathbf{z}^{\mathrm{T}} f_{\mathrm{aug},\mathbf{vv}}\, \mathbf{z}$
    - With bounds: $\mathbf{v}_{\mathbf{min}} \leq \mathbf{v} + \mathbf{z} \leq \mathbf{v}_{\mathbf{max}}$
    - 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 $\mathcal{F}_{\mathrm{QUBO}} = \mathbf{b}^T \mathbf{A} \mathbf{b}$
    - QUBO optimization $\mathbf{b} = \arg\min_{\mathbf{b}'} \mathcal{F}_{\mathrm{QUBO}}(\mathbf{b}'; \mathbf{A})$

User programmable parameters

  - Binary-decimal conversion of a scalar field
    - Definition of a L-bit string under the form $\mathbf{b_1} = [b_0\ \ldots b_{L-1}]^{\mathrm{T}}$ with $b_i \in \{0, 1\}$
    - Conversion $b_{L-1}\ \ldots b_0 \equiv \sum_{j=0}^{L-1} b_j\ 2^j = \boldsymbol{\beta}^{\mathrm{T}} \mathbf{b_1}$ with $\boldsymbol{\beta} = [2^0\ 2^1\ \ldots\ 2^{L-1}]^{\mathrm{T}}$
    - Introduce the bounds $z \in [z^{\min}, z^{\max}]$

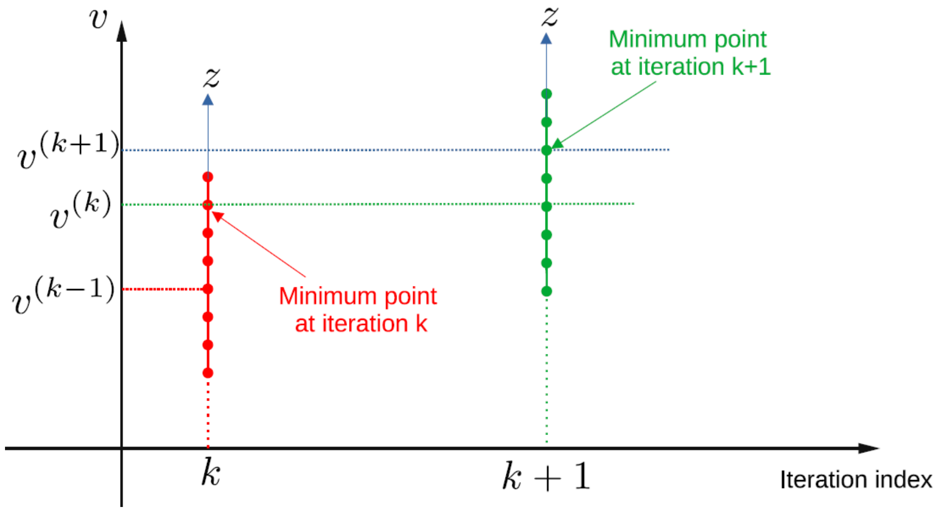
      ⇨ $z = z^{\min} + \epsilon_1 \boldsymbol{\beta}^T \mathbf{b_1}$ with the scaling $\epsilon_1 = \frac{z^{\max} - z^{\min}}{2^L - 1}$
    - One scalar is represented (in a discrete way) by L qubits
  - Binary-decimal conversion of a vector field
    - Vector of size N represented by $N \times L$ qubits
    - $\mathbf{z} = \mathbf{z}^{\min} + [\epsilon_i \boldsymbol{\beta}^T \mathbf{b}_i\ \text{ for }\ i = 0..N-1]$ ⇨ $\mathbf{z} = \mathbf{a} + \mathbf{D}(\boldsymbol{\epsilon})\mathbf{b}$

Double-minimization process solved by Quantum annealing

- Transform each continuous quadratic optimization problem into a binarized one
  - Optimization problems to be solved
    - $\mathbf{z} = \arg\min_{\mathbf{z}'} \mathrm{QF}(\mathbf{z}', f_{\mathrm{aug},\mathbf{v}}, f_{\mathrm{aug},\mathbf{vv}})$ & $\mathrm{QF}(\mathbf{z}; f_{\mathrm{aug},\mathbf{v}}, f_{\mathrm{aug},\mathbf{vv}}) = \mathbf{z}^{\mathrm{T}} f_{\mathrm{aug},\mathbf{v}} + \frac{1}{2} \mathbf{z}^{\mathrm{T}} f_{\mathrm{aug},\mathbf{vv}} \mathbf{z}$
    - With bounds: $\mathbf{v}_{\mathbf{min}} \leq \mathbf{v} + \mathbf{z} \leq \mathbf{v}_{\mathbf{max}}$
  - Binarization of $z \in \mathbb{R}^N$ 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 $\epsilon = \frac{\mathbf{z}^{\max} - \mathbf{z}^{\min}}{2^L - 1}$

