HYBRID QUANTUM COMPUTING

Applications for Combinatorial Problems in the Energy Sector

Sergio López Baños, DLR-VE, 16.01.2024

Content

1. | Motivation: why energy optimization problems? >

Source: April 2023 - Mckinsey - Quantum Technology Monitor

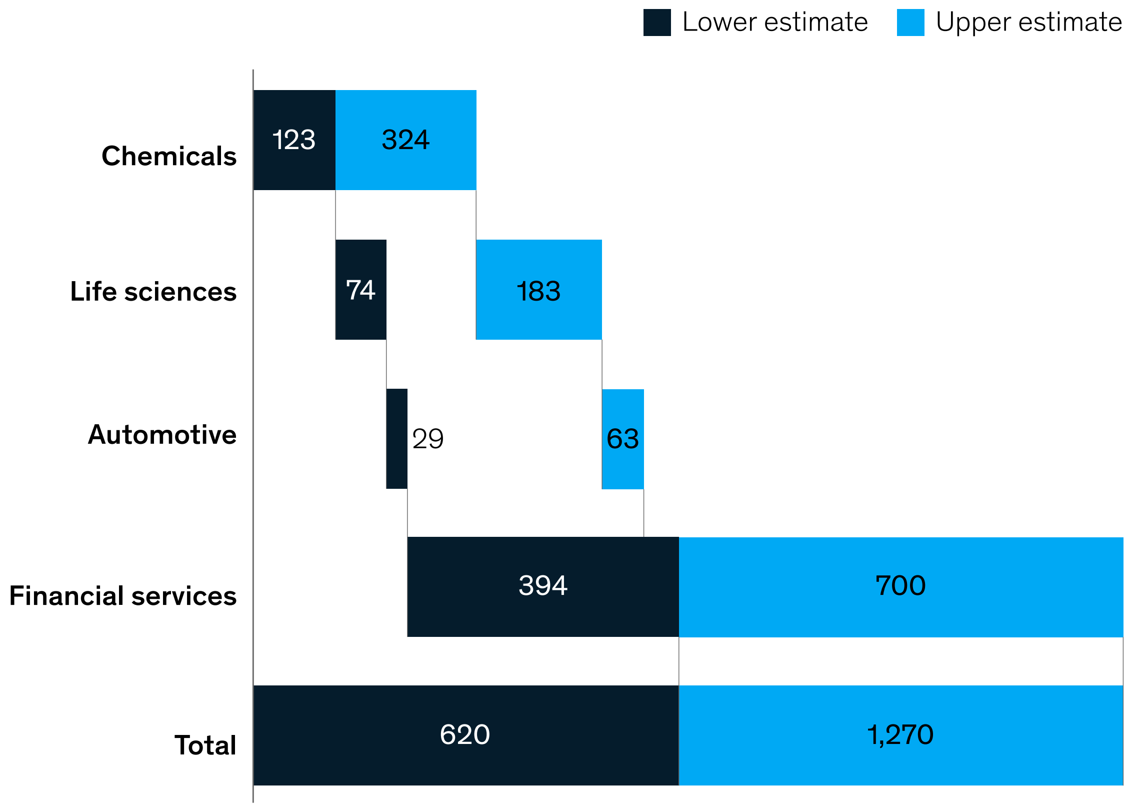
The estimated value at stake for QC in the four industries most likely to see impact first has now reached nearly $1.3 trillion.

Economic value + Incremental ++ Significant +++ Disruptive

Industry	Key segment for QC	2025–30	2030–35
Global energy and materials	Oil and gas	+	++
	Sustainable energy	+	+++
	Chemicals	++	+++
Life sciences	Pharmaceuticals	++	+++
Advanced industries	Automotive	++	++
	Aerospace and defense	+	++
	Advanced electronics	+	++
	Semiconductors	+	++
Finance	Financial services	++	+++
Telecom, media, and technology	Telecom	+	++
	Media	+	+
Travel, transport, and logistics	Logistics	+	++
Insurance	Insurance	+	+

