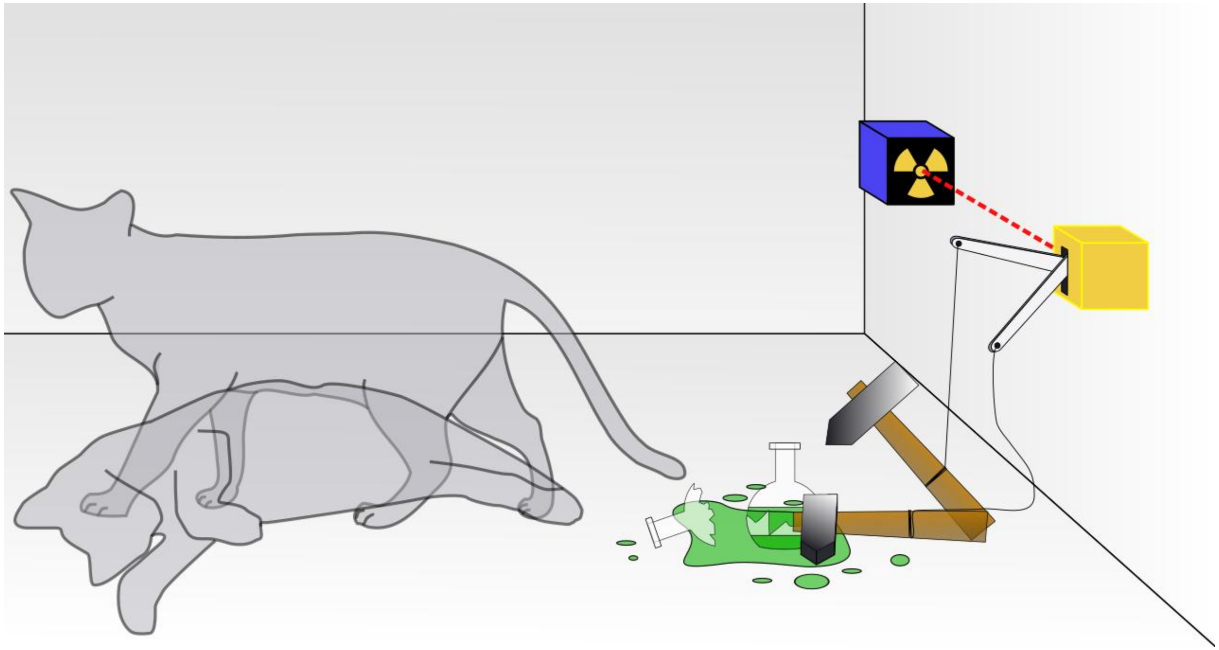
Elasto-Plastic Finite Element Simulations on Quantum Annealers

Van Dung Nguyen, Ling Wu, Françoise Remacle, and Ludovic Noels



V.-D.N acknowledges the support of the Fonds National de la Recherche (F.R.S.-FNRS, Belgium). F.R. acknowledges the support of the Fonds National de la Recherche (F.R.S.-FNRS, Belgium), #T0205.20. This work is partially supported by a “Strategic Opportunity” grant from the University of Liege

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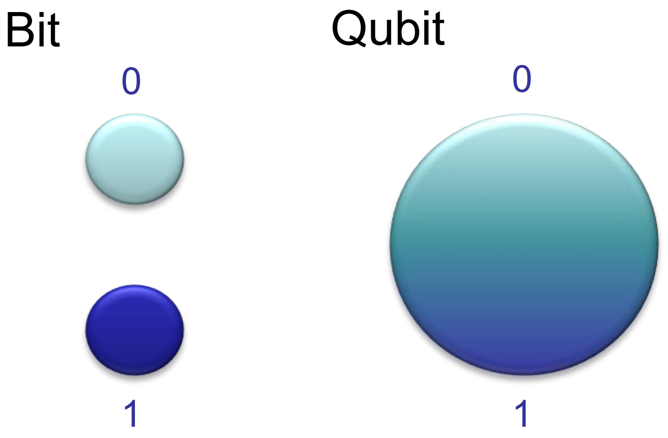
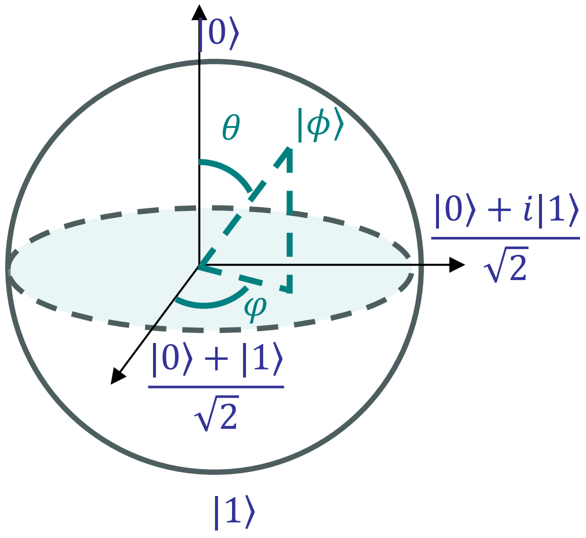
Introduction to Quantum Computing

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

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

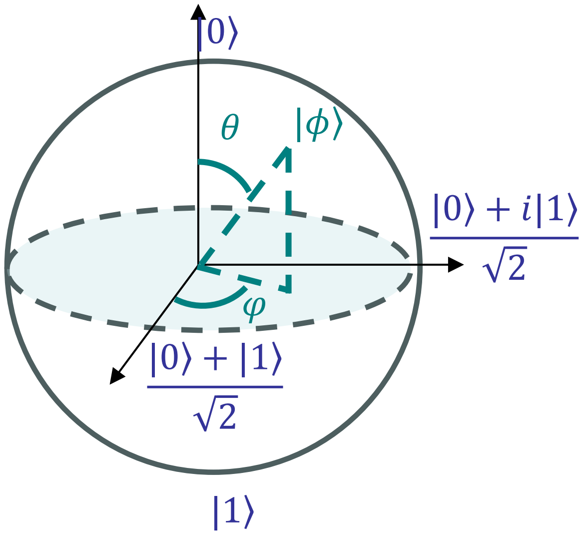
$$|\boldsymbol{\phi}\rangle = \alpha_{00}|00\rangle + \alpha_{01}|01\rangle + \alpha_{10}|10\rangle + \alpha_{11}|11\rangle$$

Because of entanglement, a K-qubit state is more general

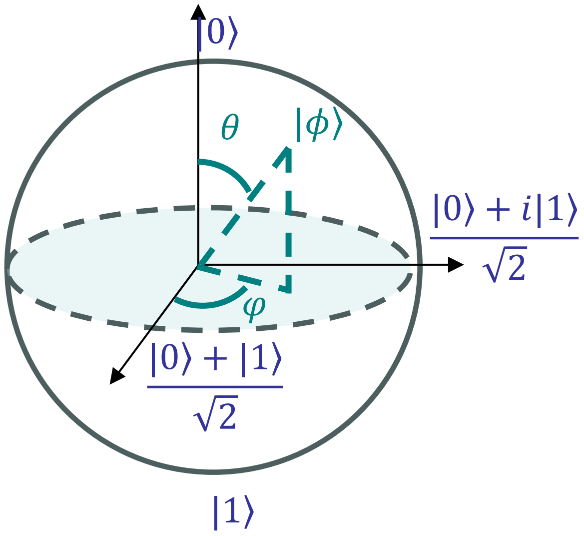
(it cannot always be written as the product of K 1-qubit states)