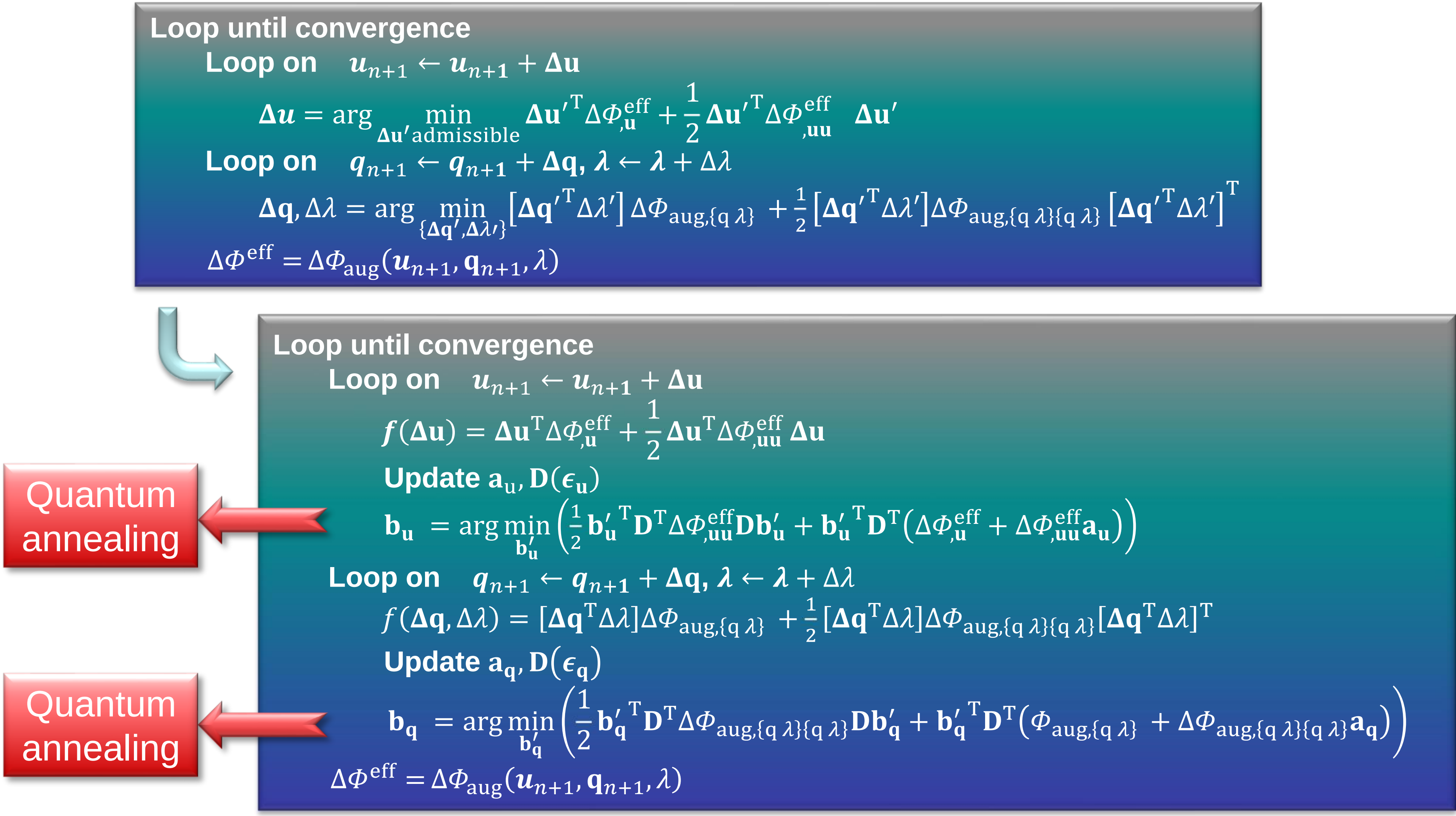
$$\Rightarrow \mathrm{QF}(\mathbf{z}; f_{\mathrm{aug},\mathbf{v}}, f_{\mathrm{aug},\mathbf{vv}}) = \underbrace{\frac{1}{2} \mathbf{b}^{\mathrm{T}} \mathbf{D}^{\mathrm{T}} f_{\mathrm{aug},\mathbf{vv}} \mathbf{D} \mathbf{b} + \mathbf{b}^{\mathrm{T}} \mathbf{D}^{\mathrm{T}} \left(f_{\mathrm{aug},\mathbf{v}} + f_{\mathrm{aug},\mathbf{vv}} \mathbf{a} \right)}_{\mathcal{F}_{\mathrm{QUBO}}(\mathbf{b}; \mathbf{A})} + \frac{1}{2} \mathbf{a}^{\mathrm{T}} \left(f_{\mathrm{aug},\mathbf{vv}} \mathbf{a} + f_{\mathrm{aug},\mathbf{v}} \right)$$

  - 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 $\boldsymbol{u}_{n+1} \leftarrow \boldsymbol{u}_{n+1} + \mathbf{\Delta u}$

$$\boldsymbol{\Delta u} = \arg \min_{\mathbf{\Delta u}' \text{admissible}} \mathbf{\Delta u}'^{\mathrm{T}} \Delta \Phi^{\text{eff}}_{,\mathbf{u}} + \frac{1}{2} \mathbf{\Delta u}'^{\mathrm{T}} \Delta \Phi^{\text{eff}}_{,\mathbf{uu}} \quad \mathbf{\Delta u}'$$

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

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

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

Loop until convergence

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

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

Update $\mathbf{a}_{\mathrm{u}}, \mathbf{D}(\boldsymbol{\epsilon}_{\mathbf{u}})$

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

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

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

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

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

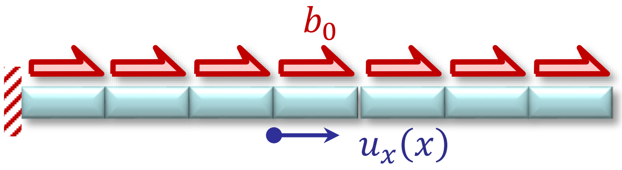
$$\Delta\Phi^{\text{eff}} = \Delta\Phi_{\text{aug}}(\boldsymbol{u}_{n+1}, \mathbf{q}_{n+1}, \lambda)$$