Four industries expected to see first impact

Value at stake with incremental impact of QC by 2035, $ billion



2. | Transmission Expansion Planning Problem (TEP) >

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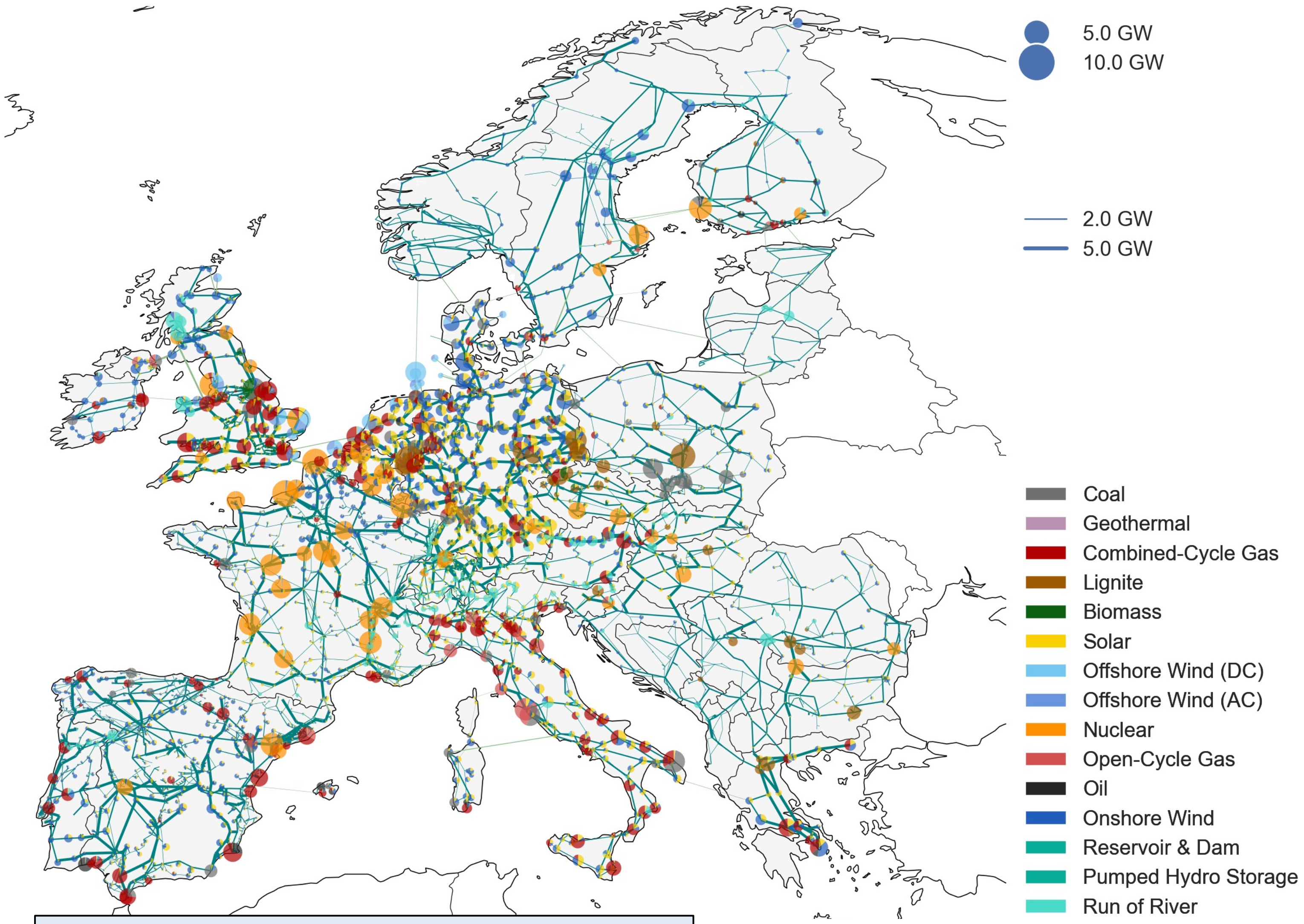


Source: PyPSA software https://pypsa.readthedocs.io/en

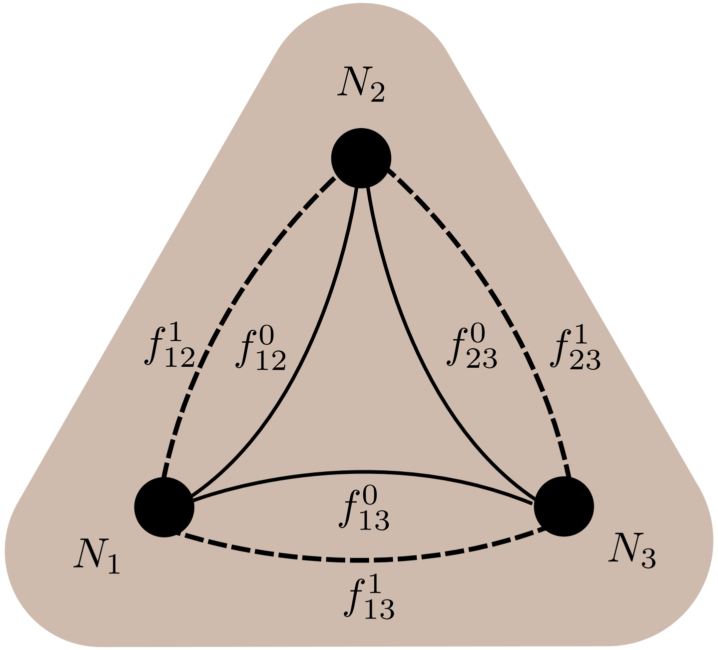
Objective: distribute the energy across a network in the most effective way so that we minimize the cost.

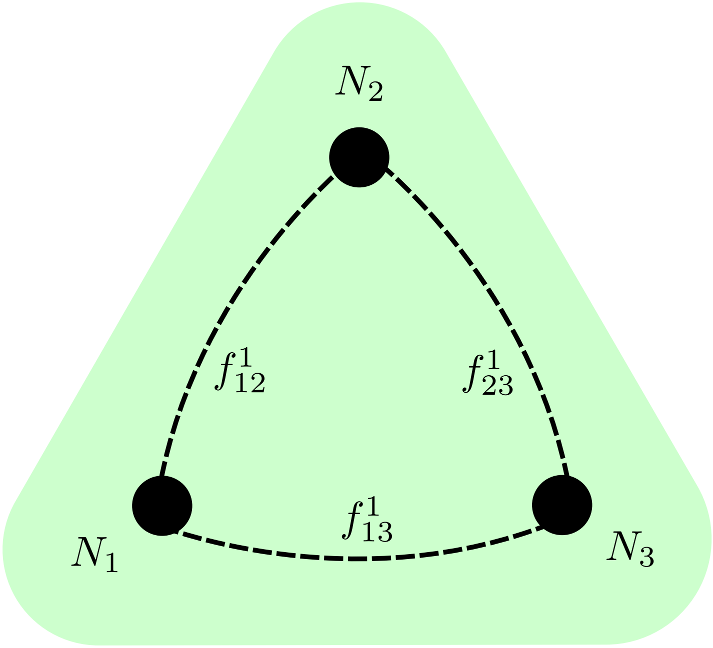
How: expanding the transmission lines of a network.