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

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



Introduction to Quantum Computing



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  - Most general 2-qubit state

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

  - 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:

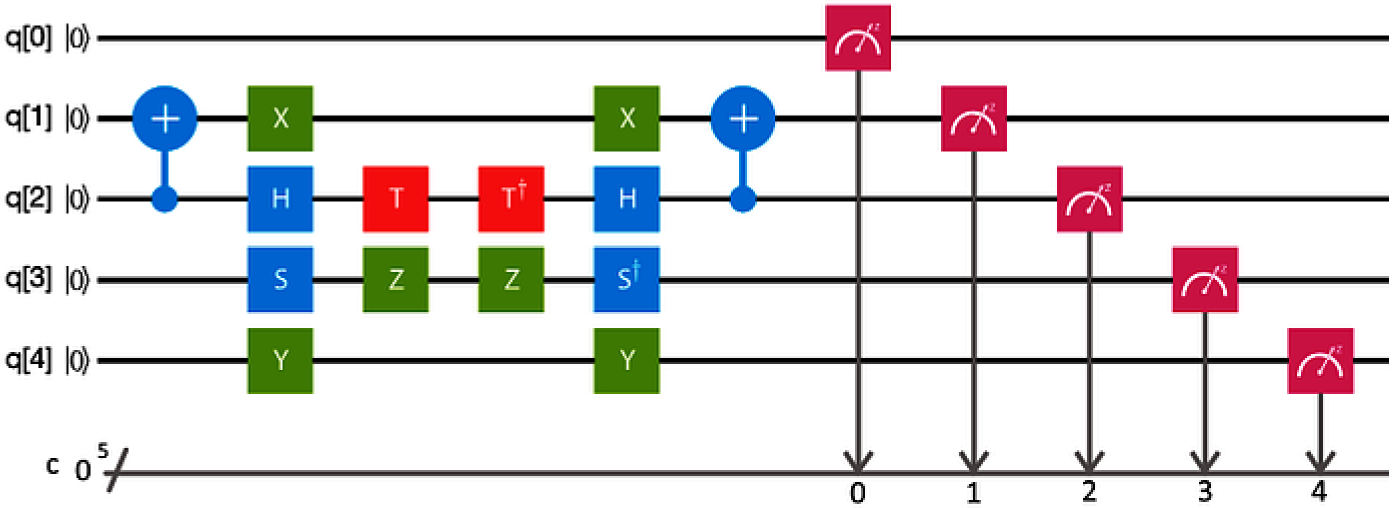
$$|\boldsymbol{\phi}\rangle = \phi_0|0\rangle \otimes |0\rangle \dots \otimes |0\rangle + \phi_1|0\rangle \otimes |0\rangle \dots \otimes |1\rangle + \cdots + \phi_{2^K-1}|1\rangle \dots \otimes |1\rangle \otimes |1\rangle$$

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

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 $\mathbf{H}$

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

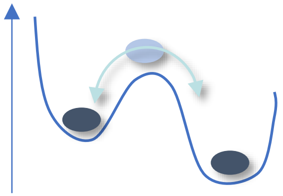
  - Based on quantum adiabatic theorem:
    - Considering a time-varying Hamiltonian $\mathbf{H}_{\mathbf{QA}}(t)$ initially at ground state, if its time evolution is slow enough, it is likely to remain at the ground state
  - Adiabatic quantum computing:
    - Starts from the ground state of an easy to prepare Hamiltonian $\mathbf{H}_i$
    - Evolves to the ground state of the Hamiltonian $\mathbf{H}$ which encodes the sought solution

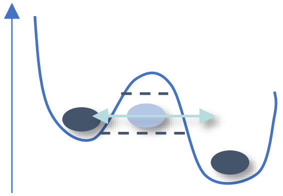
$$\mathbf{H}_{\mathbf{QA}}(t) = \frac{(t_a - t)}{t_a}\,\mathbf{H}_i + \frac{t}{t_a}\,\mathbf{H}$$

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

      We still need to design error-contained algorithm !!!
    - Less versatile than Gate-based QC

      But minimizing energy in mechanics is natural !!!


Thermal annealing


Quantum annealing

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 $V = \{0, \dots K-1\}$
    - 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: $\mathbf{Z}_i = \underbrace{\mathbf{I}}_{0} \otimes \cdots \otimes \mathbf{I} \otimes \underbrace{\mathbf{Z}}_{i} \otimes \mathbf{I} \otimes \cdots \otimes \underbrace{\mathbf{I}}_{K-1}$
    - 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 $\mathbf{H}$

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

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

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

User programmable parameters

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 $\quad b_i \in \{0,1\}$
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with $\quad \mathbf{h} = [h_i \;\; \forall i \in V] \qquad$ & $\mathbf{J} = \left[J_{ij} \;\; \forall (i,j) \in E\right]$

User programmable parameters

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

  - 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 $\; b_i^2 = b_i$

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

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

User programmable parameters

Quantum computing & finite elements

- Set of PDEs to be solved
  - Strong form → Weak form:

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

  - Constitutive model:

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

Quantum computing & finite elements

- Set of PDEs to be solved
  - Strong form ⇒ Weak form:

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

  - Constitutive model:

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

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

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

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

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

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

Omitting surface tractions

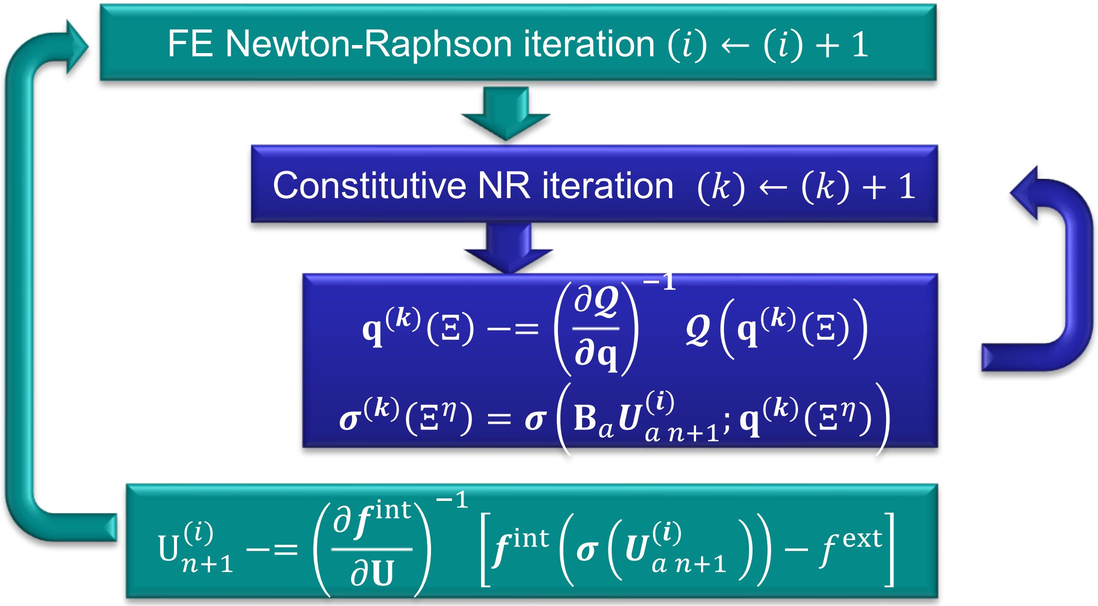
$$\Rightarrow \boldsymbol{f}_b^{\mathrm{int}} = \sum_{\Xi} \mathbf{B}_b^{\mathrm{T}}(\Xi)\, \boldsymbol{\sigma}(\Xi)\omega^{\Xi} = \sum_{\Xi} N_b(\Xi)\, \boldsymbol{b}_0(\Xi)\omega^{\Xi} = \boldsymbol{f}_b^{\mathrm{ext}}$$

