

Séminaire TQCI dédié au calcul quantique

Jeudi 31 mars 2022 de 10h00 à 16h30

Amphithéâtre Sophie Germain, Bâtiment Turing, Inria Saclay

Perspectives on the Numerical Resolution of Partial Differential Equations on Quantum Computer

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Séminaire



Teratec
Quantum
Computing
Initiative



EDF-THALES PDEs resolution : context

- EDF and Thales devote hundreds of millions of hours of CPU per year to solve Partial Differential Equations (PDEs).
- These resolutions are expensive and limited in precision.
- We are at the edge of what we can do on classical machines. The numerical solution of such equations generally involves the resolution of sparse linear systems.

Any speedup, any gain in the electrical consumption of these computations would be an advantage.

EDF-THALES Agreement : « Numerical resolution of partial differential equations by Quantum algorithms and computing »

Global Objective

- Quantum acceleration could help reducing computing time and increase the size of the problems that will be addressed.

Contribution of the Study

- Accelerate their respective research in the field of solving PDEs to study what advantages quantum computers could provide.
 - Bibliography review
 - Coding and implementation of algorithms
 - Results obtained on certain use cases

EDF-THALES Agreement : « Numerical resolution of partial differential equations by Quantum algorithms and computing »

February – March 2022:

- Framework definition between EDPS experts
- Co-editor of the bibliography review

April 2022

- Restitution of the bibliography review and sharing of avenues to be tested jointly

April – December 2022

- Joint modeling and coding work on the respective use cases.

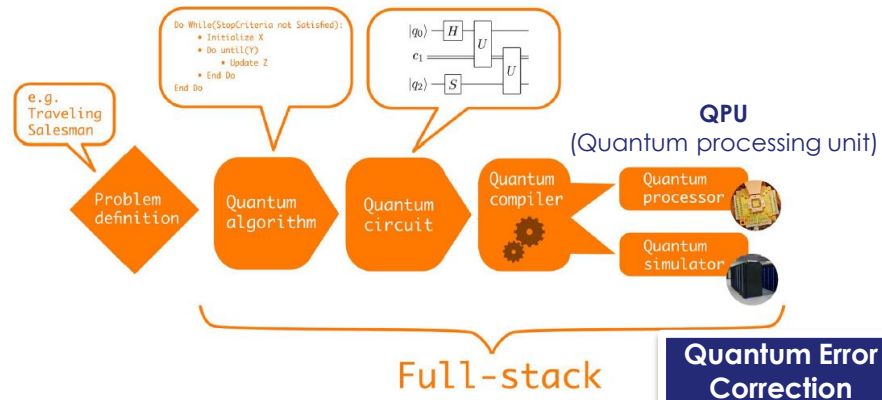
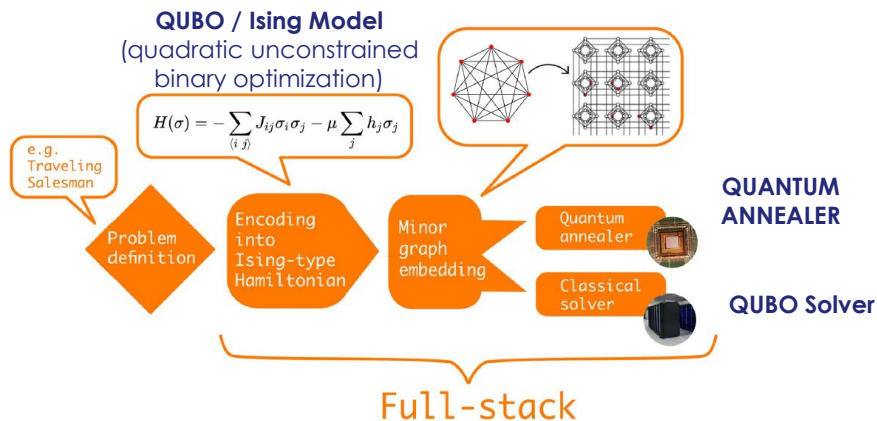
January – April 2023

- Joint benchmarking of respective use cases on NISQ machines and simulators.

