Gaspard Monge Program for Optimization, operational research and their interactions with Data Sciences

2020 Call for projects

IROE appendix

SUMMARY

1 Introduction

This paper aims to describe in detail some of the problems encountered within the field of energy management. This paper also gives an idea of the work already completed or in progress on these topics, and the main difficulties already encountered. The listed research directions are given as an example. The submitted projects may address other issues than those listed below, consider methods of resolution that are completely different or that are a continuation of the work referenced.

Proposers wishing to submit B or A1 projects are strongly encouraged to contact the experts at EDF R&D on each subject in order to have a thorough knowledge of the issues and research work already completed or planned for on each topic. To this end, please contact the PGMO board (mailto: pgmo@fondation-hadamard.fr).

2 Background: the main issues in Energy Management

2.1 Managing the Supply-Demand balance

In order to generate electricity, a diverse portfolio of physical and financial assets (supply) is available in order to meet the customers' consumption (demand). The balance between supply and demand must be achieved within each time period in order to avoid the risk of physical system failures. The objective of Generation Management is to achieve this balance at minimal cost.

2.1.1 Uncertainties

Many uncertainties significantly impact the management of production, from both the system safety and economic points of view. These uncertainties are mainly due to climate (temperature, which strongly influences the demand for electricity, hydraulic inflows, wind, cloud cover, sun), outages of power plants, prices on the energy markets, renewable production (wind and photovoltaic). Those uncertainties are strongly correlated with each other.

2.1.2 A diversified generation and flexibility assets portfolio

The physical offer comprises all generation and flexibility assets, including load management. It includes both traditional centralised assets and distributed assets. Centralised means are connected to the transmission network. Centralised assets are generating units (power plants incl. renewables, hydro valleys), demand management, multi-energy assets and storage. Distributed means of production are connected to the distribution network. Distributed assets are generating units incl. renewables, load management, electric mobility, storage and multi-energy assets. Distributed assets may be aggregates of elementary assets with diverse representations of aggregation (aggregators).

- **Thermal assets**, consisting of nuclear and conventional thermal power plants: coal, oil, gas turbines, combined cycle gas turbines (CCGT). Each plant has to respect a set of operational constraints (production ranges, minimum outage or operational periods, start-up curves, possible shared fuel stocks with other plants, etc.) and is characterized by a complex cost structure (fixed costs or variable with respect to the amount of fuel, start-up costs, etc.), specific contributions to ancillary services, emissions, etc.
- **Hydraulic assets**, consisting of hydraulic plants (including pumped storage) located in valleys with water route between plants whose flow duration vary depending where the plants are located, constraints on reservoirs (minimum and maximum volumes, water value, etc.) and plants (power limitations, discrete operating points, gradient constraints, change of direction constraints, flow delays, water head effects, etc.);
- **Intermittent renewable generation :** e.g. wind, solar
- **Electricity load**, including nonflexible demand and flexible demand (e.g. load shifting) both centralized and distributed;
- **Distributed and centralised storage**;

- **Aggregators** i.e., actors that provide aggregation services through the management of a set of distributed assets (generation, storage, demand response through contracts with some flexible customers, etc.);
- **Multi-energy assets** providing flexibilities to the electricity system (power-to-gas, power-to-heat…).

2.1.3 Markets

- Electricity and commodities spot markets
- Future markets
- Capacity markets
- Intra-day markets

2.1.4 Environmental constraints

The directives and guidelines initiated by the European Union in order to foster a general approach against climate change and for environmental protection have a strong impact on the management of the supply-demand balance for energy producers:

- control of greenhouse gas emissions: management of pollutant emissions;
- taking the increase of the renewable generation (wind, photovoltaic ...) into account, inducing high uncertainties.