Quantum annealing

Quantum annealing

Application on 1D problems

- 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: $b_{L-1}\ \dots b_0 \equiv \sum_{j=0}^{L-1} b_j\ 2^j = \boldsymbol{\beta}^{\mathrm{T}}\mathbf{b}_{\boldsymbol{i}}$
  - Resolution by quantum annealing on DWave Advantage QPU

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

$$\boldsymbol{f}(\boldsymbol{\Delta}\mathbf{u}) = \boldsymbol{\Delta}\mathbf{u}^{\mathrm{T}}\Delta\Phi^{\mathrm{eff}}_{,\mathbf{u}} + \frac{1}{2}\boldsymbol{\Delta}\mathbf{u}^{\mathrm{T}}\Delta\Phi^{\mathrm{eff}}_{,\mathbf{uu}}\,\boldsymbol{\Delta}\mathbf{u}$$

Update $\mathbf{a}_{\mathrm{u}}, \mathbf{D}(\boldsymbol{\epsilon}_{\mathbf{u}})$

$\mathbf{b'}^{\mathrm{T}}_{u}\mathbf{A}\mathbf{b'}_{u}$

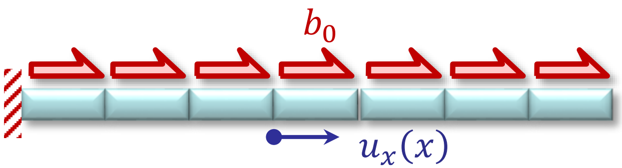
$$\mathbf{b}_{\mathbf{u}} = \arg\min_{\mathbf{b}'_{\mathbf{u}}}\left(\frac{1}{2}\mathbf{b}'_{\mathbf{u}}{}^{\mathrm{T}}\mathbf{D}^{\mathrm{T}}\Delta\Phi^{\mathrm{eff}}_{,\mathbf{uu}}\mathbf{D}\mathbf{b}'_{\mathbf{u}} + \mathbf{b}'_{\mathbf{u}}{}^{\mathrm{T}}\mathbf{D}^{\mathrm{T}}\left(\Delta\Phi^{\mathrm{eff}}_{,\mathbf{u}}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

Quantum annealing

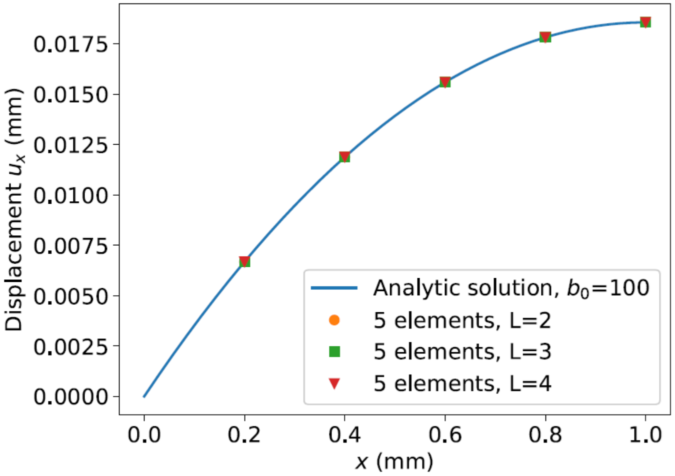
```
from dwave.system import DWaveSampler, EmbeddingComposite
sampler = EmbeddingComposite(DWaveSampler())
sampleset = sampler.sample_qubo(A, num_reads=100, annealing_time=20)
b = sampleset.first.sample
```

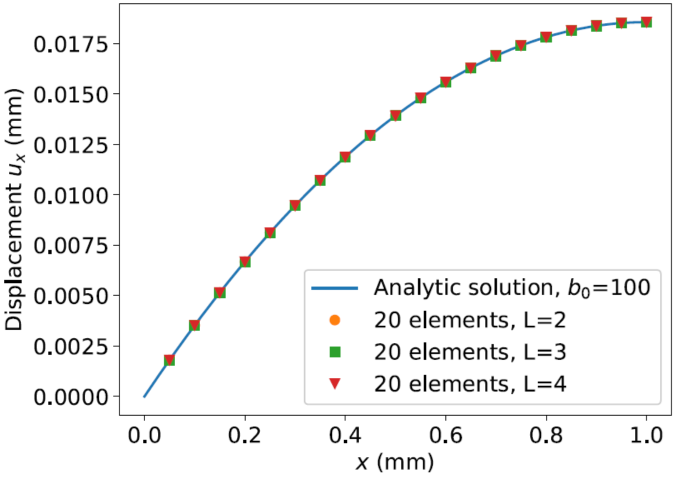
Application on 1D problems

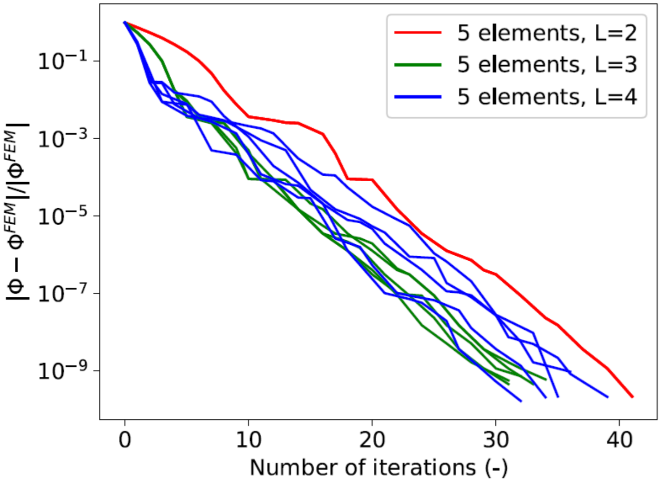
- Uniaxial-strain test
- Elastic case
    - Error analysis for 5 realizations for different total numbers of qubits

