TOWARDS OPTIMAL GRAPH COLORING USING RYDBERG ATOMS

Introduction

Quantum computing
Quantum mechanics laws provide the foundation for implementing the building blocks of a new computing paradigm, i.e., Quantum Computing.

Quantum Computers (QC) are theoretically able to outperform any classical (super)computer for specific tasks

Quantum Computers are effective in:

- Executing algorithms like traditional digital computers (universal gate-based quantum computers)
- Simulating physical systems by evolving a Hamiltonian target function
- Optimize computationally hard problems via quantum annealing

Physical Quantum Computer Implementations
There are many candidate (and competing) technologies for implementing Quantum Computers:

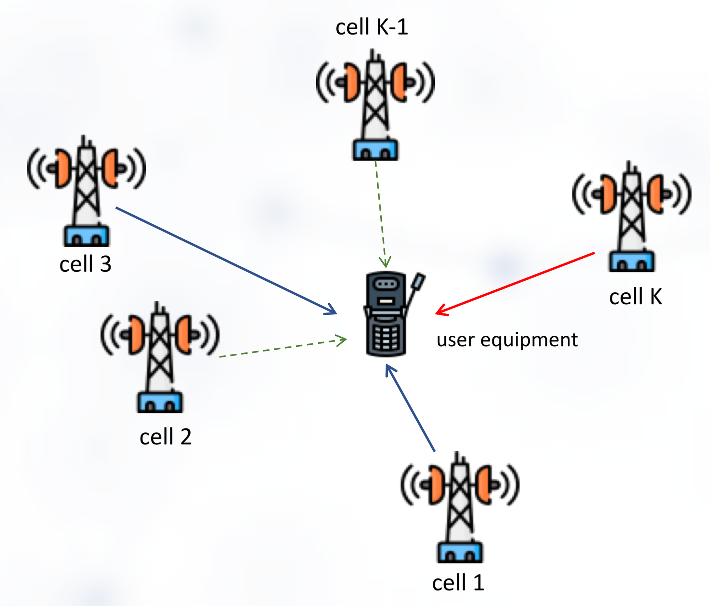
- Superconducting transmon-based devices (gate-based QC)
- Ion-trap based devices
- Optical-based devices
- Neutral Rydberg atoms-based devices

Motivation

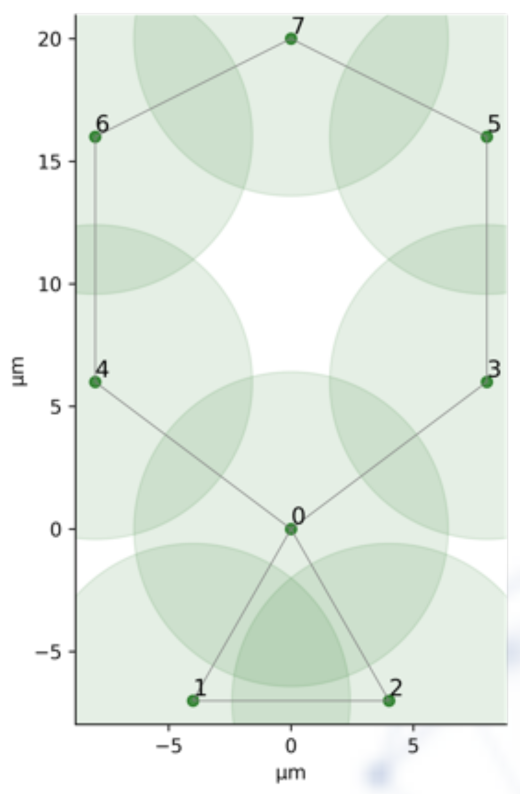
Industrial applications – Physical cell identification
Many scientific and industrial applications require to solve complex optimization problems (typically NP-hard or NP-complete)

Here we focus on Graph Coloring (GC) problem since it provides the foundation for efficiently solving the Physical Cell Identifier (PCI) Assignment problem in cellular networks.

Since the number of PCI is limited w.r.t. the number of nodes on the cellular communication network, the problem is to properly assign them to minimize conflicts.
This can be directly mapped to the Graph Coloring problem.