2.2 The challenge : manage a diversified portfolio that's very large in size

The goal is to manage the portfolio (generation assets and contracts) with the objective of minimizing costs while considering uncertainties. This problem is not solvable in the present state of knowledge, because of its very large size and mathematical complexity. Thus, it has to be decomposed into a set of different problems per time frame. Different considerations are taken into account at different time frames. At distant time horizons, the most important hazards (weather hazards, hazards on the operation of power plants, market risks ...) are represented very accurately (in practice as a random process or a very large number of scenarios), while the power generation assets are described only approximately. By the same token, at close time horizons, generation assets are described very precisely but uncertainties are not represented. Each time horizon provides a set of indicators for the time horizons that are closer to real-time, this is in order to keep the real time operation coherent with our vision of the future.

Despite decomposing the problem into different sub-problems at different time frames, the optimization problems within each time frame remain very large. The challenge remains to obtain accurate solutions within reasonable computing times to allow for effective production planning.

2.2.1 Long-Term

In the long term (five to twenty years), the challenges are:

- **Simulating the evolution of fuel and electricity prices**, which are based on the calculation of underlying fundamentals, i.e., a model of the supply-demand balance over a set of interconnected geographical areas;
- **Planning investments in new generation assets**. Investment planning methods are based on a minimization of the supply-demand balance cost, the result being the optimal (and robust to uncertainties such as physical hazards, economic and regulatory uncertainties) distribution of technologies to meet base and peak demand.

More details may be found in [LAB2011].

2.2.2 Medium-Term

In the medium-term (one to five years), the challenges are:

- **Defining the optimal outage schedule for the refuelling and maintenance of nuclear reactors**: the objective is to minimize generation and refuelling costs while satisfying demand and reactor operation constraints (operational and outage constraints), all in the presence of various uncertainties. A detailed description can be found on the PGMO web site and in [ROAD2010].

- **Defining coordinated management strategies for a set of stocks** (lakes, fuel stocks, stocks of (load) sheddings, pollutant emission stocks): the aim is to calculate optimal strategies that adapt themselves to uncertainties (feedback, "multi-stage" with scheduling modifications). One of the main issues is related to the joint optimization of all stocks. The techniques currently used (dynamic programming) become difficult to solve when more than three different stocks are considered. In addition, the uncertainties models are not very accurate, which raises many questions of how to describe those hazards in the optimization problem. (see [L2008], [G2010] for more details).

2.2.3 Short-Term

In the short-term (a few days to a few hours), the challenge is to define a day-ahead production plan and to adjust near real-time schedules to meet the actual demand. The main issues are:

- **Calculating minimum cost generation schedules for the next day**, including all constraints on generation assets, meeting the demand constraint (power and reserves) while providing recourse schedules in order to take into account future uncertainties;
- **Optimizing intra-day rescheduling** ("redéclarations" in French): at each hour of the day, the producer must change the schedules of a limited number of assets (thermal assets or parts of hydro-valleys) in order to reduce the real-time difference between production and consumption due to uncertainties on demand and availability of assets;
- **Calculating generation margins and optimizing reserves**;
- **Calculating balancing offers** for the adjustment market.

More details are available in [HBML2010]. A very detailed description of the problem, as well as presentations explaining the state of the art on this issue are available on the PGMO website.

3 IROE Main research topics

The list of all already funded PGMO projects may be found on the PGMO website.

3.1 Energy Management

3.1.1 Long-term and investments

Fundamentals models are designed to calculate the long-term prices of energies on a set of interconnected areas. In the case of electricity, the main difficulties come from the representation of strategies for the management of many stocks with various seasonalities (water stocks in particular), the intermittence of renewable energy production, the representation of the transmission network and the amount of flexibility made possible by demand response. Another difficulty is to anticipate the impact of the competition between primary energies on the long term electricity demand. The mathematical model dealing with these issues is a problem of economic stability across Europe, each area aiming at minimizing its costs while providing energy to its customers and contributing to the global European equilibrium. Balance prices calculated with this model can be interpreted as price indicators of electric energy.