May – June 2023

- Drafting of a roadmap on the theme for next steps

3 kinds of computers: Quantum Annealers, NISQ, Full-Tolerant LSQ



QA Quantum Annealer

Non Universal Machine. No Entanglement but Quantum Tunneling

Solve QUBO (Quadratic Unconstrained Binary Optimization) modelled as Ising Model (Hamiltonian Functional)

Limitations due to connectivity: Ancillary connections required

QUADRATIC UNCONSTRAINED BINARY OPTIMIZATION

BINARY INTEGER LINEAR PROGRAMMING

NISQ

Noisy Intermediate Scale Quantum

Medium-sized imperfect (noisy) computer

Short quantum coherence duration

VARIATIONAL ALGORITHMS (Polynomial speed-up)

VQE: Variational Quantum Eigensolver

LSQ

Full-Tolerant Large Scale Quantum

Full-Tolerant with stabilized Qubits

Error Correction & Full Connectivity

LARGE SCALE ALGORITHM (Expon. Speed-up)

HHL: Linear Systems of Equations Solver

QUANTUM COMPUTERS PERFORMANCES BENCHMARKING

Consolidate Quantum Benchmarking Rules/Tools

⇒ DARPA Quantum Benchmarking Program: establish key quantum-computing metrics

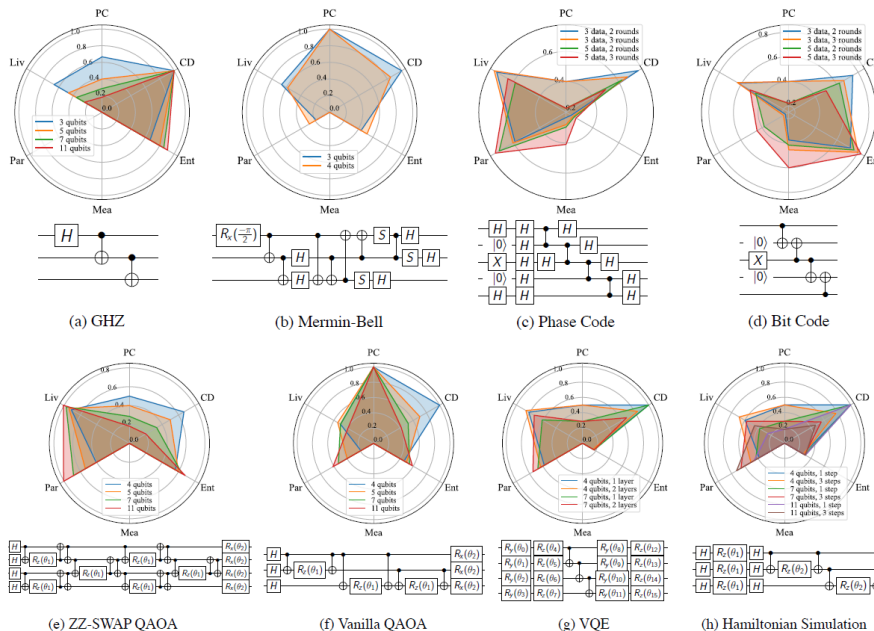
Q-Score
(ATOS)

SupermarkQ
Suite
(Super-Tech)

Quantum
LINPACK
(Berkeley Lab)

CLOPS
(IBM)

BCG - The Race to Quantum Advantage
Depends on Benchmarking



SupermarQ:
A Scalable
Quantum
Benchmark
Suite

Séminaire



OPEN



Quantum Computing Simulator

THALES BENCHMARK OF QUANTUM COMPUTER SIMULATORS



cuQuantum

200 Qubits

(dedicated algos)



40 Qubits



36 Qubits



50 Qubits



Microsoft

30 Qubits



40 Qubits

EDF/THALES
Use-Cases



Benchmark

Selection of
Simulators

Séminaire



OPEN



THALES
Building a future we can all trust

Quantum Algorithms & Computing STACK

Quantum Functional Programming

New Quantum Algorithms

Quantum Algorithms Library

Classical Algorithms

Hybrid Computing Partitioner (HPC & Quantum Accelerator)

Quantum Compiler to Q Gates
(HW-Agnostic Compiler)

HPC Compiler

Quantum Gates Optimizer (+ error correct.)