Motivation:

- Larger and more Complex models.
- Bad at Integer Problems (IP)
- Decentralized weather-dependent renewable energy.
- Increase of Storage Components.

2.1 | Transmission Expansion Planning Problem (TEP) > ⊗ |Brownfield and Greenfield Models >

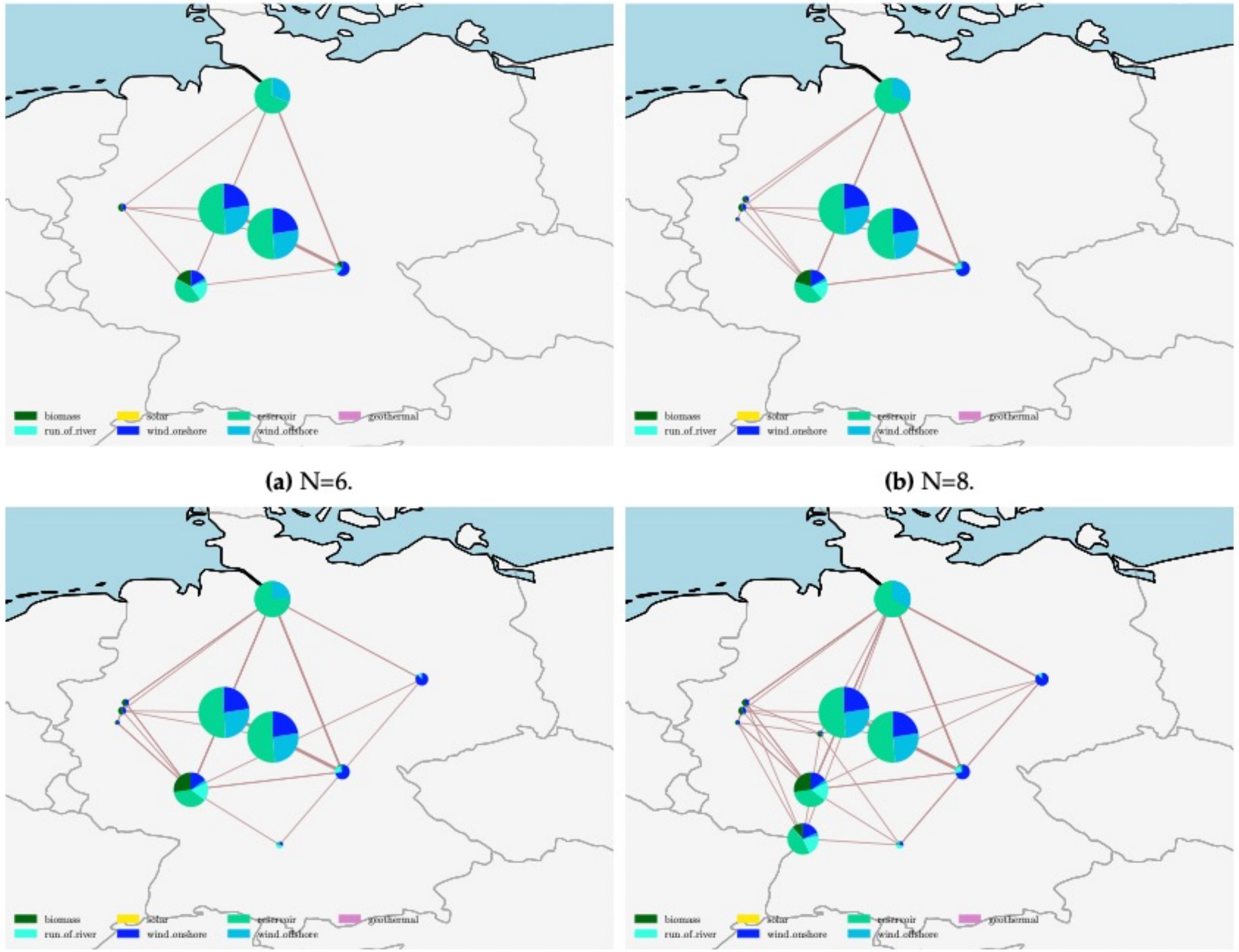




Brownfield model: Network considering current transmission lines (solid lines) and candidate lines (dashed lines).

Greenfield model: Network considering just candidate lines (dashed lines).

2.2| Transmission Expansion Planning Problem (TEP) > ⊗ |Test Cases>



(a) N=6.

(b) N=8.

(c) N=10.

(d) N=12.

Figure: European network generated with PyPSA for N clusters from eGo100 data.

- Scalable Test Cases.
- Enable to work only with renewable energies.
- Greenfield or Brownfield model.
- Number of snapshots.

2.3 | Transmission Expansion Planning Problem (TEP) > ⊗ |Parameters and Variables>

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Parameters

Variables

Symbol	Description	Type
N	Set of nodes of the network	Set
H	Set of snapshots	Set
C	Set of candidate transmission lines	Set
C_k	Set of candidate transmission lines from all nodes to node k	Set
E	Set of existing transmission lines	Set
E_k	Set of existing transmission lines from all nodes to node k	Set
x_{kl}	Transmission line from node k to l	Binary
f_{kl}^0	Power flow in existing line from node k to l	Real
$\bar{f}_{kl}^0$	Maximum power flow in existing line from node k to l	Real
f_{kl}^1	Power flow in candidate line from node k to l	Real
$\bar{f}_{kl}^1$	Maximum power flow in candidate line from node k to l	Real
r_k	Shedding load at node k	Real
$d_k(h)$	Demand of node k at snapshot h	Real
$g_k(h)$	Current generation at node k at snapshot h	Real
$\bar{g}_k$	Maximum generation at node k	Real
c_{kl}	Investment cost of transmission line from node k to l	Real
$c_k^{(oc)}$	Annualised operational cost per MWh of generator g_k	Real
c_k	Cost of shedding load at node k	Real

Table: Description of variables and parameters involved in TEP problems.