with

$$\begin{cases} \boldsymbol{\sigma}(\Xi, t_{n+1}) = \boldsymbol{\sigma}\big(\mathbf{B}_a(\Xi)\boldsymbol{U}_{a\,n+1}; \mathbf{q}(\Xi, t_{\boldsymbol{n+1}})\big) \\ \boldsymbol{Q}\big(\boldsymbol{\sigma}(\Xi, t_{n+1}), \mathbf{q}(\Xi, t_{n+1}), \mathbf{q}(\Xi, t_n)\big) = \mathbf{0} \end{cases}$$

Quantum computing & finite elements

- Consider classical finite element resolution on Quantum Computers?



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

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

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

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

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

Iterations on whole mesh nodal unknowns

Iterations on quadrature point state variables

Quantum computing & finite elements

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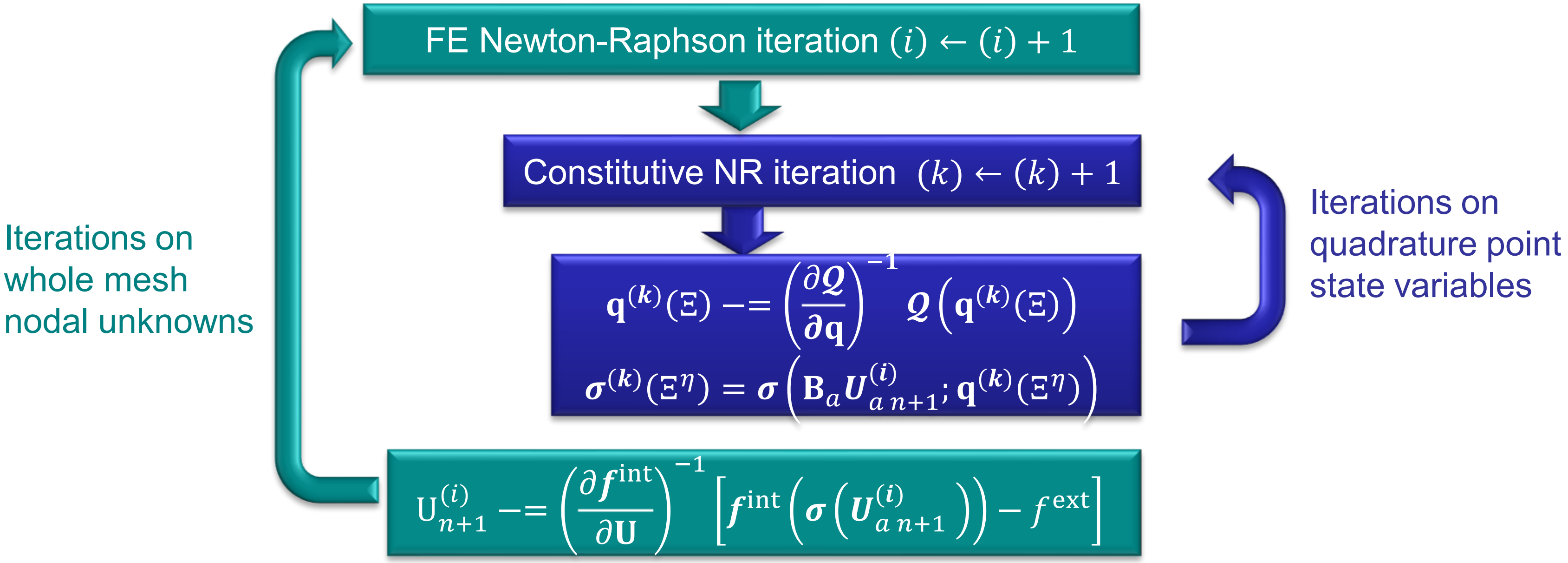

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$$\boldsymbol{\sigma}^{(k)}(\Xi^{\eta}) = \boldsymbol{\sigma}\left(\mathbf{B}_a \boldsymbol{U}_{a\,n+1}^{(i)}; \mathbf{q}^{(k)}(\Xi^{\eta})\right)$$

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

Iterations on whole mesh nodal unknowns

Iterations on quadrature point state variables

  - 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

- 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 $\Psi\big(\boldsymbol{\varepsilon}(x)\big)$ 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 $\int_V \frac{\partial \Psi(\boldsymbol{x})}{\partial \boldsymbol{\varepsilon}} : \boldsymbol{\delta\varepsilon}(\boldsymbol{x}) dV = \int_V \boldsymbol{b}_0 \cdot \boldsymbol{\delta u} dV$

Quantum computing & finite elements

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    ⇨ The weak form becomes $\int_V \dfrac{\partial\Psi(\boldsymbol{x})}{\partial\boldsymbol{\varepsilon}}:\boldsymbol{\delta\varepsilon}(\boldsymbol{x})dV = \int_V \boldsymbol{b}_0\cdot\boldsymbol{\delta u}dV$
  - 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: $\boldsymbol{u}(V) = \arg\min_{\boldsymbol{u'}(V)} \Phi\left(\boldsymbol{u}'(V)\right)$

Quantum computing & finite elements

- Non-linear finite element resolution on Quantum Computers?
  - Weak form: $\int_V \boldsymbol{\sigma}(\boldsymbol{x}) : \nabla \otimes^s \boldsymbol{\delta u}(\boldsymbol{x}) dV = \int_V \boldsymbol{b}_0 \cdot \boldsymbol{\delta u} dV$
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  - Introduction of a functional
    - $\Phi(\boldsymbol{u}(V)) = \int_V \Psi(\nabla \otimes^s \boldsymbol{u}(\boldsymbol{x})) dV - W^{\text{ext}}(\boldsymbol{u}(V))$ & $W^{\text{ext}} = \int_V \boldsymbol{b}_0 \cdot \boldsymbol{u}(\boldsymbol{x}) dV$
    - The weak form results from nulling the Gâteaux derivative