Quantum Compiler to HW

Classical Compiler to HW

QAnnealer
Emulation

QPU
Emulation

QAnnealer

QPU

CPU

GPU

TPU

Secure Cloud Access

THALES Electromagnetic Simulation

THALES QUANTUM ALGORITHM for PDE Solver of Electromagnetic Simulation

Electromagnetic Simulation for Antenna Design & Performance

Assessment

- Maxwell equations : core business of electronic equipment and systems development. Simulation is one of the main lever of competitiveness and is hugely used all along the V development cycle.
- The realm of physics around the Maxwell equations is closely tied to the electronic equipment/system development, a core aspect of business.

THALES Applications

- Radar and EW antennas in Defence Mission System
- Microwave tubes in Defence, spatial or medical applications

Maxwell equation solver:

- **Finite Element Method (FEM)** : the variationnal form
- **Boundary Element Method (BEM)** : the integral form
- **Finite Difference Time Domain (FDTD)**
- **Coupling BEM and FEM** : domain decomposition techniques

⇒ need the **resolution of linear system in complex algebra**:

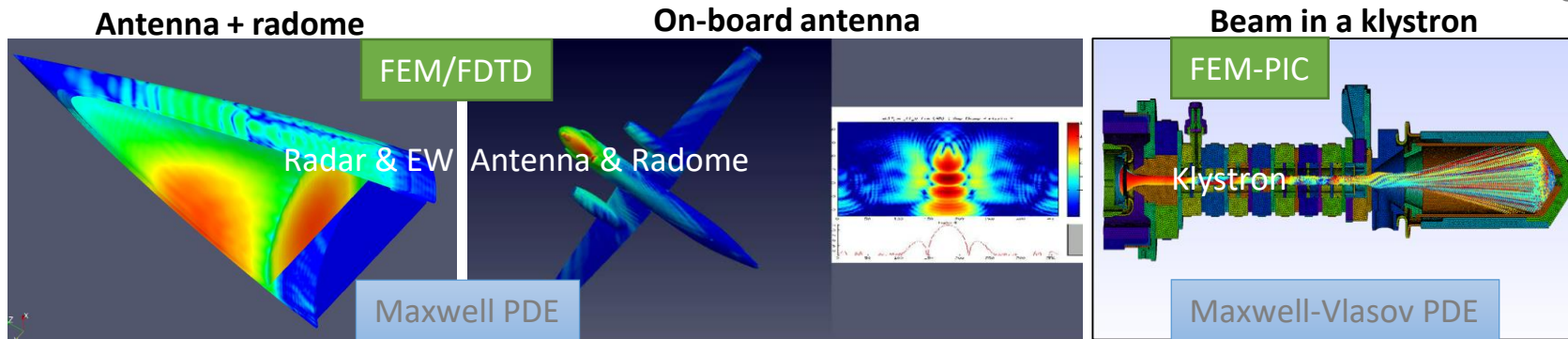
- BEM: **Full Linear system**
- FEM/FDTD: **Sparse Linear system**

Nota: BEM linear system Solver SoA:

- Based on **SVD (Singular Value Decomposition)**



HHL Algo
on LSQ &
HHL Algo
on NISQ



THALES Use-Cases (1/3)

EM sensors radiating performances

- **Pain:** Simulation of the radiating performances of radar or interferometer panel as they are measured in development or in their environment (radome for radar or on-board for radar and EW systems) requires huge computing resource. At this level HPC facilities are required. To do so, DMS uses internal Maxwell solver with different and complementary numerical methods. Although numerical breakthrough has been developed and applied these last 20 years (Domain Decomposition, H-matrix, HPC) cpu time remains a research axis
- **Gain:** The objective of this Use-Case is to evaluate if and how Quantum computing could give an opportunity to decrease drastically or not cpu time of complex antenna simulations
- **UC:** The use-case will be focused on radar application in the presence of radome

Electromagnetic Tube Simulations

- **Pain:** Thales MIS uses Standard computer when using reduced Particle-In-Cell (PIC) codes. But Full 3D Time PIC codes are required to
 - Simulate future high frequency tubes (Bande V or W) where the design margins to reach performances are very thins
 - Simulate Time loop oscillations in tubes which sometimes stop tubes productionNew simulation resources (codes are available) are required to perform these simulations.
- **Gain:** More faster and realistic Simulation to take into account industrial difficulties (assembly, tolerances)
- **UC:** Telecom & Space Business lines (ground space and/or space ground connections), satellites with mini-tubes Twt's, Klystrons for radar