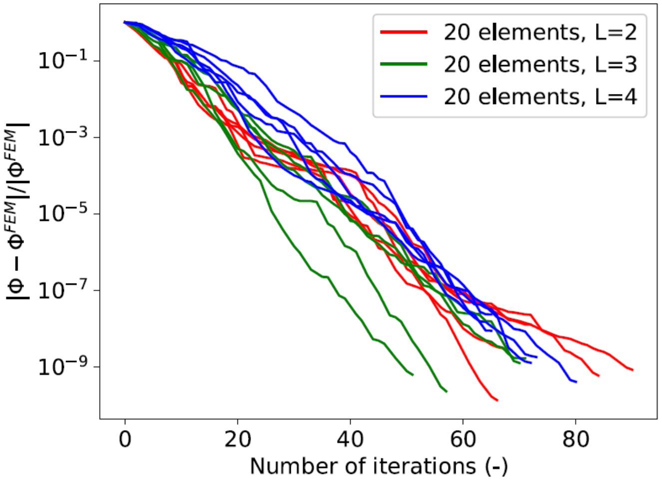


$$b_{L-1}\ \dots b_0 \equiv \sum_{j=0}^{L-1} b_j\ 2^j = \boldsymbol{\beta}^{\mathrm{T}}\mathbf{b}_{\boldsymbol{i}}$$







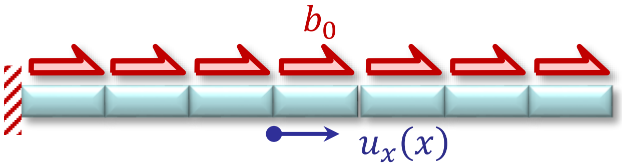


With increasing total number $N \times L$ of qubits

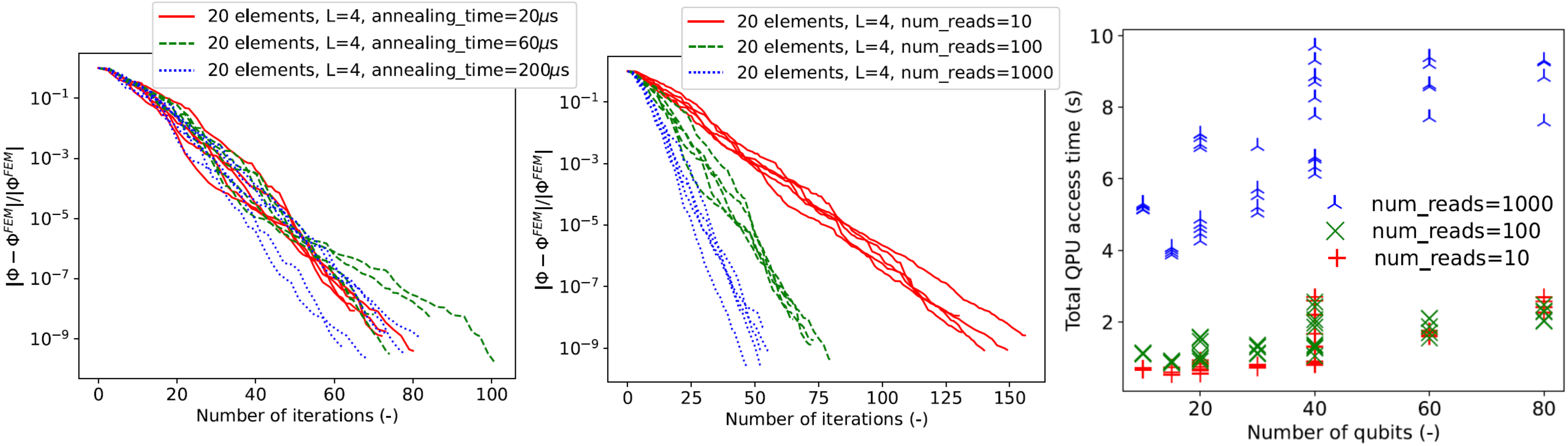
- Discrepancy between realizations increases
- Required number of iterations increases

Application on 1D problems

- Uniaxial-strain test
- Elastic case
  - – Effect of annealing time and number of reads