2.4 | Transmission Expansion Planning Problem (TEP) > ⊗ |Mathematical Model MILP>

MILP problems can be decomposed in IP and LP

$$\min_{\mathbf{x},\mathbf{g},\mathbf{r},\mathbf{f}^0,\mathbf{f}^1} \underbrace{\sum_{kl\in C} c_{kl}x_{kl}}_{\text{Investment cost}} + \underbrace{\cancel{\sum_{h\in H}\sum_{k} c_k^{(oc)} g_k(h)}}_{\text{Operational cost}} + \underbrace{\sum_{h\in H}\sum_{k} r_k(h)c_k}_{\text{Load shedding cost}}$$

(Power Balance) $d_k(h) - \left(\sum_{l\in E_k} f^0_{kl}(h) + \sum_{l\in C_k} f^1_{kl}(h) + g_k(h) + r_k(h)\right) = 0\,,$

(Existing circuit flow limits) $\left|f^0_{kl}(h)\right| - \bar{f}^0_{kl}(h) \leq 0\,,$

(Candidate circuit flow limits) $\left|f^1_{kl}(h)\right| - \bar{f}^1_{kl}(h)x_{kl} \leq 0\,,$ ← Complicated Constraint

(Node generation limits) $g_k(h) - \bar{g}_k(h) \leq 0\,,$

(Node loads limits) $r_k(h) - d_k(h) \leq 0\,,$

(Positive variables) $\mathbf{g},\mathbf{r} \geq 0,$

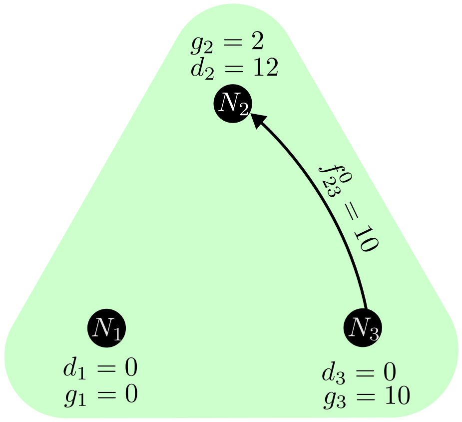
(Binary type) $x_{kl} \in \{0,1\}\,,$

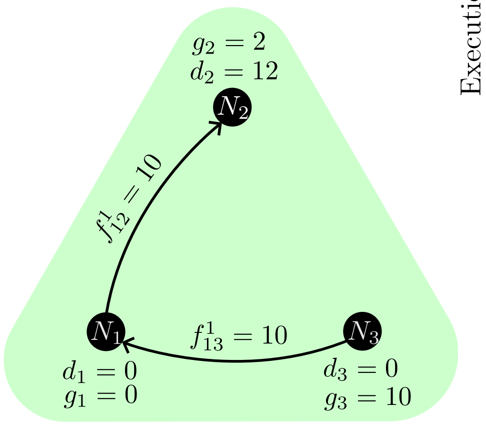
Conference Paper: Dilwali, K., Gunnaasankaraan, H., Viswanath, A., & Mahata, K. (2016). Transmission expansion planning using benders decomposition and local branching. In 2016 IEEE Power and Energy Conference at Illinois (PECI). 2016 IEEE Power and Energy Conference at Illinois (PECI). IEEE. https://doi.org/10.1109/peci.2016.7459265