Cooling process simulation

- **Pain:** Dispersed particle transport equation, being akin to the Maxwell-Vlasov equation, has proven to be rather hard to compute, even more when coupled with a fluid in a liquid-solid phase transition.
 - The implicit numerical scheme used to simulate the cooling process of an ammunition requires the inversion of massive matrices, and thus requires vast amounts of computing power.
 - Optimizing the cooling process is difficult, as it requires to solve a system that becomes exponentially harder to solve the higher the amount of degrees of freedom in it.
- **Gain:** In order to conduct this simulation in a reasonable timespan, many approximations are required. Therefore, using quantum algorithms may lead to more complex modelizations while keeping acceptable computing times.
- **UC:** cooling process of an ammunition

THALES Use-Cases (2/3)

TOPIC: Maxwell

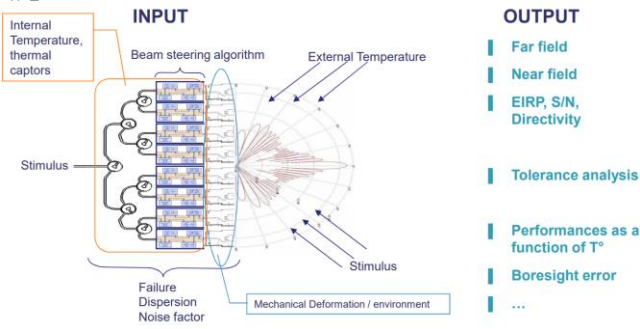
- Radar and EW antennas in Defence Mission System
- Finite Element Method (FEM) / Finite Difference Time Domain (FDTD)

GOVERNING EQUATIONS

- Maxwell's equation in the frequency domain with constant permittivity and permeability

TEST MODEL & DATA DESCRIPTION

- **Sphere 1D:** A metallic sphere coated or not with a dielectric material can be used for frequency domain, Mie series being the analytical solution



TOPIC: Maxwell-Vlasov

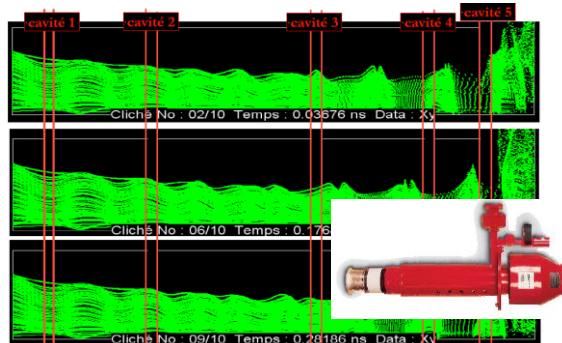
- A klystron, with two or three resonant cavities, representative of THALES MIS products.
- FEM-PIC

GOVERNING EQUATIONS

- Maxwell's equations in the time domain, possibly coupled with the Vlasov equations (Lorentz force)

TEST MODEL & DATA DESCRIPTION

- **Vlasov 1D:** A metallic resonant cavity (rectangular or spherical) can be used for time domain, cavity modes being the analytical solution



TOPIC: PDF powder

- Polydispersed gunpowder burning in an ammunition propulsion system
- Solved by averaging over particle size

GOVERNING EQUATIONS

- Population balance equation coupled with particle transport equation

TEST MODEL & DATA DESCRIPTION

- **Polydispersed powder sedimentation:** Sedimentation of polydispersed particles in a viscous liquid which solidifies at constant speed in the opposite direction of gravity



THALES Use-Case: Electromagnetic Simulation (3/3)

Topic: Solving Sparse Linear Systems in complex algebra (THALES DMS & LAS)

Use case: Resolution of Maxwell's equations by domain decomposition based on the use of transmission operators (BEM/FEM).

Part of the simulation code concerned: Part of Antenna Design dealing with the calculation of the transmission operator from a domain solved by the FEM method (use of high-order finite elements)

Current dimension of the linear systems solved in simulations: a few tens of millions

Dimension of linear systems for the future needs of simulations: several hundred million.