The issue of Investment decision problems is to determine the technologies in which it will be best to invest in the future in order to meet energy demand. Due to the nature of those investments (building power plants or storage capacity, network expansion etc.) it is necessary to anticipate them far in advance. In other words it is necessary to take all relevant information into account to determine the right sizing of production facilities for a horizon of 15-20 years in the future.

3.1.2 Decentralized Optimization, local actors

The energy systems in Europe have originally been designed in order to reach the best possible economical objective in each country for satisfying a given demand. Economy of scale principles were applied and lead to the construction of a generation mix mainly composed of large generation assets. Moreover, a centralised generating mix was seen to be the best solution to serve demand. This is because centralisation allows for the aggregation of multiple highly uncertain and variable demands thus reaching a relatively stable global demand.

The emergence of a high share of intermittent renewable energy sources in the energy system leads to many difficulties, due to their characteristics (intermittent, hardly predictable, usually non flexible, usually not contributing to frequency stability services, spread all over the country/continent - not always close to demand, connected to the distribution network thus constrained by its size).

Furthermore, recent and forthcoming regulatory and technical evolutions will deeply transform the system with the upcoming local demand management tools and a more proactive stance of actors in the field, including customers.

Therefore, the energy management tools will need to change significantly and contributions to flexibility will gain “significant” value which will make their precise valuation essential.

The energy generation management process at medium-term horizons is conventionally done in France in a centralized way.

Decentralised Optimization covers many interesting problems:

- Integrated optimization. Integrated optimization means that all means of generation/flexibility in a specific geographic area are considered, either with a ‘centralised’ point of view or not. New constraints and mechanisms are to be dealt with
- Optimization of local players. At a local level, new problems appear related to the emergence of local players. They are facing local specific constraints (among them those coming from the distribution network). The modelling of these problems, especially in a context of intermittent energy is a topic in itself.
- Relationships between centralized power system management (supply-demand balance on a global scale and network balance management) and decentralized management (local management, due to the emergence of new players and means of production: photovoltaic, wind, smart grids, storage, etc.). Regarding the global supply-demand balance, one can address various questions: i) what is the role and impact of local actors on the centralized management? ii) What will be the signals that are

transmitted between the different actors and how will we model them? iii) How should local constraints be considered with a global point of view?

- The emergence of local actors also requires considering problems related to (transmission and distribution) network and joint 'network-generation-demand flexibilities' optimization problems (considering mainly the distribution network). Problems relating to modelling the behaviour of consumers in a competitive context also arise.
- Contributions of multi-energy assets will need to be integrated.

This topic is fairly new and deals with issues at different levels of the supply-demand balance process.

Some mathematical approaches were identified including:

- Decomposition Methods
- Bilevel Optimisation,
- Game Theory

3.1.3 Grid stability in a system with a high share of renewable energy sources

The growing share of variable renewable energy sources VRES (such as windpower or photovoltaic) raises major challenges for the electricity systems:

- The spatial repartition of the variable renewable generation does not always coincide with areas of high demand (e.g. urban centers) and, as a consequence, can lead to transportation of the electricity over long distances. Such power flows may create congestion issues at distribution and transmission levels.
- In an AC network, any imbalance between supply and demand results in a frequency deviation. On-line synchronous spinning machines (i.e. nuclear, hydro, coal, etc.) currently ensure the stability of the grid by providing inertia (linked to the amount of kinetic energy stored in the rotating masses of spinning machines) and frequency regulation. The substitution of the conventional generation by VRES may decrease the capacity to maintain the frequency at a satisfactory level.
- As energy losses and supply quality depend on the voltage value, voltage control is essential for reliable and cost-effective transmission of electricity. Traditionally, specific regulators and provision of reactive power by the conventional generators ensure the voltage control respectively at distribution and transmission level.

The main challenge is then to improve grid dynamics considerations such as frequency regulation and voltage control within all energy management optimization models.

3.1.4 Short-term Generation Scheduling

The "Unit Commitment" problem consists of finding a minimum cost operating program for all power plants:

- providing adequate system services;
- ensuring the supply-demand balance at every time period (currently defined as every half-hour but will soon change to every quarter of an hour);
- respecting all operational constraints.