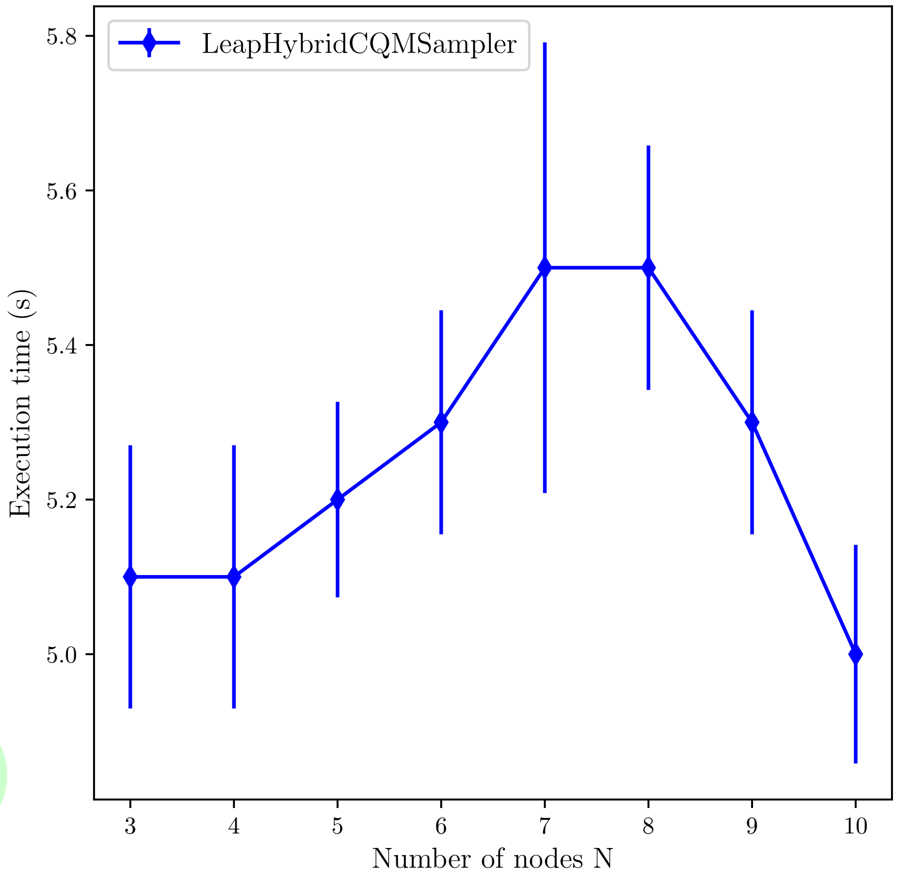
LeapHybridCQMSampler

Main features:

- 20 min of free trial.
- Solve MILP problems.
- Cannot know how much quantum solver was involved in the resolution.







We do not have control of how much QA is involved in the calculations. The D-Wave hybrid solvers are black boxes.

x_{12}	x_{13}	x_{23}	f_{12}	f_{13}	f_{21}	f_{23}	f_{31}	f_{32}	g_1	g_2	g_3	r_1	r_2	r_3	Prices
0	0	1	0	0	0	10	0	0	0	2	10	0	0	0	60
1	1	0	0	10	10	0	0	0	0	2	10	0	0	0	60

3.2 | Methods for addressing large problems >
⊗ | Simulated Annealing vs Quantum Annealing >

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Source: Transmission Expansion Planning by Quantum Annealing (MSc Thesis)

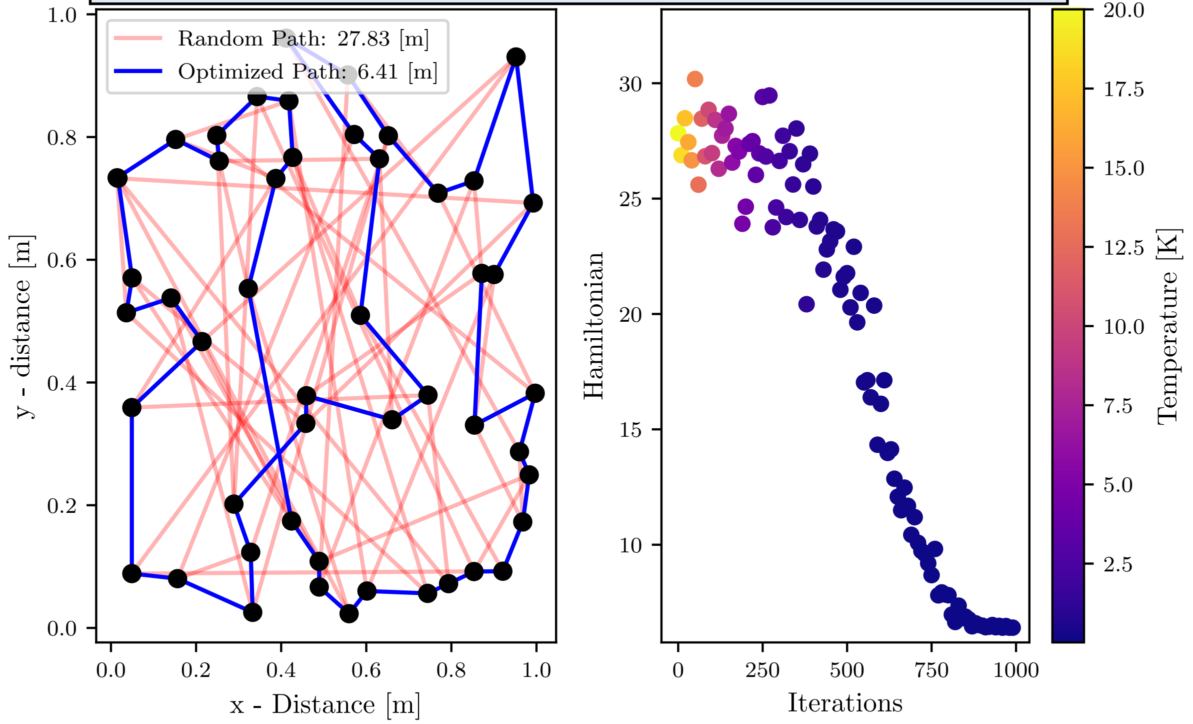


Figure B.1: Simulated annealing process for a 20-nodes travelling salesman problem, where nodes are represented by black dots. The code to produce the figure can be found in Appendix D. **Left:** Plot showing a random path (red) to travel the nodes and the path (blue) obtained for an instance of simulated annealing. **Right:** Hamiltonian as a function of iterations and temperature.