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

    The solution of the weak form minimizes the energy: $\boldsymbol{u}(V) = \arg\min_{\boldsymbol{u\prime}(V)} \Phi(\boldsymbol{u}'(V))$
  - 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 $\Theta^*(\mathbf{Y})$
    - $\Theta(\dot{\mathbf{q}}) = \max_{\mathbf{Y}} [\mathbf{Y} \cdot \dot{\mathbf{q}} - \Theta^*(\mathbf{Y})]$ $\dot{\mathbf{q}} = \frac{\partial \Theta^*(\mathbf{Y})}{\partial \mathbf{Y}}$ & $\mathbf{Y} = \frac{\partial \Theta(\dot{\mathbf{q}})}{\partial \dot{\mathbf{q}}}$

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

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 $\left\{\begin{array}{l} \text{internal variables } \mathbf{q}(x) \\ \boldsymbol{\varepsilon}(x) = \nabla \otimes^{s} \boldsymbol{u}(\boldsymbol{x}) \end{array}\right.$
  - Dissipation $\mathcal{D}$ and Clausius-Duhem inequality
    - $\mathcal{D} = \boldsymbol{\sigma} : \dot{\boldsymbol{\varepsilon}} - \dot{\Psi} \geq 0$ with $\dot{\Psi} = \dfrac{\partial \Psi}{\partial \boldsymbol{\varepsilon}} : \dot{\boldsymbol{\varepsilon}} + \dfrac{\partial \Psi}{\partial \mathbf{q}} \cdot \dot{\mathbf{q}}$
    - Equality holds in case of a reversible transformation

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

      ⇒ $\dfrac{\partial \mathcal{E}}{\partial \dot{\mathbf{q}}} = -\mathbf{Y} + \dfrac{\partial \Theta(\dot{\mathbf{q}})}{\partial \dot{\mathbf{q}}} = \mathbf{0}$ ⇒ $\mathcal{E}$ 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 $\boldsymbol{\sigma} = \dfrac{\partial \Psi}{\partial \boldsymbol{\varepsilon}} = \dfrac{\partial \mathcal{E}^{\mathrm{eff}}}{\partial \dot{\boldsymbol{\varepsilon}}}$
  - 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
    - $\boldsymbol{u}(V) = \arg\min_{\boldsymbol{u}'(V)} \Phi\left(\boldsymbol{u}'(V)\right)$ with $\Phi\left(\boldsymbol{u}(V)\right) = \int_V \Psi\left(\nabla \otimes^s \boldsymbol{u}(\boldsymbol{x})\right) dV - W^{\text{ext}}\left(\boldsymbol{u}(\boldsymbol{x})\right)$
  - Double minimization problem in inelasticity
    - Power functional $\mathcal{E}$

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

    - Volume power functional

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

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Quantum computing & finite elements

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    - Volume power functional

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

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

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

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

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

Quantum computing & finite elements

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

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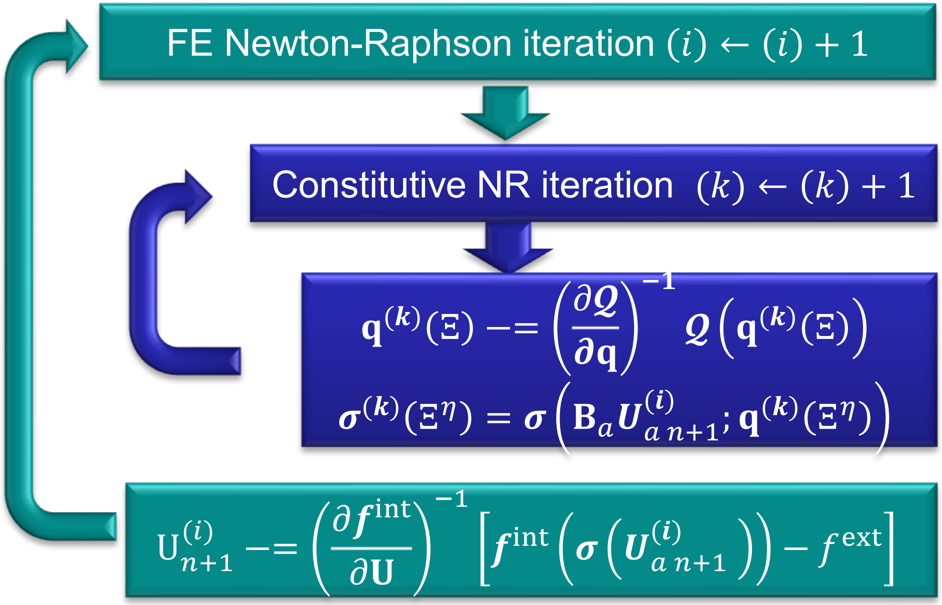
    - The problem solution reads

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

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

Quantum computing & finite elements

- Classical finite element resolution



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

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

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

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

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

- Finite element as a double-minimization problem

Loop until convergence

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

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

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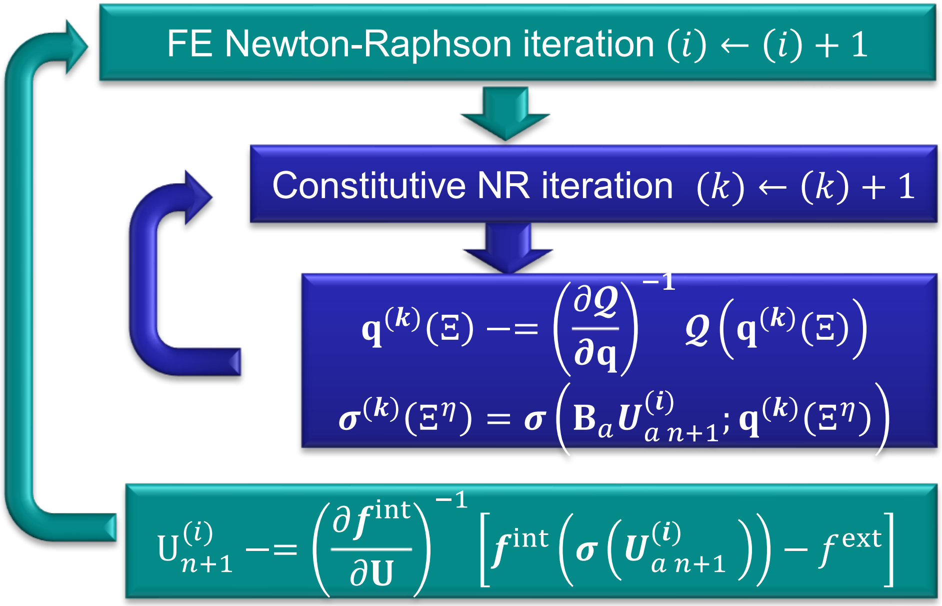
Internal variables can be constrained (e.g. $\mathbf{N}:\mathbf{N} = \frac{3}{2}, \Delta\gamma \geq 0)$

Quantum computing & finite elements

- Classical finite element resolution



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- Finite element as a double-minimization problem

Loop until convergence

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

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Internal variables can be constrained (e.g. $\mathbf{N}:\mathbf{N} = \frac{3}{2}, \Delta\gamma \geq 0$)