Daily and Weekly Optimization

The objective is to determine the optimal generation schedule which minimizes costs (production costs and start-up costs), while meeting a set of constraints. Constraints include numerous operational constraints that affect thermal and hydraulic power plants and meeting exactly a set of "demands" (consumption, reserve capacity and system services). Solving this problem provides a reference schedule for the day to come.

This Unit Commitment problem is already well-known and researched. The current solution is a combination of Lagrangian dualization, price-decomposition and bundle algorithms (see [LS1994]). This gives a first schedule which will then be adapted using an Augmented Lagrangian technique combined with the use of the auxiliary problem principle to get the reference schedule (see [CZ1984], [BR1992], [MS1983], [DGL2005]). This solution gives excellent results on the historical deterministic problem.

Recently, the strong increase of "new" renewable energies (wind, solar) has forced us to rethink this problem. "Historical" uncertainties (consumption, water intake, failures) could be neglected on a very short-term horizon, it is no longer the case for these new hazards. This is due to their high non-predictability (we have no reliable forecasts beyond a few hours) and their intermittent nature (e.g. passing clouds can reduce the photovoltaic generation abruptly to 0). It is essential to address these new phenomena.

- Firstly, all operational constraints must be finely modelled in order to benefit from the flexibility of all production facilities, particularly in hydraulics. This leads to the introduction of many non-convex or binary constraints. Detailed modelling of the constraints induces difficulties on the overall resolution of the problem because the sub-problems arising from the price decomposition become more difficult to solve, so are solved in an approximate way which is not compatible with the traditional algorithm. To solve this problem, a new bundle method capable of dealing with an inaccurate Oracle was developed. A PGMO project (Consistent Dual Primal Signals and Optimal Solutions) aims to improve the resolution by Lagrangian dualization through incorporating heuristics and improving the bundle algorithm. A new line of highly prospective research concerning the non-convex duality and interpretation of dual variables associated is also identified;
- Secondly, uncertainties must be taken into account through the calculation of robust production programs, i.e. where the cost of adapting to the occurrence of intra-day hazards is minimal. This problem can be formalized as a problem with recourse. Work has been done on a robust approach without recourse decisions, as well as a robust approach with recourse decisions but on small convex problems (cf. [BS2011] [Ap2007] [AHMZ2011]). More recently, advances were made through a PhD thesis [A2013b], and a PGMO project (optimization under uncertainty for the "Unit Commitment" problem) looking at the real problem is ongoing. An approach based on stochastic optimization using uncertainty trees is also addressed in a PGMO project (A Stochastic Programming Approach to Finding Robust Reference Schedules for the Unit Commitment problem). See also PGMO project “Optimization & stability of stochastic unit-commitment problems”.

Intra-Day Optimization and Re-Scheduling

Regulatory developments have led to formulate a new problem on the intra-day horizon : recalculating production schedules by solving the same problem as above plus a so-called re-scheduling constraint which specifies the maximum number of plants (about 30 out of 150) for which the reference schedule can be changed. This constraint is both coupling and combinatorial. Heuristic methods were considered: the problem is decomposed into a phase of selection of plants in which the schedule will be changed then a phase of optimization of the schedules of these plants.

Work is currently being undertaken around a method consisting in using a supervised learning algorithm to decide the list of plants whose program will be changed and a classic Unit-Commitment problem.

Some "Group Sparsity" approaches are also under investigation (see [ABLEGRZ2014], and the PGMO project “Robust Sketching for Structured Multi-Instance Optimization with Uncertainty, Application to Energy Management”).

Recent regulatory evolutions may make it necessary to reduce the time steps of the models. Typical timestep in the daily/intraday process is 30 minutes which may go down to 15 or even 5 minutes. An answer to these changes may be to have a time continuous model, which may lead to developing completely different optimization methodologies.

See also PGMO project “short term re-planning”.