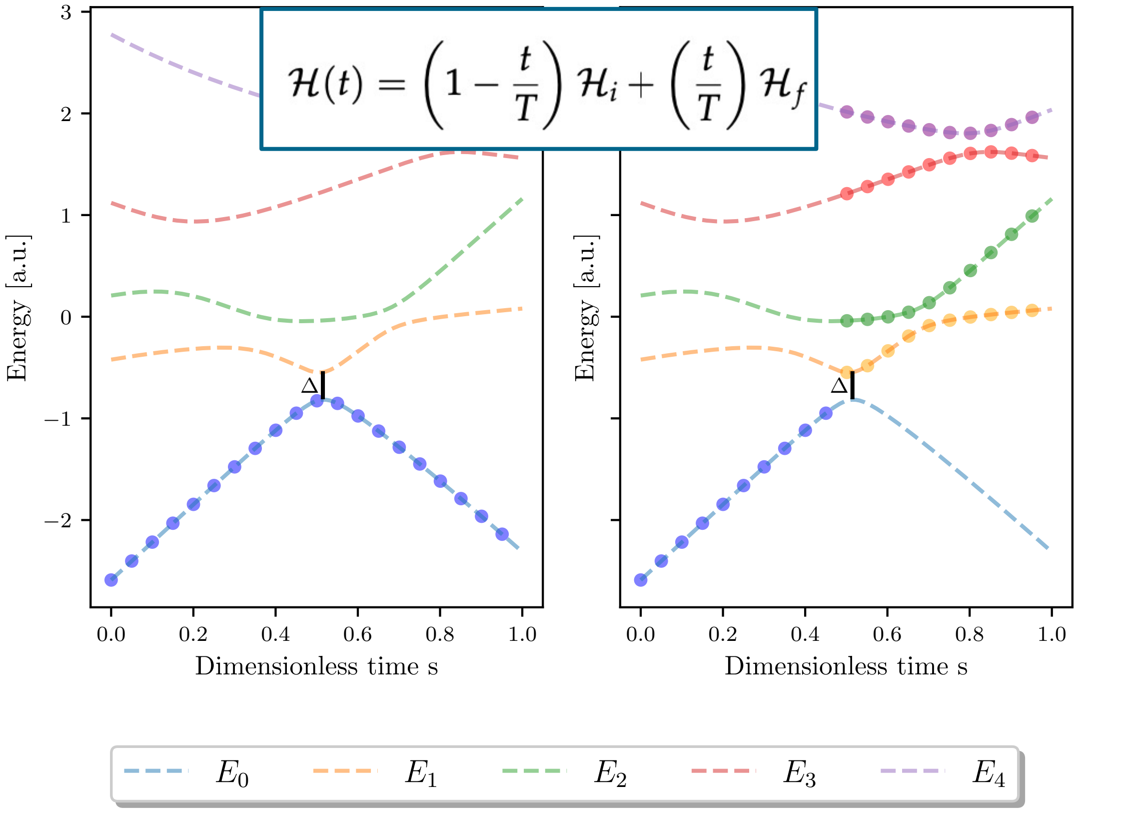
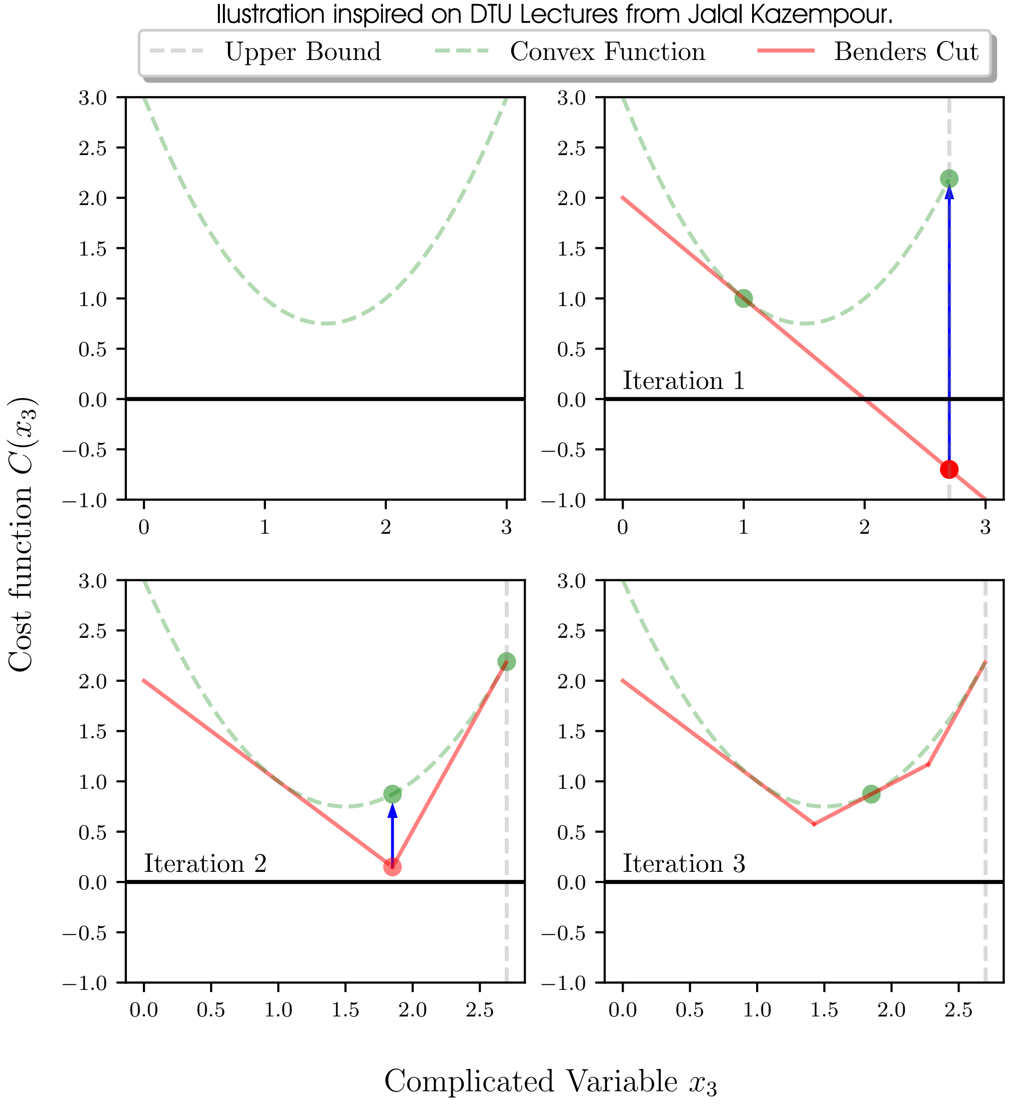