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

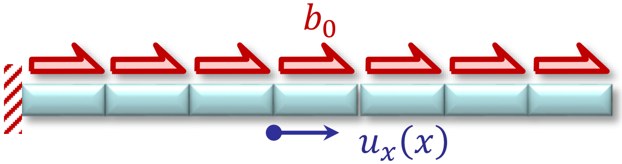


With increasing number of reads

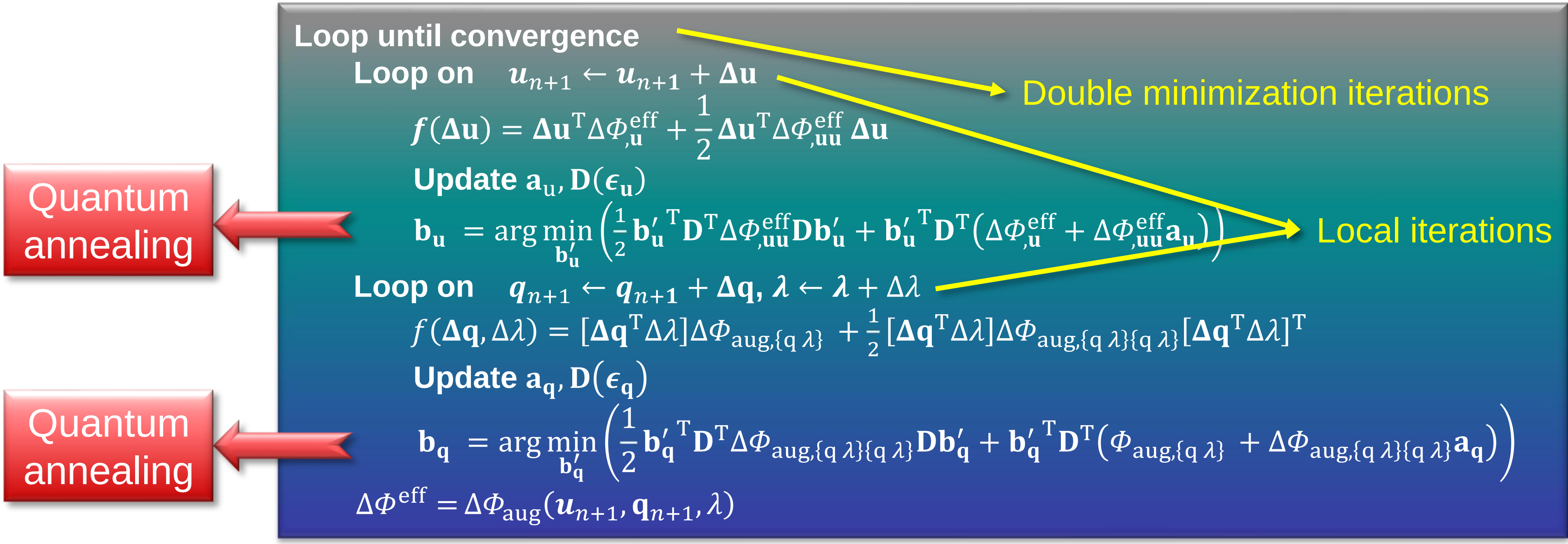
- Required number of iterations decreases
- But not necessarily the quantum processing unit (QPU) access time

Application on 1D problems

- Uniaxial-strain test



- Elasto-plastic case
  - Double minimization
    - Binarizations L of each nodal displacement and internal variable: $b_{L-1}\dots b_0 \equiv \sum_{j=0}^{L-1} b_j\ 2^j = \boldsymbol{\beta}^{\mathrm{T}}\mathbf{b}_{\boldsymbol{i}}$
  - Resolution by quantum annealing on DWave Advantage QPU



```
Loop until convergence
    Loop on $\boldsymbol{u}_{n+1} \leftarrow \boldsymbol{u}_{n+1} + \boldsymbol{\Delta}\mathbf{u}$
        $f(\boldsymbol{\Delta}\mathbf{u}) = \boldsymbol{\Delta}\mathbf{u}^{\mathrm{T}}\Delta\Phi^{\mathrm{eff}}_{,\mathbf{u}} + \frac{1}{2}\boldsymbol{\Delta}\mathbf{u}^{\mathrm{T}}\Delta\Phi^{\mathrm{eff}}_{,\mathbf{uu}}\,\boldsymbol{\Delta}\mathbf{u}$
        Update $\mathbf{a}_{\mathrm{u}}, \mathbf{D}(\boldsymbol{\epsilon}_{\mathbf{u}})$
        $\mathbf{b}_{\mathbf{u}} = \arg\min_{\mathbf{b}'_{\mathbf{u}}}\left(\frac{1}{2}{\mathbf{b}'_{\mathbf{u}}}^{\mathrm{T}}\mathbf{D}^{\mathrm{T}}\Delta\Phi^{\mathrm{eff}}_{,\mathbf{uu}}\mathbf{D}\mathbf{b}'_{\mathbf{u}} + {\mathbf{b}'_{\mathbf{u}}}^{\mathrm{T}}\mathbf{D}^{\mathrm{T}}\left(\Delta\Phi^{\mathrm{eff}}_{,\mathbf{u}} + \Delta\Phi^{\mathrm{eff}}_{,\mathbf{uu}}\mathbf{a}_{\mathbf{u}}\right)\right)$
    Loop on $\boldsymbol{q}_{n+1} \leftarrow \boldsymbol{q}_{n+1} + \boldsymbol{\Delta}\mathbf{q}, \boldsymbol{\lambda} \leftarrow \boldsymbol{\lambda} + \Delta\lambda$
        $f(\boldsymbol{\Delta}\mathbf{q}, \Delta\lambda) = [\boldsymbol{\Delta}\mathbf{q}^{\mathrm{T}}\Delta\lambda]\Delta\Phi_{\mathrm{aug},\{\mathrm{q}\ \lambda\}} + \frac{1}{2}[\boldsymbol{\Delta}\mathbf{q}^{\mathrm{T}}\Delta\lambda]\Delta\Phi_{\mathrm{aug},\{\mathrm{q}\ \lambda\}\{\mathrm{q}\ \lambda\}}[\boldsymbol{\Delta}\mathbf{q}^{\mathrm{T}}\Delta\lambda]^{\mathrm{T}}$
        Update $\mathbf{a}_{\mathbf{q}}, \mathbf{D}(\boldsymbol{\epsilon}_{\mathbf{q}})$
        $\mathbf{b}_{\mathbf{q}} = \arg\min_{\mathbf{b}'_{\mathbf{q}}}\left(\frac{1}{2}{\mathbf{b}'_{\mathbf{q}}}^{\mathrm{T}}\mathbf{D}^{\mathrm{T}}\Delta\Phi_{\mathrm{aug},\{\mathrm{q}\ \lambda\}\{\mathrm{q}\ \lambda\}}\mathbf{D}\mathbf{b}'_{\mathbf{q}} + {\mathbf{b}'_{\mathbf{q}}}^{\mathrm{T}}\mathbf{D}^{\mathrm{T}}\left(\Phi_{\mathrm{aug},\{\mathrm{q}\ \lambda\}} + \Delta\Phi_{\mathrm{aug},\{\mathrm{q}\ \lambda\}\{\mathrm{q}\ \lambda\}}\mathbf{a}_{\mathbf{q}}\right)\right)$
    $\Delta\Phi^{\mathrm{eff}} = \Delta\Phi_{\mathrm{aug}}(\boldsymbol{u}_{n+1}, \mathbf{q}_{n+1}, \lambda)$
```