3.1.5 Optimization of hydro-electric valleys

In the long and medium-term, the objective is to calculate good management strategies for the hydro valleys, taking some constraints on reservoir levels into account. In the short term, the problem amounts to computing feasible programs (i.e. satisfying the constraints) in order to allow the use of all flexibilities of the hydraulic park.

Long and medium term

The main difficulty is to calculate the management strategies for coordinated reservoirs while dealing with uncertainties. Some solutions to the classical problem where the reservoirs have to respect a coupling demand constraint already exist. For more complex structures, for instance ‘Cascade’ e.g. when it comes to coordinating all the reservoirs of one hydraulic valley, effective methods are still being defined (see [E2008], [L2008], [B2004], [D2006], [CCD2009], [PDG2011], [VP2011], [RS2011]). The stochastic decomposition method developed in the context of the global supply-demand balance [G2010] has been extended to the case of cascade reservoirs by [A2013].

A formulation with probability constraints (for taking into account the volume probability constraints on reservoirs) was proposed in [A2013]; the resolution method is based on the dualisation of the probabilistic constraint.

Short-term

The main difficulty is to solve accurately, and in a very short calculation time, a large mixed integer problem, characterized by very strong constraints.

A thesis and a PGMO project (Optimality for Tough Combinatorial Problems Valley Hydro) are working on solving this problem by combining mathematical methods and combinatorial optimization heuristics. The PGMO project "Decomposition and feasibility restoration for Cascaded Reservoir Management" is ongoing.

Local approaches are also investigated (see PGMO project "Hybrid approaches for solving bi-objective energy problems with low-carbon constraints").

The need to take into account the short-term uncertainties also requires a solution to the problem that considers the hazards. To this end, a PGMO Project ("Hydro-electric scheduling under uncertainty") aims to combine methods from stochastic optimization and combinatorial optimization.

3.2 Electric Vehicles

The development of electric mobility leads to multiple research questions, which include:

- **[long-term "strategic" decisions]** Electric Vehicle (EV) charging infrastructure location and sizing - for standard individual / fleet mobility usage, or new mobility services (autonomous / shared mobility);
- **[short-term "operational" decisions]** "Smart charging" (i.e. EV consumption profile(s) scheduling) of one or multiple EVs (at home, in a car park, on public charging stations), which can be done at a local scale, in presence of Renewable Energy Sources;
- **[EV user services]** Design of user-centric information / incentive mechanisms (to share EV charging infrastructure in space and / or time).

In particular, the following research aspects could be very beneficial for this field:

- coordination/optimisation of charging decisions for a large set of EVs, and with constraints at hierarchical levels;
- the integration of EV battery aging modeling;
- the integration of load-flow based local electricity network constraints/metrics;
- the analysis of the specificity of EV as a "moving" electricity appliance (not always connected to the grid, not always at the same location).

3.3 Routing Problems

The scheduling and routing problem for technician interventions on the electricity distribution networks is difficult and of high interest due to the number of kilometers and mobilized resources (manpower, vehicles and equipment).

This problem can be decomposed into several coordinated stages:

- **Strategic**: deciding where to place sites (i.e. the premises where the technicians and their vehicles are based), taking into account all different activities organized there, and the site capacity (number of employees, number of vehicles), as well as needs and constraints. When the workload changes, decision makers can explore the interest of reducing or increasing the number of sites and their location, looking at several criteria;
- **Operational**: determining the daily routing of all technicians of a given site, while meeting the demand (list of operation applications, e.g. maintenance of an electric line), and taking into account several criteria (e.g. distances, equipment that have to be loaded in each vehicle at the beginning of the day, necessary qualifications to perform the operations);
- **Real-Time**: adjusting the routing schedule to the occurrence of unforeseen events (e.g. cancellations and weather).

This problem can be seen as a multiple Vehicle Routing Problem with Time Windows. Current work was conducted on a simplified problem (operational stage only), using local search techniques and mixed integer linear programming.