Figure 2.1: Eigenenergies of a random Hamiltonian as function of dimensionless time s = t/T. The dots indicate the state of the system at each point in time. **Left:** when adiabatic conditions are fulfilled, i.e., if the evolution is carried out suffi- ciently slowly, then our system evolves continuously in time along the ground state. **Right:** when the evolution is carried out not fulfilling the adiabatic con- ditions, it could happen that we end up in a different eigenstate if our system absorbs enough energy to jump to next level over the evolution, something that is more likely to happen close to the minimum gap Δ. If that happens we would end up in a different eigenstate of the target Hamiltonian which does not encode the optimal solution.

Proceeding: Romero, R., Gallego, R. A., & Monticelli, A. (n.d.). Transmission system expansion planning by simulated annealing. In Proceedings of Power Industry Computer Applications Conference. Power Industry Computer Applications Conference. IEEE. https://doi.org/10.1109/pica.1995.515195

3.2 | Methods for addressing large problems >
⊗ | Benders' Decomposition Algorithm >



1. Fix integer variables to feasible integer values.
2. Solve the resulting LP for fixed integer variables.
   1. Upper Bound for the objective function.
   2. Sensitivities (dual variables).
3. Solve the IP problem again with the newly added cuts.
   1. Lower Bound for the objective function.
   2. New Integer Values.
4. Check Stopping Criterion:

   Upper_bound – Lower_bound < precision

Book: Conejo, A. J., Castillo, E., Minguez, R., & Garcia-Bertrand, R. (2010). Decomposition techniques in mathematical programming. Berlin, Germany: Springer.

3.2 | Methods for addressing large problems > ⊗ | Benders' Decomposition Algorithm >

Step 1: Initialization of Benders' decomposition

$$t = 1 \quad \text{Benders' iteration} \tag{4.8}$$
$$\underline{z}^0 = -\infty \quad \text{Lower bound} \tag{4.9}$$
$$\bar{z}^0 = \infty \quad \text{Upper bound} \tag{4.10}$$
$$\alpha^0 = 0 \quad \text{Load shedding and operational cost} \tag{4.11}$$
$$\Pi^0_{f^1_{kl}} = 0 \quad \forall kl \in C \quad \text{Lagrange multipliers} \tag{4.12}$$

Step 2: Master problem solved by a quantum annealer

$$\min_{\mathbf{x}^t} \quad \underline{z}^t \tag{4.13a}$$
$$\text{s.t.} \quad \underline{z}^t \geq \sum_{kl \in C} c_{kl} x^t_{kl} + \alpha^{t-1} - \sum_{kl \in C} \Pi^\tau_{f^1_{kl}} \left(x^t_{kl} - x^\tau_{kl}\right) \quad \forall \tau = 1, \dots, t-1, \tag{4.13b}$$
$$x_{kl} \in \{0, 1\}, \quad \forall kl \in C. \tag{4.13c}$$

- The cuts produced cannot be real numbers. (Otherwise we have to discretize)
- If the cuts are big integers numbers →many slack variables.

Step 3: Slave problem solved by a classical solver

$$\min_{\mathbf{g}, \mathbf{r}, \mathbf{f}^0, \mathbf{f}^1} \quad \alpha^t \equiv \underbrace{\sum_k c^{(oc)}_k g_k}_{\text{Operational cost}} + \underbrace{\sum_k r_k c_k}_{\text{Load shedding cost}} \tag{4.14a}$$
$$\text{s.t.} \quad d_k - \left(\sum_{l \in E_k} f^0_{kl} + \sum_{l \in C_k} f^1_{kl} + g_k + r_k \right) = 0, \quad \forall k \in N, \tag{4.14b}$$
$$\left|f^0_{kl}\right| - \bar{f}^0_{kl} \leq 0, \quad \forall kl \in E, \tag{4.14c}$$
$$\left|f^1_{kl}\right| - \bar{f}^1_{kl} x^t_{kl} \leq 0, \quad \forall kl \in C, \tag{4.14d}$$
$$g_k - \bar{g}_k \leq 0, \quad \forall k \in N, \tag{4.14e}$$
$$r_k - d_k \leq 0, \quad \forall k \in N., \tag{4.14f}$$
$$\mathbf{g}, \mathbf{r}, \quad \geq 0 \tag{4.14g}$$

Step 4: Stopping criterion

Update the upper bound,

$$\bar{z}^t = \min\{\bar{z}^{t-1}, \sum_{kl \in C} c_{kl} x^t_{kl} + \alpha^t\}. \tag{4.15}$$

If $\left(\bar{z}^t - \underline{z}^t\right) / \bar{z}^t \leq \epsilon$, then we found the (sub)-optimal solution, else $t = t + 1$ and we have to repeat the algorithm from step 2 until the stopping criterion is satisfied.

