Quantum Computing for Combinatorial Optimisation
PHD Thesis « CIFRE » funded by EDF R&D

Contents

Context

The Osiris Department of EDF R&D conducts researches and developments in the fields of Optimization, Simulation, Risk and Statistics for energy markets.

The resolution of huge discrete/combinatorial optimization problems is at the core of many applications tackled by this Department. As a typical example, one may mentioned the so-called « Unit-Commitment Problem » which consists in deciding which unit productions have to be stopped/started on a given time period, in order to satisfy a load demand at lower cost, while fulfilling numerous operating constraints relating to production units and to the electricity network. These applications are of great importance for EDF in a context where the field of *energy management* has experienced the emergence of numerous new problems in the past few years: increasing of the exchanges on energy markets, production decentralization and smart grids, energy storage, growing part of the Renewable Energies in the energy-mix engendering new issues due to their intermittence …

Many of these applications take the form of optimization and constraint-satisfaction problems that can be expressed as instances of typical NP-complete problems: *travelling salesman, bin-packing, job-shop scheduling, SAT, knapsack*, etc., or generally as *Linear (Mixed) Integer Programs*.

Therefore, there is no known efficient (polynomial) algorithm available to solve them.

The OSIRIS Department is thus deeply involved in the fields of Operational Research and Combinatorial Optimization and conducts , in collaboration with the Academic Community, researches and developments on the different approaches dedicated to this class of problems : reformulation and decomposition techniques (e.g. column and cut generation), meta-heuristics (e.g. local search, simulated annealing, genetic algorithms).

Major progress have been made in Quantum Computing in the past few years, opening new and promising perspectives in the field of “hard” problems solving, typically in the NP-class. Some important results demonstrate that machines and computing models relying on quantum properties of *qubits* can be used to obtain significant —sometimes up to exponential— speedups on some of these problems, compared to the best classical algorithms known: Grover’s algorithm for “unstructured” search [Grover 96], the famous Shor’s algorithm for integer factorisation [Shor 97], adiabatic approaches and QAOA algorithm for combinatorial optimization [Fahri et al 00] [Fahri et al 01][Fahri et al 14] … While dedicated to a problem in the P-class, the HHL algorithm [Harrow et al 2009] also deserves to be mentioned in this non-exhaustive list, due to its huge potential contribution to many problems based on the resolution of linear systems.

Although many issues, both theoretical and practical, still need to be overcome before the achievement of some “Universal Quantum Turing Machine”, whatever the quantum computing model it would implement, it appears to us that Quantum Computing and its applications to hard Optimisation Problems is a field which is by now sufficiently advanced to be investigated in a framework of “applied researches”.

This is why we propose a PhD thesis on this subject, funded by a “Cifre Industrial Research Training Agreement”.

Thesis Intentions

The main objective of the thesis is to investigate and characterize the potential contributions of Quantum Computing to the resolution of hard Combinatorial Optimization problems, buy testing different approaches on use-cases drawn from industrial applications treated by EDF.

Considered Research Directions

The Osiris Department proceeded to a first state of the art of the domain, and has identified *Adiabatic Computing* and the *Quantum Approximate Optimization Algorithm (QAOA)* as two promising research directions that will guide the thesis, without excluding other directions that could be identified in the course of the PhD.

These two approaches take advantage of the quantum properties of *qubits* system in order to solve specific types of Combinatorial Optimization problems. Theoretically, they should outperform exact and heuristic classical methods dedicated to this type of problems by using quantum properties (quantum parallelism inherent to superposition, entanglement, tunnel effect …)

Their principles can be summed up as follows:

- represent the problem in an *ad*-hoc quantum system, 2^n binaries variables x being mapped to n *qubits* q;
- apply specified operators to this quantum system, in order to make it evolve to a final state $|Q_f>$ encoding the solution :
    - *Adiabatic computing* : GroundState $\{|Q_f>\} \Leftrightarrow$ MinObjectiveFunction($<x_i>$)
    - *QAOA :* $|Q_f> = |x_1 \ldots x_n>$, where $x_1 \ldots x_n$ maximizes the number of satisfied constraints

Because they didn't not aim at defining some general computing and quantum information processing model, neither to build some "Universal Quantum Computer" implementing such a model, these approaches seem to be less subject to issues inherent to more general ones.

Adiabatic Computing/Quantum annealing

This approach, proposed in the early 2000 by a MIT research team [Fahri et al 00] [Fahri et al 01], relies on the correspondence between the formulation of Quadratic Unconstrained Binary Optimization problem « QUBO ») and a particular Hamiltonian, the Ising's Hamiltonian [Lucas 14], modelling the temporal evolution of a quantum system which *qubits* represent the binary variables of the problem and their connections the relationships between the variables.
Once this correspondence has been set — a process that ca be viewed as a kind of compilation of the QUBO problem in the *qubits* lattice— the *adiabatic theorem* is used to make the quantum system evolve to a configuration corresponding to the solution of the problem. This theorem guaranties that if a quantum system is in its *ground state*, i.e. a state of minimum energy, then it stays in this lowest energy state provided that the Hamiltonian of the system changes "slowly enough". Thus, the method consists in initializing the *qubits* system in a starting *ground state* that can be "easily" prepared, then making it slowly evolve by the application of a time dependant Hamiltonian up to a final Hamiltonian which *ground state* is the solution of the minimization problem under concern.