Topic: Sparse Linear System Solving (THALES AVS/MIS)

Use case: Simulation of electric fields in electron guns

Part of the simulation code concerned: determination of the electric fields which are used to "push" the electrons in the microwave tubes

Current size of linear systems solved in simulations: a few million (2-3)

Dimension of linear systems for the future needs of simulations: several tens of millions (30-40) which will make it possible to refine the meshes and to massively use the high order of resolution.

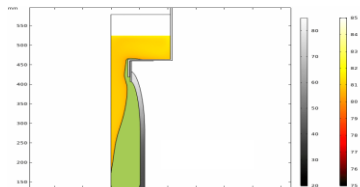
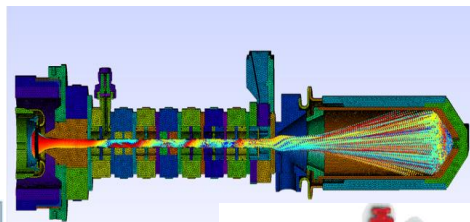
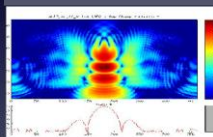
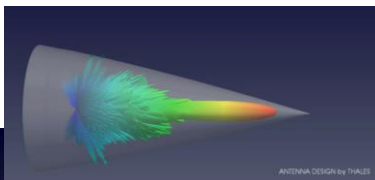
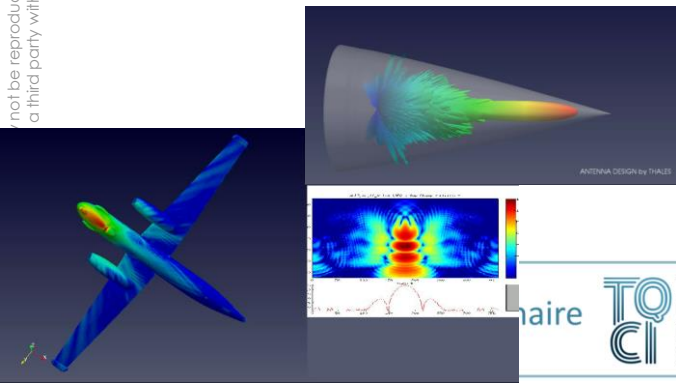
Topic: Sparse Linear System Solving (THALES LAS/VTS)

Use case: Simulation of the cooling of an ammunition containing an initially liquid explosive

Part of the simulation code concerned: Calculation of the temperature and the different fluxes over time in the explosive

Current dimension of the linear systems solved in simulations: about 30,000 elements in axisymmetric 2D

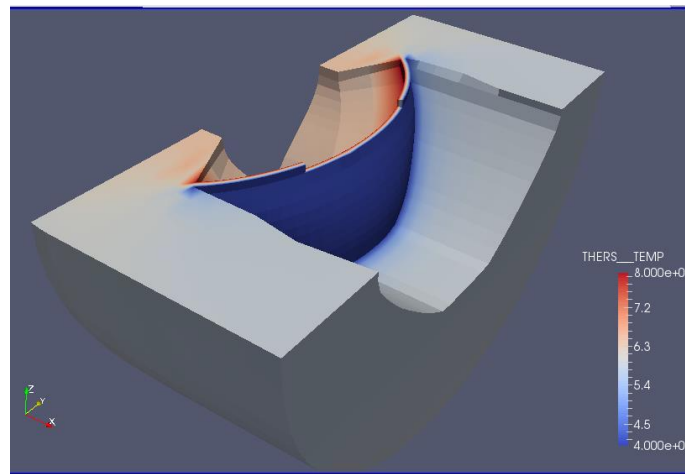
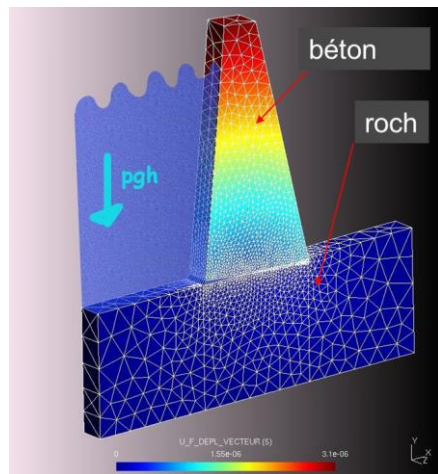
Dimension of linear systems for the future needs of simulations: around 107 elements to switch to 3D, refine the mesh, potentially increase the number of transport equations as well as the order of the digital diagram



EDF Use-Case (1/3): Mechanical structure Simulation

The current resolution of equations of mechanical structure deformation involve involves the resolution of linear system $Ax = B$

Such resolution may be done with the help of HHL or VQLE as we may not need the whole description of x .