- Quantum annealers: ground state of an Ising-Hamiltonian
  - No need for Jacobians
  - No problem of convergence (but needs to be noise-contained)
- 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

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

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

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

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

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 $b_i \in \{0, 1\}$
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⇒ $\mathbf{b} = \arg \min_{\mathbf{b}'} \mathcal{F}_{\text{QUBO}}(\mathbf{b}'; \boxed{\mathbf{A}})$ 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 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
    - $f_{\text{aug}}(\mathbf{v}) = f_{\text{aug}}(\mathbf{w}, \lambda) = f(\mathbf{w}) + c^h\left(h(\mathbf{w})\right)^2 + c^l(l(\mathbf{w}) + \lambda)^2$ 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

Double-minimization process solved by Quantum annealing

- Transform the constrained minimization problem into an unconstrained one
  - Constrained multivariate minimization problem
    - $\min\limits_{\mathbf{w}} f(\mathbf{w})$ with $\mathbf{w}^{\min} \leq \mathbf{w} \leq \mathbf{w}^{\max}$
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  - Unconstrained minimization problem
    - $\min\limits_{\mathbf{v}} f_{\text{aug}}(\mathbf{v})$ 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 optimization problem into a series of quadratic ones
  - Unconstrained optimization problem
    - $\min_{\mathbf{v}} f_{\mathrm{aug}}(\mathbf{v})$ with $\mathbf{v}^{\min} \leq \mathbf{v} \leq \mathbf{v}^{\max}$
  - Taylor's expansion
    - $f_{\mathrm{aug}}(\mathbf{v}+\mathbf{z}) \simeq f_{\mathrm{aug}}(\mathbf{v}) \underbrace{+ \mathbf{z}^{\mathrm{T}} f_{\mathrm{aug},\mathbf{v}} + \frac{\mathbf{1}}{\mathbf{2}} \mathbf{z}^{\mathrm{T}} f_{\mathrm{aug},\mathbf{vv}}\, \mathbf{z}}_{\mathrm{QF}(\mathbf{z};\, f_{\mathrm{aug},\mathbf{v}},\, f_{\mathrm{aug},\mathbf{vv}})}$
  - New series of optimization problems
    - Iterate on z with: $\mathbf{z} = \arg\min_{\mathbf{z}'} \mathrm{QF}(\mathbf{z}'; f_{\mathrm{aug},\mathbf{v}}, f_{\mathrm{aug},\mathbf{vv}})$

$$\begin{cases} {f_{\mathrm{aug},\mathbf{v}}}_{\,i} = \left.\dfrac{\partial f_{\mathrm{aug}}}{\partial v_i}\right|_{\mathbf{v}} \\[2ex] {f_{\mathrm{aug},\mathbf{vv}}}_{\,ij} = \left.\dfrac{\partial^2 f_{\mathrm{aug}}}{\partial v_i \partial v_j}\right|_{\mathbf{v}} \end{cases}$$

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
    - $f_{\text{aug}}(\mathbf{v}+\mathbf{z}) \simeq f_{\text{aug}}(\mathbf{v}) + \underbrace{\mathbf{z}^{\mathrm{T}} f_{\text{aug},\mathbf{v}} + \frac{1}{2}\mathbf{z}^{\mathrm{T}} f_{\text{aug},\mathbf{vv}}\,\mathbf{z}}_{\mathrm{QF}(\mathbf{z};\, f_{\text{aug},\mathbf{v}},\, f_{\text{aug},\mathbf{vv}})}$
  - New series of optimization problems
    - Iterate on $\mathbf{z}$ with: $\mathbf{z} = \arg\min_{\mathbf{z}'} \mathrm{QF}(\mathbf{z}'; f_{\text{aug},\mathbf{v}}, f_{\text{aug},\mathbf{vv}})$
  - 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 $\boldsymbol{u}_{n+1} \leftarrow \boldsymbol{u}_{n+1} + \boldsymbol{\Delta}\mathbf{u}$

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

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

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

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

Allow to contain the noise !!!

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: $\mathbf{v}_{\mathbf{min}} \leq \mathbf{v} + \mathbf{z} \leq \mathbf{v}_{\mathbf{max}}$
  - Binarization of $z \in \mathbb{R}^N$ into $N \times L$ qubits
    - $b_{L-1} \ldots b_0 \equiv \sum_{j=0}^{L-1} b_j\ 2^j = \boldsymbol{\beta}^{\mathrm{T}} \mathbf{b}_{\boldsymbol{i}}$ $\Rightarrow$ $z_1 = z_i^{\min} + \epsilon_i \boldsymbol{\beta}^T \mathbf{b}_{\boldsymbol{i}}$
    - $\mathbf{z} = \mathbf{a} + \mathbf{D}(\boldsymbol{\epsilon})\mathbf{b}$ with the bounds defining $\mathbf{a} = \mathbf{z}^{\min}$ & the scale $\boldsymbol{\epsilon} = \frac{\boldsymbol{z}^{\max} - \boldsymbol{z}^{\min}}{2^L - 1}$

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: $\mathbf{v}_{\mathbf{min}} \leq \mathbf{v} + \mathbf{z} \leq \mathbf{v}_{\mathbf{max}}$
  - Binarization of $z \in \mathbb{R}^N$ into $N \times L$ qubits
    - $b_{L-1} \dots b_0 \equiv \sum_{j=0}^{L-1} b_j\, 2^j = \boldsymbol{\beta}^{\mathrm{T}} \mathbf{b}_i$ ⇨ $z_1 = z_i^{\min} + \epsilon_i \boldsymbol{\beta}^T \mathbf{b}_i$
    - $\mathbf{z} = \mathbf{a} + \mathbf{D}(\boldsymbol{\epsilon})\mathbf{b}$ with the bounds defining $\mathbf{a} = \mathbf{z}^{\min}$ & the scale $\boldsymbol{\epsilon} = \frac{\boldsymbol{z}^{\max} - \boldsymbol{z}^{\min}}{2^L - 1}$

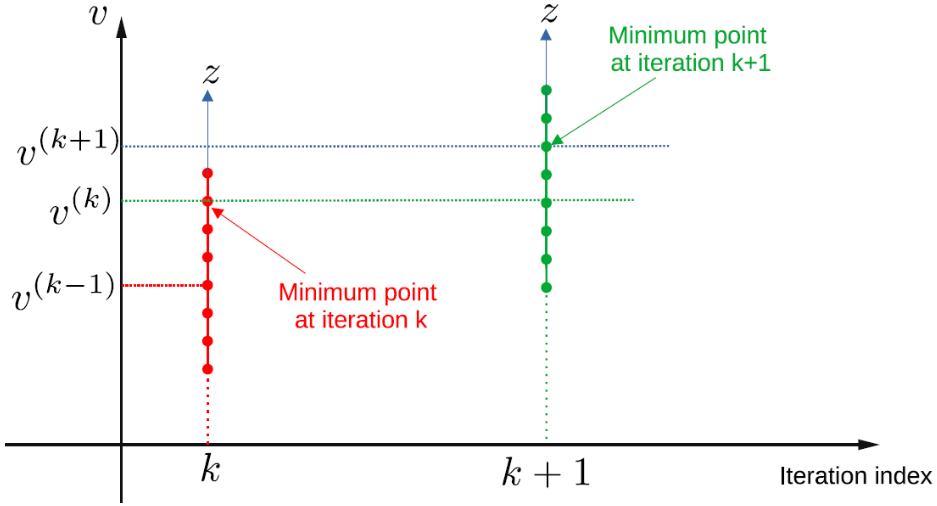
$$\Rightarrow \mathrm{QF}\left(\mathbf{z}; f_{\mathrm{aug},\mathbf{v}}, f_{\mathrm{aug},\mathbf{vv}}\right) = \underbrace{\frac{1}{2} \mathbf{b}^{\mathrm{T}} \mathbf{D}^{\mathrm{T}} f_{\mathrm{aug},\mathbf{vv}}\, \mathbf{D}\mathbf{b} + \mathbf{b}^{\mathrm{T}} \mathbf{D}^{\mathrm{T}} \left(f_{\mathrm{aug},\mathbf{v}}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