Further research could focus on the following difficulties:

- Integrating all accurate constraints of operational planning within a strategic planning model, while modelling the evolution of the load;
- Looking at future business needs: routing can be single or multiple i.e. taking into account vehicles with only one technician or several technicians. Multi-modal touring: conventional vehicle, electric vehicle, bicycle and / or walking;
- Multi-site problem: technicians of a given site may take charge of operations that are at the border of neighbouring sites;
- Robust approaches (e.g. to deal with traffic variability) or online optimization for operational planning;
- Dynamic readjustment of the routing schedule.
- Use of previous routings to help build new ones (use of machine learning suggestions to help optimization algorithm)

3.4 Maintenance & industrial process optimisation problems

3.4.1 Optimizing maintenance programs

The idea here is to find the schedule that will optimize the Net Present Value of the maintenance program (the NPV is the economic indicator that balances investment costs and benefits created by these investments) while fulfilling various constraints (e.g. precedence between investments, limited number of investments, budget limit).

- What we have: a tool, that uses a Genetic Algorithm to does this optimization based on an evaluation function that gives expected values through Markov graphs;
- What we would like to have: a tool to be able to make the same optimization based on risk indicators and not only expected values. We have the model to assess these risk indicators based on Monte-Carlo simulation but calculations are too long for usual optimization methods.

In turn, the two proposed research areas would be to work on:

- Simulation-Optimization;
- Robust Optimization.

3.4.2 Optimizing spare parts stock

The idea here is to find the number of spare parts that will minimize the global owning cost (sum of purchases and shortage costs).

- What we have: a tool that calculates the global owning cost with a closed-form expression. The "optimization" is made with a greedy algorithm iteratively buying the spare part with the best improvement over cost ratio until budget limit is reached;
- What we would like to have: an optimization algorithm that gives better results than the greedy algorithm and which would be able to deal with budget uncertainty. In turn, the two proposed research areas would be to work on: Simulation-Optimization and Robust Optimization.

3.4.3 Algorithm-driven process design

Rational design of chemical and energy processes started in the early 20th century with the emergence of chemical engineering science. Methods evolved through the decades including more and more computer assistance as new machines and algorithms became available. Today, with the recent development in computer science and applied mathematics, a next step can be foreseen: a process can be fully designed based on an algorithm, able to find an optimal solution under physical, engineering and regulatory constraints. These approaches are starting to be developed [W2015] but are not yet applied to real industrial cases including their constraints.

The development of such algorithms driven by real industrial systems with cost of generation as the objective to be minimized could be of interest, if applied to an already very well optimized and deployed industrial system (e.g. thermal process such as steam cycle or boiler or a specific equipment such as turbine or alternator) in order to be able to assess the real added value of the approach. The key issue to address is how to produce reliable results, efficiently taking into account constraints linked to engineering constraints.

3.5 Big size

A general characteristic of all the above problems is their big size, and the operational need of fast solving.

All methods to accelerate the solving of these problems are of interest.

Some ongoing ideas are to try to exploit the fact that the operational process leads to solving a very large number of very similar instances.

Online optimization, sketching methods and learning algorithms are investigated through PGMO projects "Robust Sketching for Structured Multi-Instance Optimization with Uncertainty, Application to Energy Management', 'Reducing combinatorial by using learning methods'

Alternative methodologies would be appreciated.

3.6 Algorithmique quantique pour l'optimisation difficile (en cours de traduction)

3.6.1 Introduction

L'informatique quantique (*Quantum Computing*) constitue une des ruptures technologiques les plus prometteuses du moment.

Ces trois dernières décennies ont connu des avancées majeures dans le domaine, avec le développement d'une théorie complète du traitement de l'information quantique, la spécification des classes de complexité associées aux problèmes susceptibles d'être résolus par des « Machine de Turing Quantiques » [Deutsch 85] [Bersetin Vaziran 97] [Aaronson 10] [Nielsen, Chuang 10] [Rieffel, Polak 14], et la découverte de plusieurs dizaines d'algorithmes présentant des *speedups* significatifs (jusqu'à exponentiels) par rapport à leurs homologues classiques [Jordan 19], ceci sans que les propriétés spécifiquement quantiques à la base de ces *speedups* ne soient encore clairement établies dans tous les cas.