Neutral Rydberg Atoms Architecture



Neutral Atoms as Qubits
One of the leading Quantum Computing architectures consists in arranging ensembles of the individual (trapped) neutral Rubidium atoms separated by a few micrometres.

To generate interactions between them, they are excited by a resonating laser field to a Rydberg level, which has a large principal quantum number. At the Rydberg state, the atoms present long lifetimes and large interaction strengths and are briefly called Rydberg atoms.

Each atom holds a specific quantum state encoded in specific electronic levels. These two-level systems can be represented as qubits. The ground and Rydberg states represent |0> and |1>, respectively. Their ensemble is called a Register. The Register of Qubits can be arranged at will on a 2D plane, with some geometric restrictions on the minimum distance between atoms.

The interaction between atoms at the same Rydberg level at distance R is described by the Van der Waals force, which can be exploited to create the so-called Rydberg Blockade effect between them. For neutral atom devices, this mechanism is the key behind quantum superposition and entanglement between atoms, which in turn allows exploiting the register to perform quantum simulation and, to some extent, computation. The system behaviour obeys the following Hamiltonian:

$$\mathcal{H} = \sum_{i=1}^{N} \frac{\hbar\Omega}{2}\sigma_i^x - \sum_{i=1}^{N} \frac{\hbar\delta}{2}\sigma_i^z + \sum_{j<i} \frac{C_6}{|r_i - r_j|^6} n_i n_j$$

See Ref [1] for more details.

Results

Greedy MIS vs. BB-enhanced vs. Optimal
The tables below show the results of the simulations run on Marconi-100. The change from Pulser library to a state-of-the-art QUBO solver, to simulate the Quantum system and solve MIS instances, is needed since the computational time to simulate Quantum MIS solutions with Pulser tools scales exponentially with the number of vertices in the graphs: to solve the 17 vertices instance we needed up to 40 minutes. This because Pulser fully simulates the physics of the system of Rydberg atoms: as soon as we will get access to the real quantum machine, the computational cost of computing the MISes will fall significantly.

The proposed procedure has demonstrated the capability to generate near-optimal coloring solutions with a significantly smaller number of qubits with respect to the typical QUBO-based solution (that uses the so-called one-hot encoding) by exploiting the advantages of the quantum MIS solver. Using our approach, we solve Graph Coloring instances with a number of qubits equal to the number of vertices of the graph, gaining at least a chromatic number factor in the number of qubits required. This gain can be exploited in solving larger and more difficult GC problems, as of interest in real-world applications.

Vertices	Greedy-itMIS	BB-itMIS	Optimum
10	3 colors	3 colors	3 colors
11	3 colors	3 colors	3 colors
12	4 colors	3 colors	3 colors
13	4 colors	3 colors	3 colors
14	4 colors	3 colors	3 colors
15	4 colors	3 colors	3 colors
16	4 colors	3 colors	3 colors
17	4 colors	3 colors	3 colors

Table 1. Comparison between the optimal graph coloring and the iterative MIS-based approaches using the Pulser library.

Vertices	Greedy itMIS	BB-itMIS	Optimum
25	4 colors	3 colors	3 colors
35	5 colors	5 colors	5 colors
45	8 colors	6 colors	6 colors
55	7 colors	7 colors	7 colors
65	8 colors	8 colors	7 colors
75	10 colors	9 colors	8 colors
85	10 colors	9 colors	8 colors
95	11 colors	9 colors	8 colors