Double minimization iterations

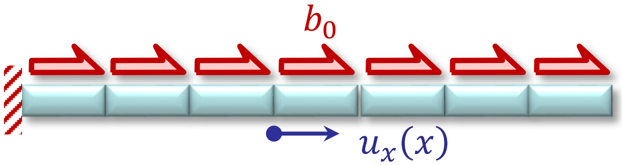
Local iterations

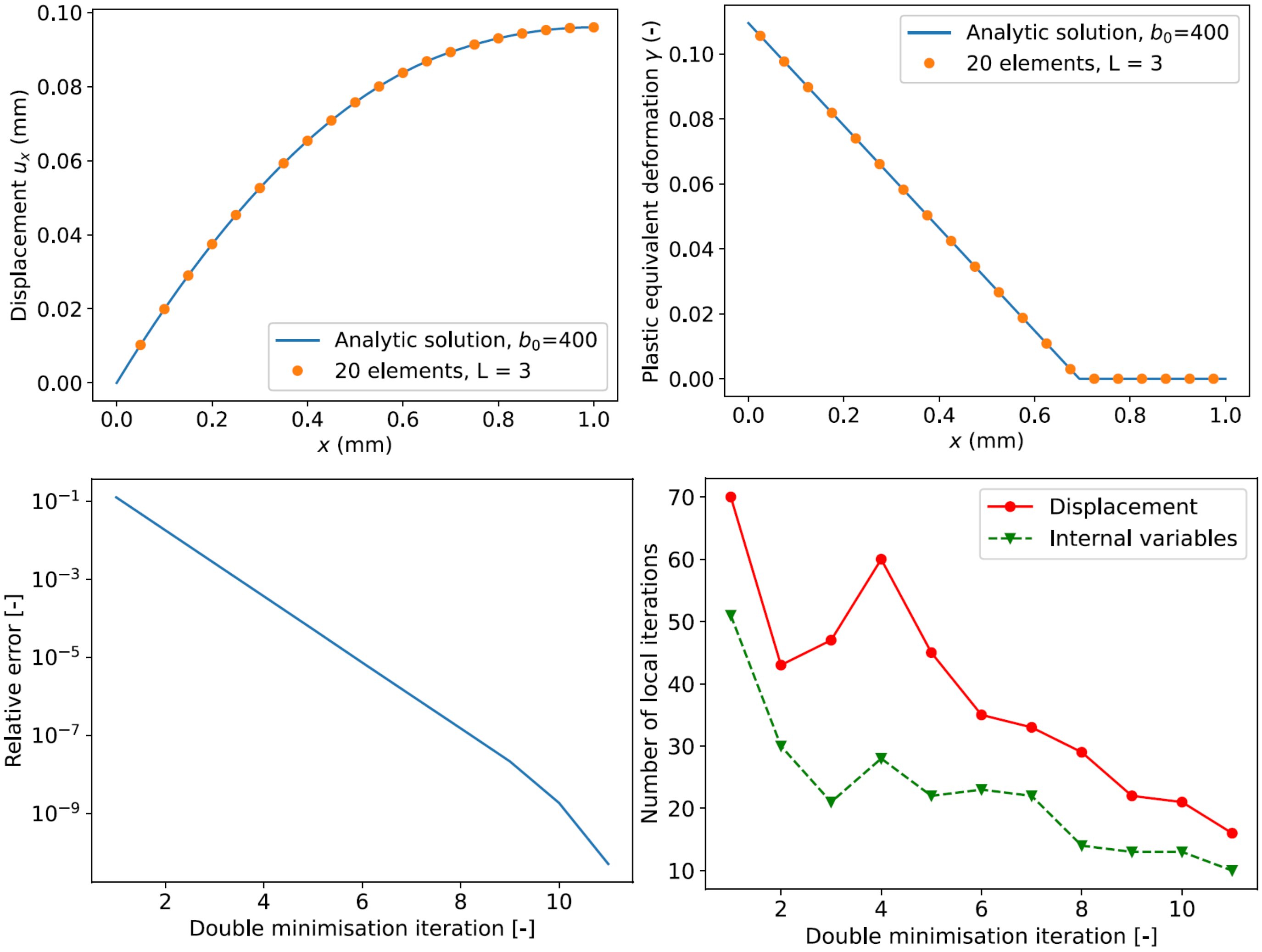
Quantum annealing

Quantum annealing

Application on 1D problems

- Uniaxial-strain test
- Elasto-plastic case
  - Effect of double-minimization & local iterations