EDF Use-cases (2/3) : Asset Management

The optimal management of EDF's portfolio of power plants may be computed with the help of HJB PDEs.

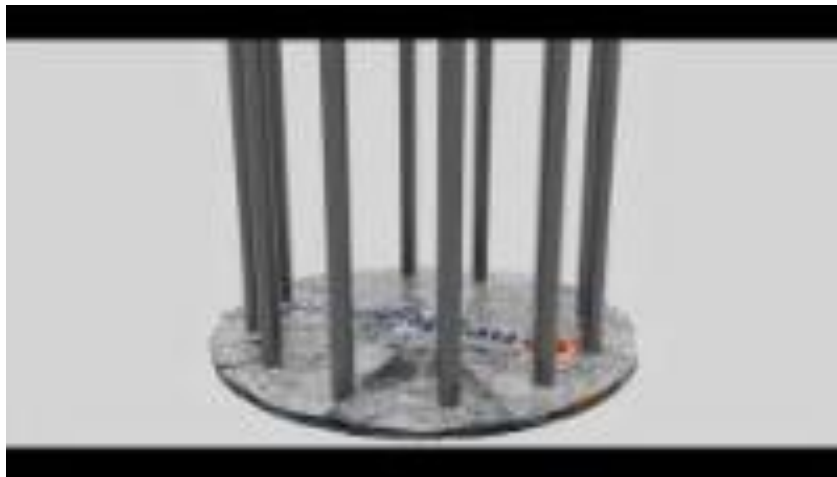
The dimension of such PDEs may be too high for traditional techniques. More recently, the use of ML methods has increased allowed overcoming the curse of dimensionality.



EDF Use-cases (3/3) Fluid dynamics

Simulation tools for nuclear thermal-hydraulics phenomena are at the core of civil nuclear industry.

Code_saturne is at the state-of-the-art of what classical machines can do. An increase in the resolution, in the execution speed would benefit to the whole civil nuclear industry.