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: $\mathbf{v}_{\mathbf{min}} \leq \mathbf{v} + \mathbf{z} \leq \mathbf{v}_{\mathbf{max}}$
  - Binarization of $z \in \mathbb{R}^N$ into $N \times L$ qubits
    - $b_{L-1} \dots b_0 \equiv \sum_{j=0}^{L-1} b_j \, 2^j = \boldsymbol{\beta}^{\mathrm{T}} \mathbf{b}_i$ $\Rightarrow$ $z_1 = z_i^{\min} + \epsilon_i \boldsymbol{\beta}^T \mathbf{b}_i$
    - $\mathbf{z} = \mathbf{a} + \mathbf{D}(\boldsymbol{\epsilon})\mathbf{b}$ with the bounds defining $\mathbf{a} = \mathbf{z}^{\min}$ & the scale $\boldsymbol{\epsilon} = \dfrac{\mathbf{z}^{\max} - \mathbf{z}^{\min}}{2^L - 1}$

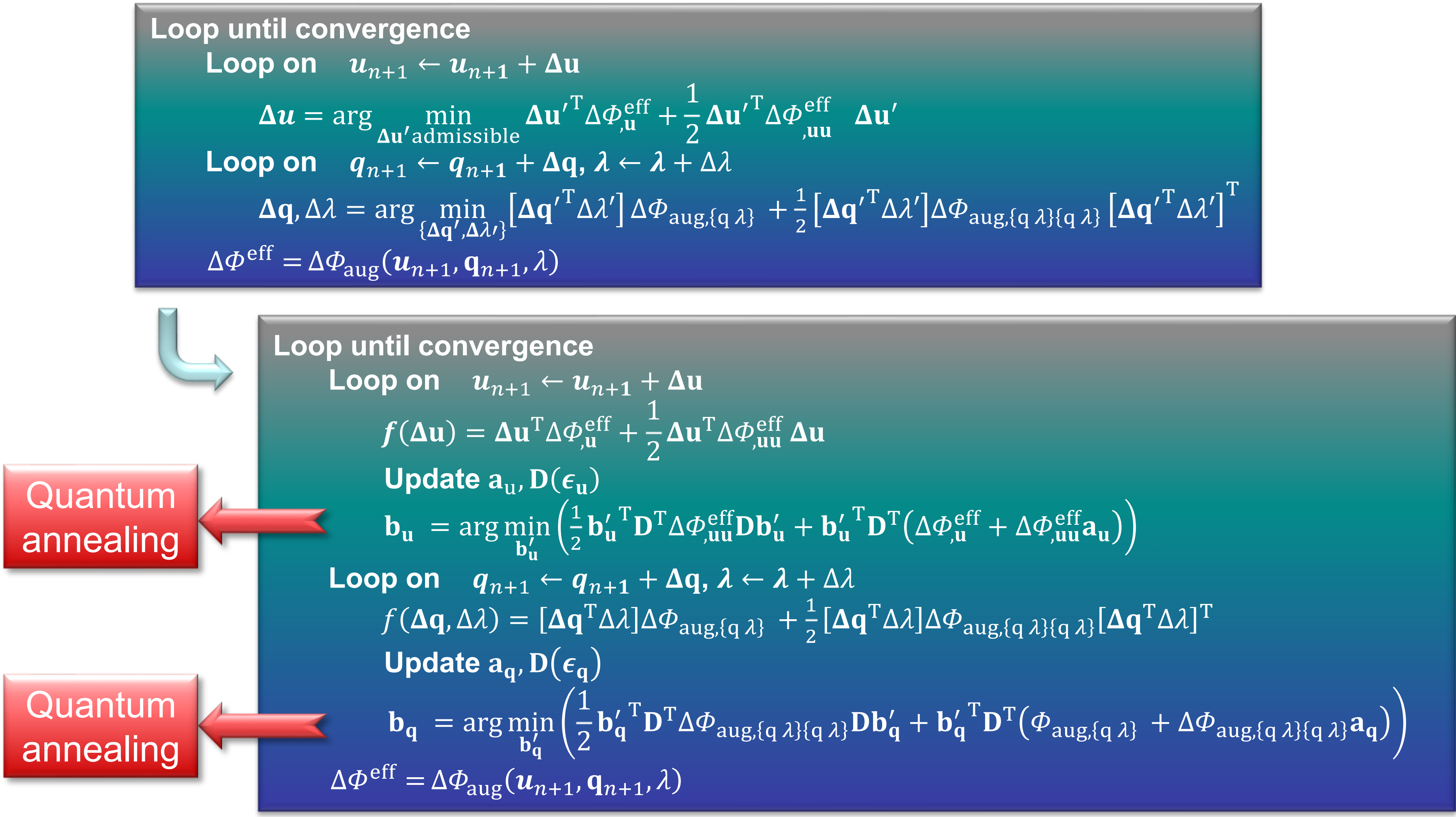
$$\Rightarrow \mathrm{QF}(\mathbf{z}; f_{\mathrm{aug},\mathbf{v}}, f_{\mathrm{aug},\mathbf{vv}}) = \underbrace{\frac{1}{2} \mathbf{b}^{\mathrm{T}} \mathbf{D}^{\mathrm{T}} f_{\mathrm{aug},\mathbf{vv}} \mathbf{D} \mathbf{b} + \mathbf{b}^{\mathrm{T}} \mathbf{D}^{\mathrm{T}} \left(f_{\mathrm{aug},\mathbf{v}}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

  - Minimization
    - Bound $\mathbf{a} = \mathbf{z}^{\min}$ and
    - Scale $\boldsymbol{\epsilon} = \dfrac{\mathbf{z}^{\max} - \mathbf{z}^{\min}}{2^L - 1}$
    - Updated when building the QUBO