The *adiabatic computing* briefly described above can be viewed as a quantum version of *simulated annealing*, a well-known heuristic method for optimisation of non-convex functions. This why it is sometimes called *quantum annealing* in the literature.

Like its classical conterpart, *quantum annealing* owns some theoretical proofs of convergence, but under hypotheses hard to satisfy in practice. Namely, the adiabatic evolution time required increases exponentially with the problem size, but with a quadratic speedup comparing to *classical annealing*. This approach thus remains in the domain of heuristic methods.

While subject to some controversy [Troels et al 14], it was experiment on some real-wold problems with significant results [Rieffel et al 14] [Venturelli et al 16] [Neukart et al 17].

It is the basis for the quantum machines commercialized by the Canadian society D-Wave, experimented in particular by Google and the NASA [Smelyanskiy et al 12] and is also at the core of the *Digital Annealer* proposed by the Japanese society FUJITSU.

Quantum Approximate Optimization Algorithm (QAOA)

This approach, recently proposed by the same team as the preceding, [Farhi et al 14], applies to combinatorial constraint satisfaction problems. The goal is there to find solutions that maximise the number of satisfied constraints in the problem. For example:

- find a *maximal cut* in a graph, i.e. un subset of vertex whose the number of edges to its complementary is maximal (MAX-CUT);
- find a variable assignation which satisfies the maximum number of *clauses* in a given propositional formula (MAX-SAT).

The QAOA uses an hybrid quantum/classical architecture. The quantum part applies a set of specific parameterized operators to a system of *n qubits* encoding the 2^n solutions.

For a fixed value of the parameters, the number of constraints satisfied by the solution encoded in the quantum state measured after the application of these operators to an initial state is evaluated. By repeating the process, one obtains a measure of the quantum expectation of the number of constraints satisfied in the resulting state. A second loop, driven by the classical part, provides the quantum one with new parameters likely to increase the expectation value. This classical part can be implemented by some conventional algorithm of *local search* (*hill climbing* …)

The whole process converges to a value of the parameters for which the ratio between the quantum expectation of the number of satisfied constraints and the maximal number of such constraints is close to one. Optimality is reached under a condition which is not accessible in practice (the number of parameters must increase to infinity). Again, this approach is thus heuristic but can provide with a good approximation of the optimal solution searched.

Applications of the HHL algorithm for Combinatorial Optimization

Besides the two above approaches, already identified as promising for Combinatorial Optimization, the study of the potential application of the HHL algorithm in the field of Integer and Mixed integer programming could also provide with a fruitful prospective research direction for the thesis. As a matter of fact, the resolution of huge systems of linear equations is at the core of many techniques used to solve this class of problems, typically when computing linear relaxations of integer programs in order to obtain bounds.

Technical support.

The PhD student will join the group “Methods, models, and tools for optimization” of the OSIRIS Department of EDF R&D division. The industrial support will be provided by expert research-engineers of this team, specialized in the combinatorial optimisation problems which will serve as applications of the works.

The Thesis will take benefits of the works carried out in the frame of the European project « Programmable Atomic Large-Scale Quantum Simulation” (PASQUANS), which precisely aims, among others objectives, to develop “programmable” adiabatic machines, and to which the OSIRIS Department participates as “End-User

Industry Partner”. This project has been accepted by the European « Quantum Technology Flagship » and begins in 2019.

Concerning the quantum computing resources available, EDF-R&D collaborates with the French society ATOS, strongly involved in Quantum Computing technologies, and which develops a simulator enabling the test of various architectures and quantum computing models. Others collaborations could be considered, according to the research directions investigated, e.g. with the Jülich Supercomputing Center in Germany, which also develops quantum simulators, among them *quantum annealers*.

Applications

As suggested in the “Context” section, many optimization problems tackled at the OSIRIS Department, and more generally at the EDF-R&D division, are candidate for these technics, given their belonging to the NP-Hard class:

- Unit commitment (to decide stops/starts of production units)
- Nuclear Power Plants : scheduling of refuelling outages, scheduling of maintenance operations during outages, permutation of assembly inserts, core fuel reload pattern optimization
- Logistic of calling centers for the Commercial Branch
- Vehicle routing problem for the Distribution Branch
- Optimisation of reload and flexibility of electrical vehicles

We intend to investigate as an application for this PhD thesis at least one of three underlined ones. The first two have been the subject of important researches and developments for many years, and various operational tools and data-sets are available for them, enabling the benchmark of the quantum approaches tested. The third one is more recent and therefore benefits of less feedback than the two others, but constitutes an important challenge for EDF.

The work of analyse and modelisation of these problems in order to evaluate the feasibility of their formulation in terms of the different quantum approaches investigated will be part of the research program. As well as the specification of instances of these problem the size of which should suit the quantum architectures available.

Location and remuneration

The OSIRIS Department of EDF-R&D division is located at EDF-Lab de Paris Saclay, at Palaiseau, in Paris area.The gross monthly remuneration of the PhD student is about 2800 €.

Sought Profile

Major competences required for the candidates are computer science and mathematical programming (optimization), especially discrete/combinatorial. A master or an equivalent degree received in this domain is mandatory. A course and an experience in quantum computing should idealistically complete this profile. Finally a competence in Quantum Physics in general should obviously be valuable.

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