Sur le plan du « hardware » quantique, si des incertitudes importantes subsistent quant à la possibilité de réaliser des « calculateurs quantiques universels » robustes aux erreurs et disposant d'un grand nombre de *qubits* – et sur les échéances auxquelles de tels calculateurs seront disponibles–, des progrès constants sont réalisés depuis plusieurs années et il existe déjà des réalisations opérationnelles de « Quantum Processor Units » (QPU) spécialisés dans des tâches pour lesquelles des « avantages quantiques » sont susceptibles d'être mis en évidence, ce dernier point faisant encore l'objet de controverses dans la communauté scientifique (processeur Sycamore de Google [Google 19], machines D-Wave [D-Wave 20] …)

On parle de « Noisy Intermediate Scale Quantum Computing » (NISQ) pour désigner l'état de l'art actuel du domaine, une période qui devrait durer encore plusieurs années dans laquelle des moyens de calcul quantiques bruités et de taille intermédiaire en terme de nombre de *qubits* seront exploitables pour accélérer des tâches spécifiques, en étant intégrés à des moyens de calcul classiques dans des architectures hybrides.

Dans le même temps, la dynamique du domaine stimule fortement *l'informatique classique* elle-même, de nombreux travaux cherchant à en repousser les limites, d'une part en mettant en œuvre des techniques avancées pour simuler efficacement les QPU sur des architectures de calcul hautes performances classiques (cf. par exemple la réponse d'IBM à la l'annonce par Google d'avoir atteint une forme de « suprématie quantique » avec son processeur Sycamore [IBM 19]), et d'autre part en proposant des algorithmes classiques *d'inspiration quantique* (*Quantum Inspired algorithms*) c'est à dire reproduisant efficacement sur des machines classiques certaines approches algorithmiques quantiques (cf. par exemple la simulation du « *recuit quantique* » par des méthodes de Monte-Carlo, pour la résolution de problèmes d'optimisation difficile [Mazzola, Troyer 17] [Fujitsu 20]).

3.7 Approches quantiques pour l'optimisation

L'optimisation, et tout particulièrement *l'optimisation combinatoire,* est un des champs les plus actifs de recherches et de développement sur les applications de l'informatique quantique.

Il n'y a rien d'étonnant à cela compte tenu du fait que les problèmes d'optimisation combinatoire appartiennent pour la grande majorité d'entre eux à des classes de complexité (**NP**, **NP-Complet** et **NP-difficile**) pour lesquelles on ne connait pas d'algorithme de résolution efficace (polynomiaux) sur les ordinateurs classiques, alors que certaines propriétés des calculateurs quantiques (nature exponentielle dans le nombre de qubits de la mémoire disponible, parallélisme quantique, intrication …) laissent espérer des accélérations importantes dans la résolution de ce type de problèmes.

Il reste que dans ce domaine comme dans tous les autres, il n'existe pas de garantie que ces propriétés spécifiques au monde quantique fournissent systématiquement des *speedups* significatifs par rapports aux meilleurs algorithmes classiques connus.

En pratique et jusqu'à aujourd'hui, un seul algorithme quantique fournit un *speedup* exponentiel sur un problème **NP** (mais non prouvé **NP-Complet**) : celui-de Peter Shor [Shor 95] pour la factorisation des nombres entiers. Cet algorithme a fait grand bruit du fait que la sécurité des clés de chiffrement « RSA » qui protège l'immense majorité des communications sur Internet, repose précisément sur la difficulté à résoudre ce problème sur une machine classique pour des entiers de grande taille.