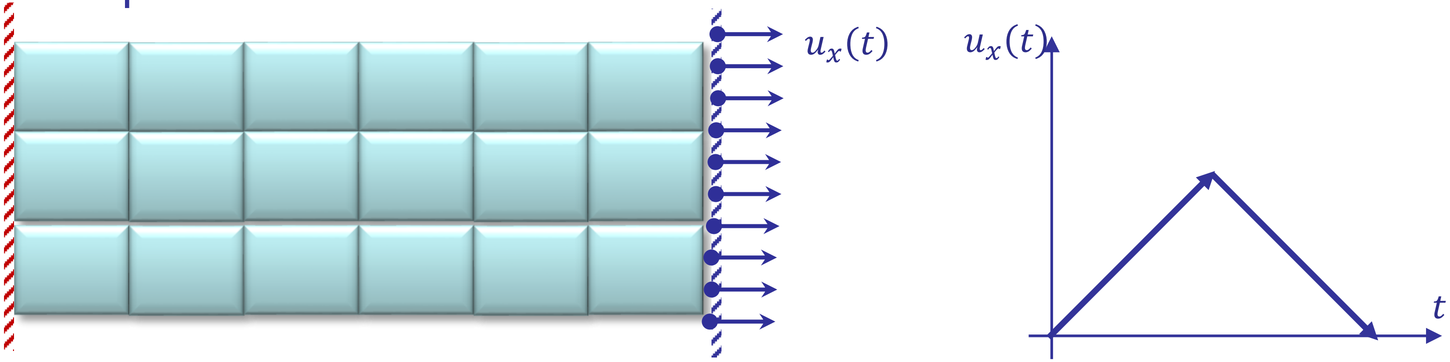




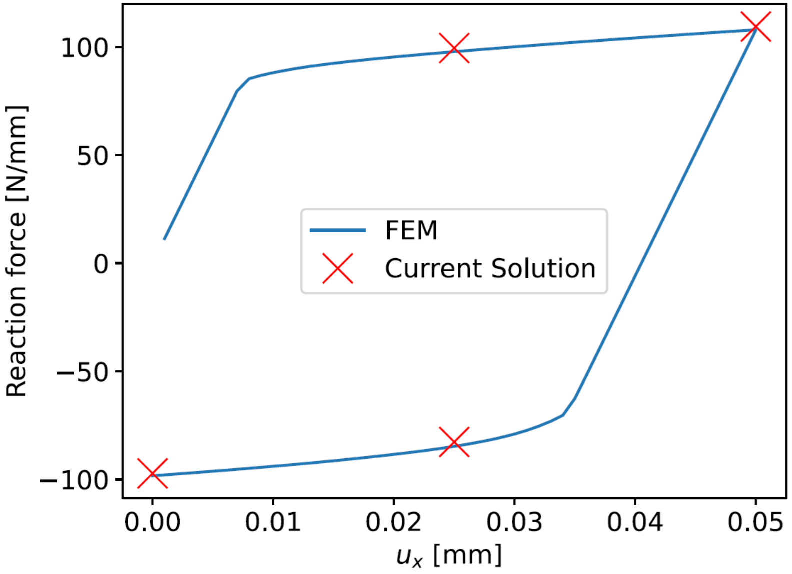
The number of local iterations decreases as the double minimisation iterations proceed