Double-minimization process solved by Quantum annealing

- Application to the double-minimization problem



```
Loop until convergence
    Loop on $\boldsymbol{u}_{n+1} \leftarrow \boldsymbol{u}_{n+1} + \mathbf{\Delta u}$
        $\boldsymbol{\Delta u} = \arg \min_{\mathbf{\Delta u}' \text{admissible}} \mathbf{\Delta u}'^{\mathrm{T}} \Delta\Phi^{\mathrm{eff}}_{,\mathbf{u}} + \frac{1}{2} \mathbf{\Delta u}'^{\mathrm{T}} \Delta\Phi^{\mathrm{eff}}_{,\mathbf{uu}} \; \mathbf{\Delta u}'$
    Loop on $\boldsymbol{q}_{n+1} \leftarrow \boldsymbol{q}_{n+1} + \mathbf{\Delta q}, \boldsymbol{\lambda} \leftarrow \boldsymbol{\lambda} + \Delta\lambda$
        $\mathbf{\Delta q}, \Delta\lambda = \arg \min_{\{\mathbf{\Delta q}', \mathbf{\Delta}\lambda'\}} [\mathbf{\Delta q}'^{\mathrm{T}} \Delta\lambda'] \, \Delta\Phi_{\mathrm{aug},\{\mathrm{q}\,\lambda\}} + \frac{1}{2} [\mathbf{\Delta q}'^{\mathrm{T}} \Delta\lambda'] \Delta\Phi_{\mathrm{aug},\{\mathrm{q}\,\lambda\}\{\mathrm{q}\,\lambda\}} \, [\mathbf{\Delta q}'^{\mathrm{T}} \Delta\lambda']^{\mathrm{T}}$
    $\Delta\Phi^{\mathrm{eff}} = \Delta\Phi_{\mathrm{aug}}(\boldsymbol{u}_{n+1}, \mathbf{q}_{n+1}, \lambda)$
```