Un certain nombre d'approches quantiques très prometteuses ont cependant été développées pour attaquer ces problèmes combinatoires :

- *L'algorithme de Grover* [Grover 96] fournit un *speedup* au plus quadratique par rapport à un algorithme d'énumération exhaustive (toujours exponentiel dans le pire cas), pour n'importe quel problème dans **NP** ;
- Dans le même esprit, des travaux récents s'appliquent au *Branch & Bound* pour en accélérer les phases de *backtracking* [Montanaro 20] **;**
- *L'algorithme quantique adiabatique (Quantum Adiabatic Algorithm QAA)* [Fahri et al 00] [Fahri et al 01], dérivé d'un modèle général de calcul quantique [Albash, Lidar 18], est exploitable pour la résolution de problèmes d'optimisation combinatoire sur des machines quantiques « analogiques », en identifiant un tel problème à la recherche d'un état d'énergie minimal d'un Hamiltonien appliqué au système de *qubits* ;
- Son approximation discrète à base de portes quantique, l'algorithme *QAOA* (*Quantum Approximate Optimization Algorithm* » [Fahri Goldstone 14] [Fahri Goldstone 16], constitue une approche hybride pour le même type de problèmes associant un circuit quantique et un ordinateur classique ;
- Le *recuit quantique* (*Quantum Annealing*) une approche adiabatique limitée à certains types d'Hamiltoniens [Albash, Lidar 18], et donc à certains types de problèmes combinatoires, peut être vue comme la version quantique du *recuit simulé*, une technique heuristique bien connue pour l'optimisation non convexe. Cette approche fait l'objet de nombreuses applications industrielles, en particulier sur les machines proposées par la société D-Wave [D-Wave 20] dont l'apport en termes d'accélération quantique reste contesté [Troels et al 14].

En dehors de l'optimisation combinatoire proprement dite, il faut également mentionner l'algorithme *HHL* de résolution de systèmes linéaires [Harrow et al 09]. Ce problème polynomial sur une machine classique et qui joue un rôle essentiel dans de très nombreuses applications, est rendu logarithmique par *HHL* sur une machine quantique, sous certaines conditions.

3.8 Domaines d'application visés et objectifs des recherches

Tous les domaines d'application de l'optimisation difficile, typiquement combinatoire/discrète, sont visés.

En particulier, un très grand nombre de problèmes issus du *management d'énergie*, du classique *unit-commitmen*t au *smart-charging* de véhicules électriques, en passant par les problèmes *d'ordonnancement* les plus divers (placement des arrêts des centrales, optimisation des tâches de maintenances à l'intérieur des arrêts, tournées de véhicules d'intervention, logistiques des centres d'appels téléphoniques ...), sont susceptibles de bénéficier de ces approches.

Un point d'intérêt particulier concerne la prise en compte des *contraintes* dans les approches issues du *calcul adiabatique* (*QAA, QAOA, QA*). En effet, ces approches reposent sur la modélisation des problèmes à résoudre sous des formes imposant le plus souvent l'absence de contraintes (typiquement *binaires quadratiques sans contraintes*, dites *QUBO* pour *Quadratic Binary Optimisation Problem*). Il est donc nécessaire de relâcher celles-ci dans la formulation, généralement sous forme de pénalisation dans la fonction objectif, ce qui complexifie la mise œuvre des Hamiltoniens associés. L'intégration efficace à ces approches des contraintes présentes dans la très grande majorité des problèmes industriels constituent un sujet de recherche important. (Cf. par exemple [Dupuy, Hullo 19] pour la formulation d'un problème de management d'énergie comme un problème de « sac à dos » contraint et son traitement par l'algorithme QAOA).

De façon générale, les recherches menées à EDF sur ce thème visent à évaluer les potentialités d'applications d'approches quantiques aux problèmes cités ci-dessus, sans en attendre à cette étape des résultats meilleurs que ceux obtenus par les approches classiques actuellement utilisées pour les résoudre. L'objectif est de qualifier ces méthodes sur des moyens de calculs « NISQ » pour de petites instances de problèmes d'intérêt pour EDF, et d'étudier leur possibilité de passage à l'échelle dans le futur.

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