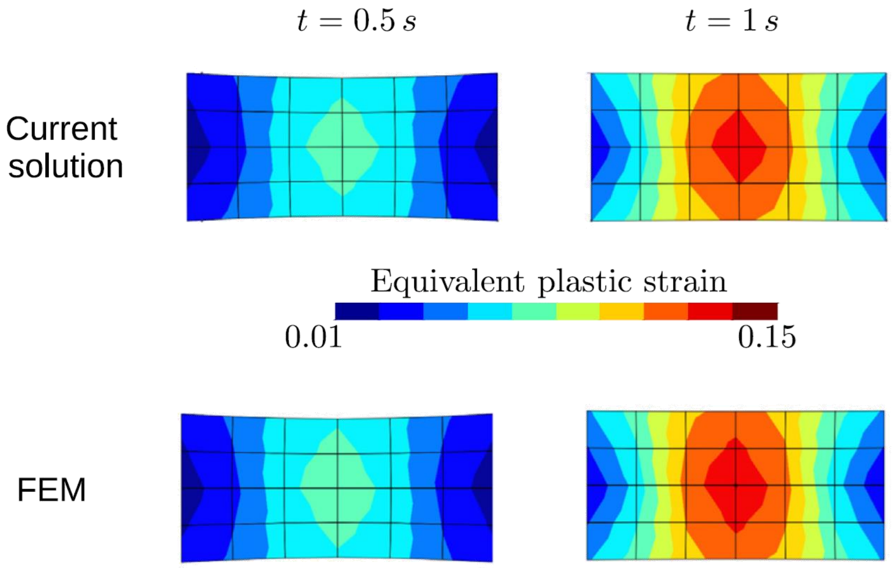
Application on 2D problems

- 2D-elasto-plastic case



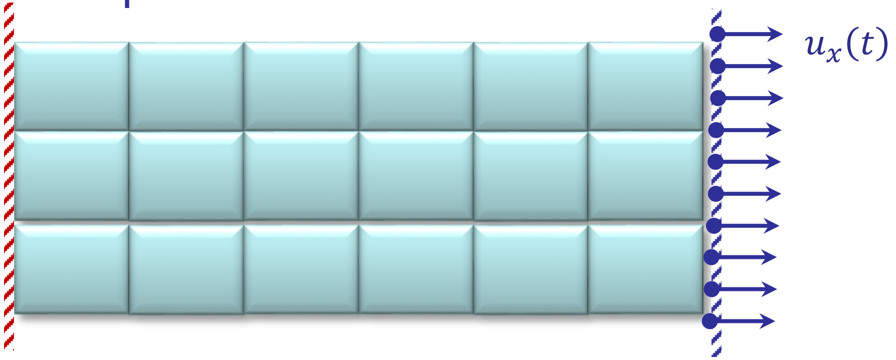
  - Double minimization
    - Binarizations L of each nodal displacement and internal variable: $b_{L-1} \dots b_0 \equiv \sum_{j=0}^{L-1} b_j\ 2^j = \boldsymbol{\beta}^{\mathrm{T}} \mathbf{b}_{\boldsymbol{i}}$
  - Resolution by quantum annealing on DWave Advantage QPU

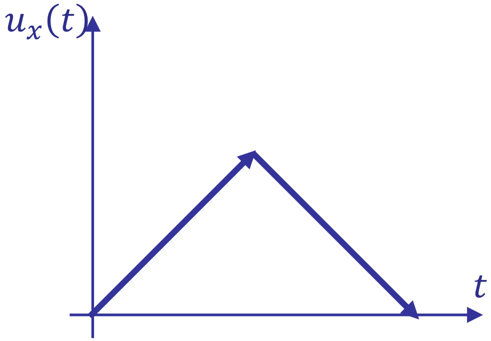




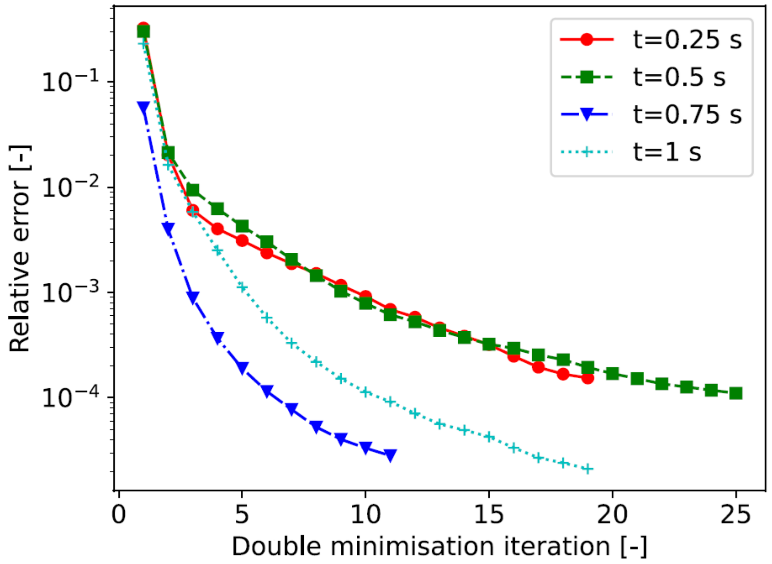
Application on 2D problems

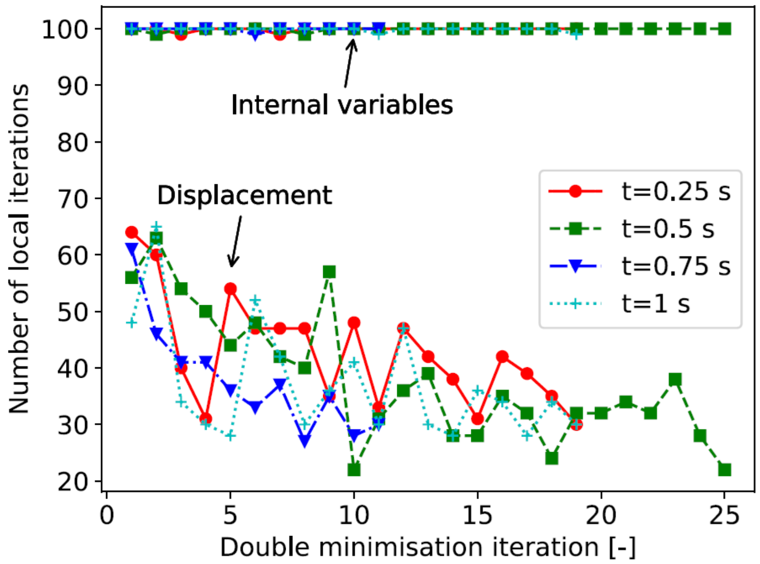
- 2D-elasto-plastic case





  - Effect of double-minimization & local iterations





Conclusions

- 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, 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
- Data and code on
  - Doi: 10.5281/zenodo.10451584