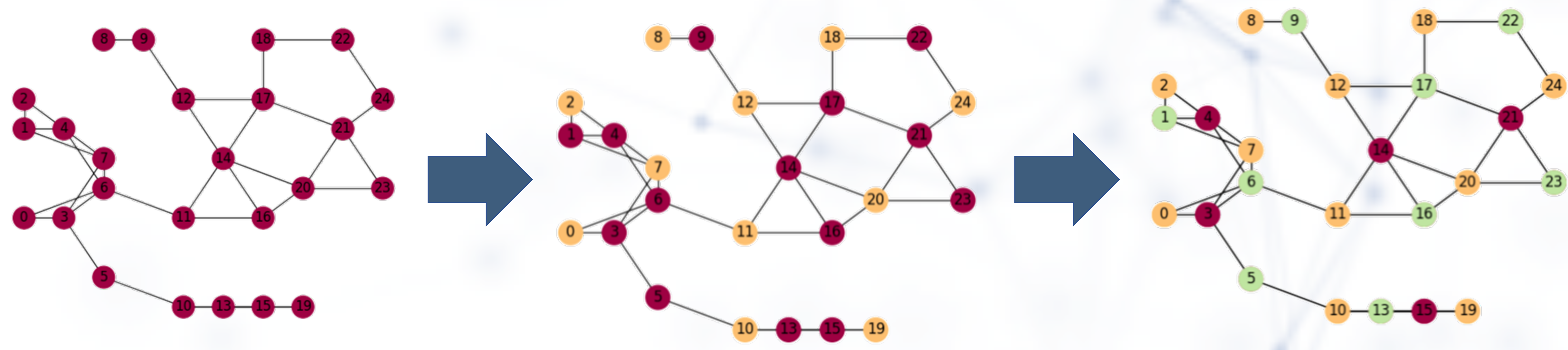
Table 2. Validation of the approach using state-of-the-art QUBO solver.

Graph Coloring Through Iterative Maximal Independent Sets

Greedy-itMIS: Unit-disk Greedy MIS Coloring
The proposed approach starts from a simple quantum-based heuristic to solve the GC problem by iteratively solving a Maximal Independent Set (MIS) problem. To this end, a register of Rydberg atoms is constructed in such a way it directly maps on the geometric graph structure of the problem (Ref [2]).

This arrangement of the register allows exploiting the Rydberg blockade phenomenon to directly obtain a set of candidates MIS solutions with a limited computing cost by using a Quantum Approximate Optimization Algorithm (QAOA) approach in analog mode (i.e., using analog control over atoms).

The GC problem can be solved by iteratively selecting one MIS of the graph: at each iteration, a new set of MIS solutions is generated, and the most promising one is chosen (i.e., it corresponds to assign a new color to the graph), then a sub-graph is derived by removing the nodes belonging to the MIS. The picture below shows the whole procedure with the color assignment.



BB-itMIS: Branch&Bound (near-)optimal Coloring
Building upon the presented heuristics, it is possible to improve over a purely greedy approach: in fact, theory guarantees that every graph has an optimal coloring in which (at least) one of the colors is a maximal independent set [3].

By implementing a Branch and Bound (BB) strategy that, at each step, optimises the choice of the MIS solutions among the set of feasible ones provided by the quantum register, it is possible to achieve a near-optimal solution.
Based on the fact that alternative solutions for the MIS are generated (i.e., the measurement of the final state of the quantum system –Rydberg atoms' register– results in a distribution of feasible solutions), a BB tree is constructed and explored in parallel.
To avoid exponential growth of the number of branches, pruning criteria based on the chromatic number Lower Bounds and graphs redundancy have been defined. The chromatic number Upper Bounds are used instead for the exploration policy. Moreover, we limited the number of BB nodes explored, each of them containing a feasible GC solution. This choice makes our BB as a heuristic, while it would, eventually, converge to an exact solution if the above mentioned limitation is removed.

To validate the itMIS approaches on small graphs, we performed experiments simulating the Rydberg atoms-based MIS process through the Pulser simulation framework using the CINECA Marconi-100 supercomputer. The framework models the physics of the Rydberg atoms, hence fully reflects the behaviour of the upcoming machine, with the drawback of a significant computational cost. For this reason, we tested both itMIS approaches for larger graphs replacing the MIS solver with a non-quantum one, while keeping the same global optimization approach.

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FUTURE WORKS

- The effect of Quantum background noise on solution quality will be evaluated
- The speed-up obtained by using a real Quantum Computer with respect to a full classical procedure will be evaluated through the use of real devices
- Explore the possibility to solve arbitrary QUBO problems on present and upcoming Neutral atoms architectures

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