No

Yes → END

3.2 | Methods for addressing large problems > ⊗ | Benders' Decomposition Algorithm >

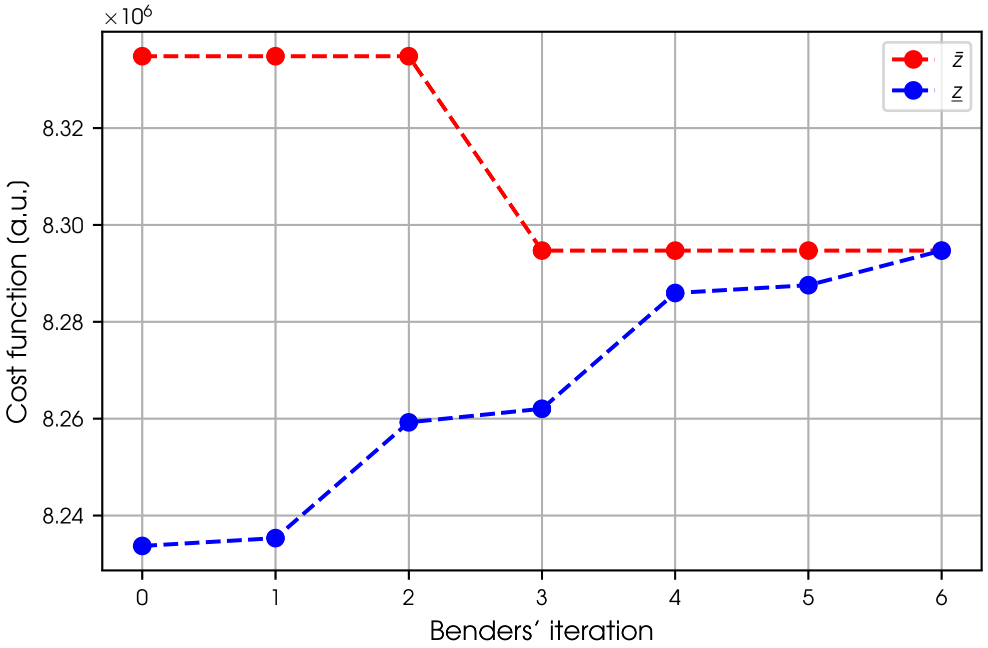


Figure: Plot of the upper and lower bounds of the hyrbrid Benders' decomposition algorithm applied to a 8-nodes PyPSA-EUR clustered network of Europe.

- PyPSA-EUR 8-Nodes Clustering of European Network.
- The data is rounded so that D-Wave can handle the problem.
- D-Wave is not capable to find an embedding for the master problem.
- The solution is optimal (dual gap is zero).

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A hybrid Quantum-Classical Algorithm for Mixed-Integer Optimization in Power Systems

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Department of Wind and Energy Systems, Technical University of Denmark (DTU)
Elektrovej, 2800 Kgs. Lyngby, Denmark

Optimization Method (1) [Pareto Cuts]:

- Guiding the choice of Binary will provide efficient cuts.

Optimization Method (2) [R solutions from QPU]:

- Run the Dual-SP for the best R-solutions provided by the annealer.
  - Add more cuts per iteration.
  - Minimize the access time to QPU

Journal Article: Magnanti, T. L., & Wong, R. T. (1981). Accelerating Benders Decomposition: Algorithmic Enhancement and Model Selection Criteria. In Operations Research (Vol. 29, Issue 3, pp. 464–484). Institute for Operations Research and the Management Sciences (INFORMS). https://doi.org/10.1287/opre.29.3.464

6.| Difficulties and Future Steps >

1. Reduce the number of slack variables (qubits that use the quantum computer to do the binary expansion of integer of your problem) by reformulating the problem and adding a post-processing.

2. The cuts added to the master problems are in the more straighforward way but there are smarter ways of adding cuts or even different "flavours" of Benders. In other words, there are redundant cuts.

3. Effect of not getting the optimal solution of the Master Problem (heuristic) for the Benders algorithm. Quality of solution. Could we avoid or improve this?

4. There exist other alternatives approaches (multi-cuts) such as the one proposed by Paterakis 10.1016/j.compchemeng.2023.108161

Impressum

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Thema: Hybrid Quantum Computing: Applications for Combinatorial Problems in the Energy Sector

Datum: 16.01.2024

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Extra | Benders' Decomposition Algorithm >

Step 2: Master problem solved by a quantum annealer

$$\min_{\mathbf{x}^t} \quad \underline{z}^t \tag{4.13a}$$

$$\text{s.t.} \quad \underline{z}^t \geq \sum_{kl \in C} c_{kl} x_{kl}^t + \alpha^{t-1} - \sum_{kl \in C} \Pi_{f_{kl}^1}^{\tau} \left(x_{kl}^t - x_{kl}^{\tau} \right) \quad \forall\, \tau = 1, \ldots, t-1, \tag{4.13b}$$

$$x_{kl} \in \{0, 1\}, \quad \forall\, kl \in C. \tag{4.13c}$$

QUBO formulation

$$\begin{aligned} \max_{\mathbf{x},\mathbf{w}} \quad & c^{\mathsf{T}}\mathbf{x} + \sum_{i=-\underline{m}}^{\bar{m}_+} 2^i w_{(i+\underline{m})} - \sum_{j=0}^{\bar{m}_-} 2^j w_{j+1+\underline{m}+\bar{m}_+} \\ \text{s.t.} \quad & (b - A\mathbf{x})^{\mathsf{T}} u^k \geq \bar{t}(\mathbf{w}), \quad \text{for } k \in \hat{K}, \\ & (b - A\mathbf{x})^{\mathsf{T}} r^j \geq 0, \quad \text{for } j \in \hat{J}, \\ & \mathbf{x} \in X, \quad \mathbf{x} \in \{0,1\}^n, \\ & \mathbf{w} \in W, \quad \mathbf{w} \in \{0,1\}^M. \end{aligned}$$