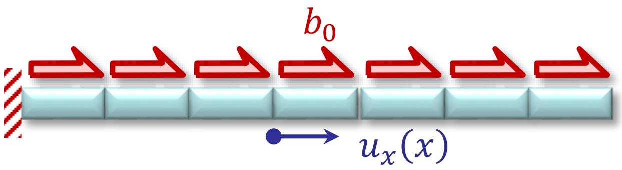
```
Loop until convergence
    Loop on $\boldsymbol{u}_{n+1} \leftarrow \boldsymbol{u}_{n+1} + \mathbf{\Delta u}$
        $f(\mathbf{\Delta u}) = \mathbf{\Delta u}^{\mathrm{T}} \Delta\Phi^{\mathrm{eff}}_{,\mathbf{u}} + \frac{1}{2} \mathbf{\Delta u}^{\mathrm{T}} \Delta\Phi^{\mathrm{eff}}_{,\mathbf{uu}}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

Quantum annealing

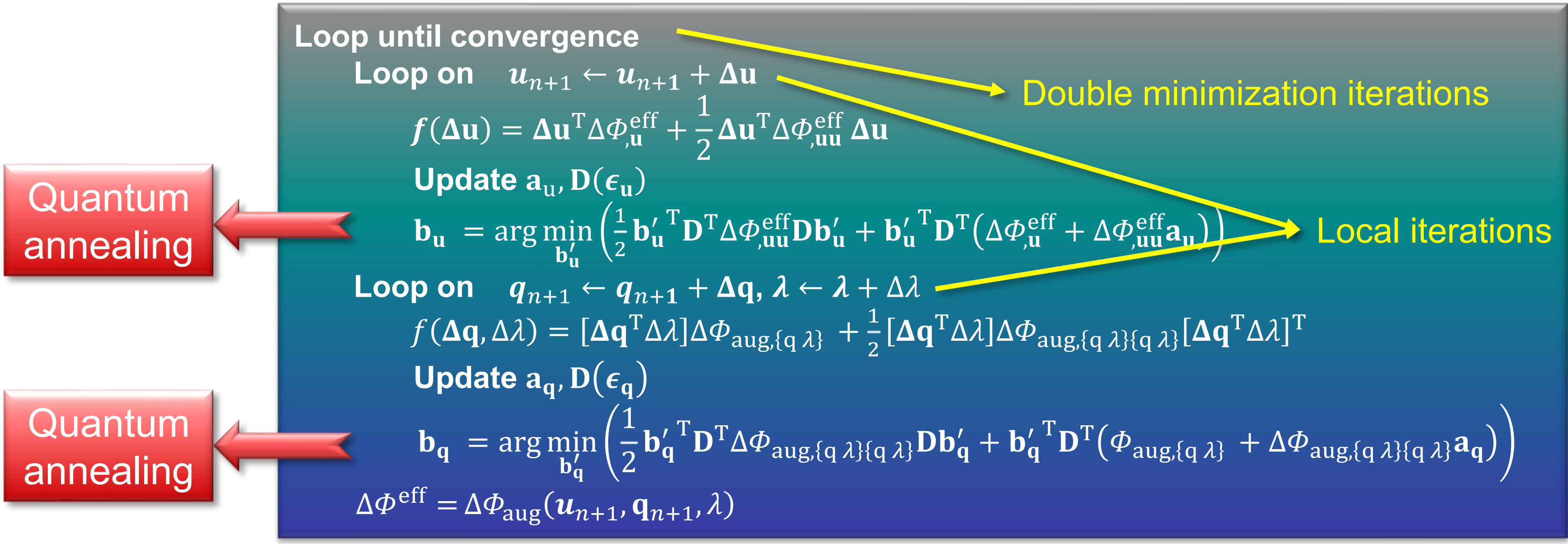
Quantum annealing

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

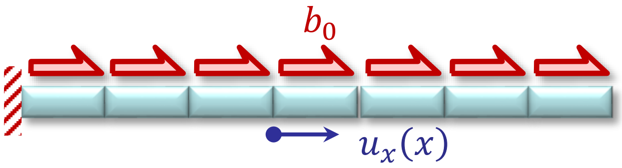
Local iterations

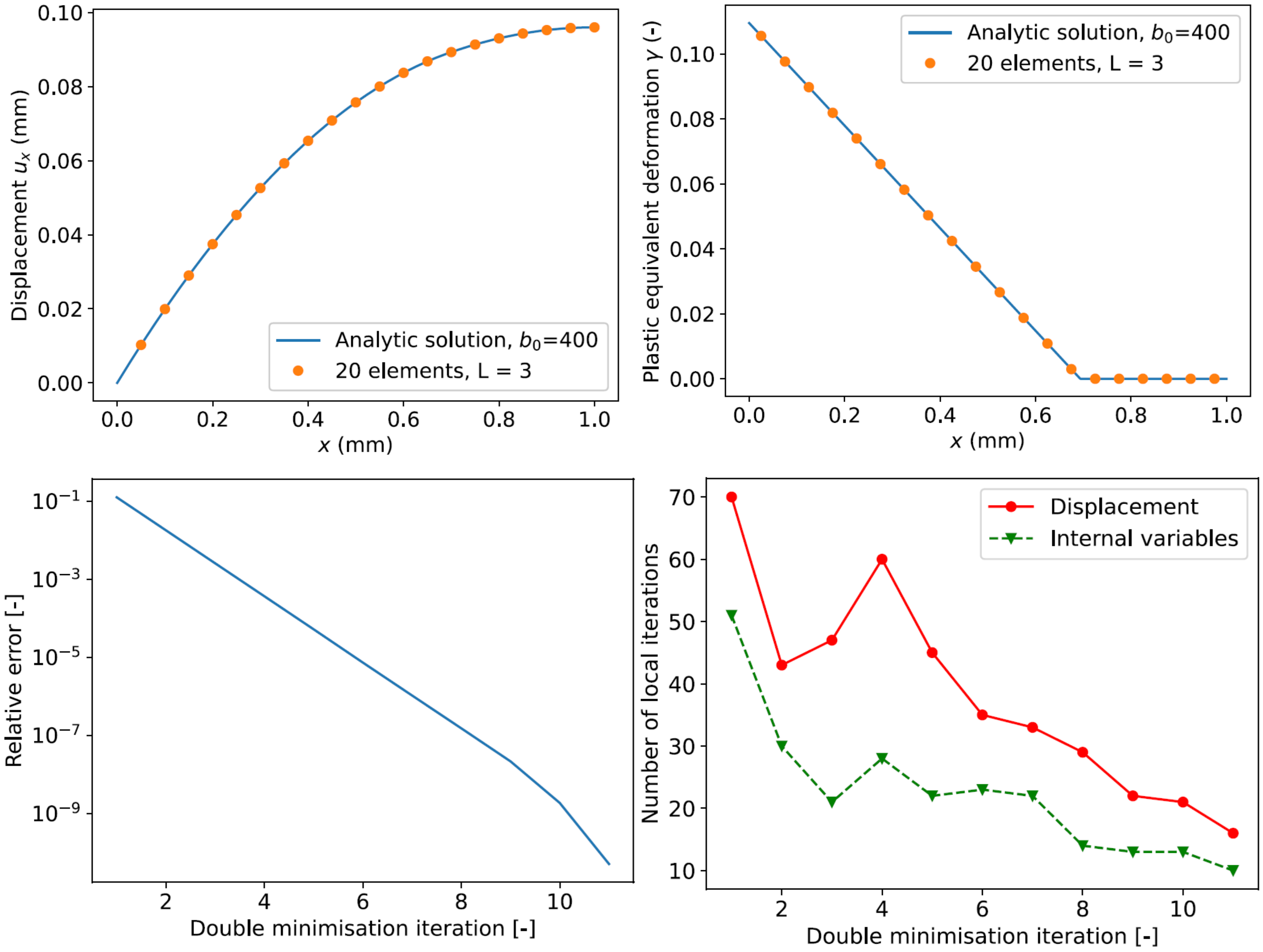
Quantum annealing

Quantum annealing

Application on 1D problems

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

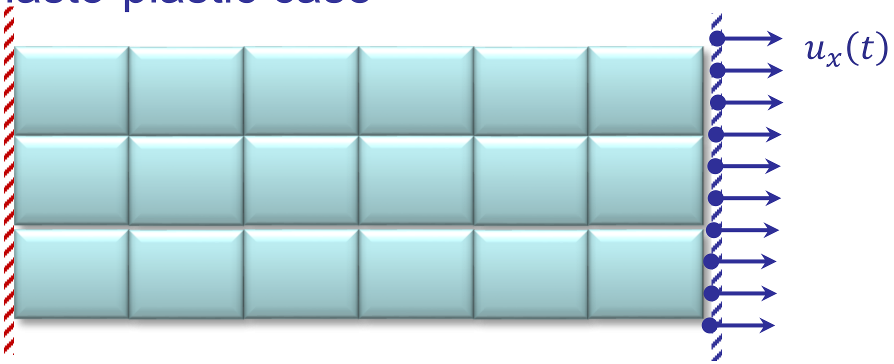


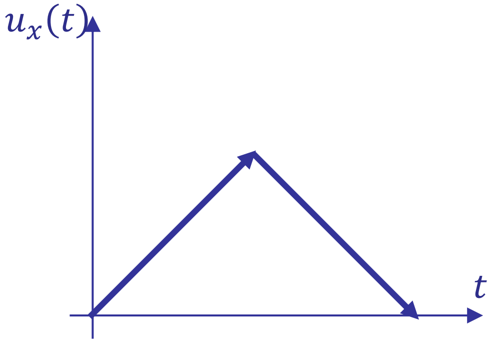


The number of local iterations decreases as the double minimisation iterations proceed

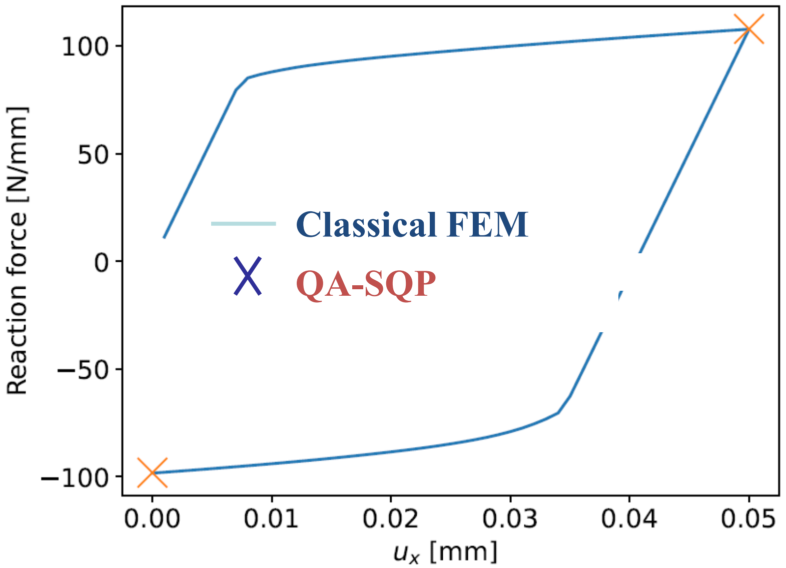
Application on 2D problems

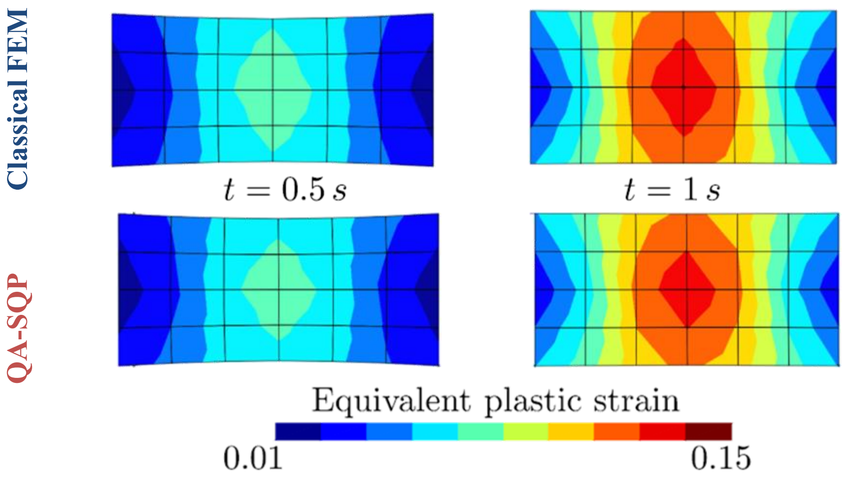
- 2D-elasto-plastic case





  - 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





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
  - Binarization remains a limitation

- 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