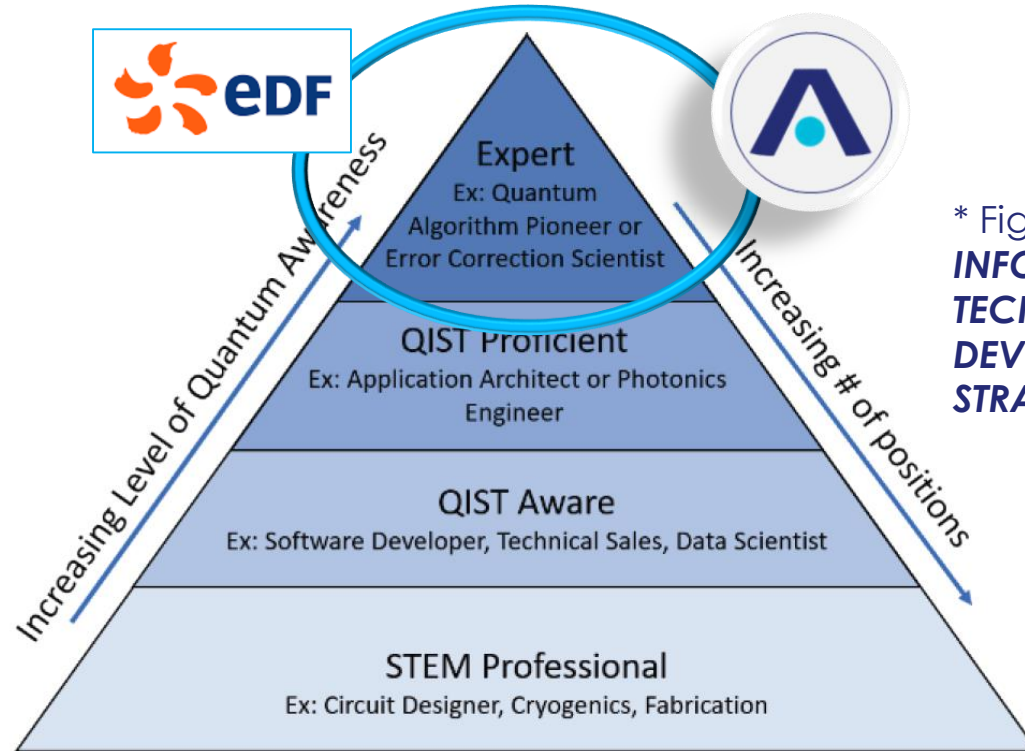


EDF & THALES Workforce Need

➤ Develop and Maintain an Understanding of Workforce Needs in the Ecosystem, with both Short-Term and Long-Term Perspectives

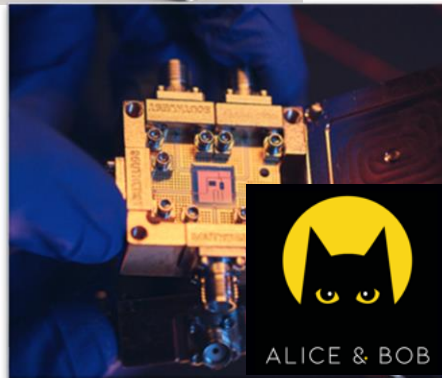
- Goal: Understand the supply of and demand for “Quantum Information” workers













**LEADERSHIP
ON DISRUPTIVE
KEY ENABLERS**



* Figure from « **US QUANTUM INFORMATION SCIENCE AND TECHNOLOGY WORKFORCE DEVELOPMENT NATIONAL STRATEGIC PLAN** »

COLLABORATION WITH QUANTUM COMPUTERS PROVIDERS



Technology	Digital Quantum Computing (gate-based systems, one-way models)	Analog Quantum Computing (quantum annealers, adiabatic systems)
Superconducting Qubits	  	
Silicon Qubits	 	
Trapped ions		
Neutral atoms		
Photons	 	

OPEN TO COLLABORATION TO BENCHMARK EDF-THALES ALGORITHMS ON QUANTUM COMPUTERS

Séminaire



OPEN



THALES
Building a future we can all trust

QUESTIONS ?

THALES PUBLICATIONS

- Timothé Presles, Cyrille Enderli, Rémi Bricout, Florence Aligne, Frédéric Barbaresco. Phase-coded radar waveform AI-based augmented engineering and optimal design by Quantum Annealing. 2021. (hal-03318130v2); <https://hal.archives-ouvertes.fr/hal-03318130/>
- Nico Piatkowski, Thore Gerlach, Romain Hugues, Rafet Sifa, Christian Bauckhage, Frederic Barbaresco. Towards Bundle Adjustment for Satellite Imaging via Quantum Machine Learning. 2022. session "Quantum Algorithms for Fusion", FUSION'22; <https://www.fusion2022.se/>
- IET UK Special Issue "Radar, Sonar & Navigation": « Radar Applications of Quantum Computer & Quantum Algorithms » by Frédéric Barbaresco, John Rarity & Hugh Griffiths, 2022

EDF PUBLICATIONS

- Algorithme quantique pour trouver les séparateurs d'un graphe orienté, Conférence Internationale Francophone sur la Science des Données (CIFSD), 2020.
- Convex Non-negative Matrix Factorization Through Quantum Annealing, The 7th IEEE International Conference on Data Science and Systems, 2021.
- Balanced K-means using Quantum annealing, IEEE Symposium Series on Computational Intelligence (IEEE SSCI 2021).
- Distance Estimation for Quantum Prototypes Based Clustering, International Conference on Neural Information Processing (ICONIP 2019).
- Pochart, T., Jacquot, P., & Mikael, J. (2021). On the challenges of using D-Wave computers to sample Boltzmann Random Variables. Proceedings of IEE 19th International Conference on Software Architecture Companion (ICSA-C)
- Dalyac, C., Henriët, L., Jeandel, E., Lechner, W., Perdrix, S., Porcheron, M., & Veshchezerova, M. (2021). Qualifying quantum approaches for hard industrial optimization problems. A case study in the field of smart-charging of electric vehicles. EPJ Quantum Technology, 8(1), 12.