

BBQ-mIS: graph coloring optimization using a hybrid quantum-classical algorithm

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Keywords : *hybrid algorithm, graph coloring, analog quantum computing*

One of the significant challenges in existing quantum machines is the limitation posed by the qubit count, especially when attempting to scale up computational tasks of substantial size, such as those derived from real-world applications. In addressing this challenge, a potential approach involves decomposing the given problems to accommodate the constraints of size-limited quantum resources.

For this purpose, we have developed a hybrid quantum-classical algorithm named **BBQ-mIS**, designed specifically to tackle graph coloring problems on Rydberg atoms quantum machines. The **BBQ-mIS** algorithm integrates the inherent representation of Maximum Independent Set (*MIS*) problems onto the machine Hamiltonian using a Branch&Bound (BB) approach for effective graph coloring identification. In this devised solution, the graph is formed through qubit interactions, where qubits correspond to graph vertices. The coloring is subsequently determined by systematically assigning one color to a maximal set of independent vertices in the graph, all while minimizing the number of colors through the application of the Branch&Bound approach.

Quantum MIS solver: Neutral atoms machines employ Rydberg atoms, *i.e.* neutral atoms, to act as *qubits*, organizing them on a 2D/3D register. The interactions among these atoms, subject to laser pulses [1], generate the machine Hamiltonian H , which depends on both the laser pulse parameters and the positions of qubits. Once measured, the qubits assume one out of two possible quantum states, the excited Rydberg state $|1\rangle$ or the ground state $|0\rangle$.

When the strength of the qubit-to-qubit interactions balances with the Rabi frequency of the laser, the quantum system undergoes the *blockade effect*, which acts as a threshold on the qubit pair distances, discriminating those closer than the *blockade radius* r_b from the farther. In this way, the interactions between qubits, which can be assimilated to the vertexes of a graph, can induce a Unit-Disk Graph (UDG): qubit positions in the quantum register are UDG's vertex positions, and edges in the UDG link two vertexes whenever their Euclidean distance is shorter than r_b . The blockade effect prevents qubits, which fall within the blockade radius, from being both in the state $|1\rangle$. Thus, retrieving the ground state of H coincides with computing the largest set of non-interacting qubits on the register, *i.e.*, the *Maximum Independent Set* (*MIS*) of the corresponding UDG.

In our experiments, we relied on *Pulser*¹ for the emulation of the quantum system on classical resources. We adopted the Quantum Approximate Optimization Algorithm (QAOA) [1, 2] to optimize the laser pulses' durations to solve *MIS* problems. Specifically, each input graph \mathcal{G} is depicted on the array of rearranged Rydberg atoms. The laser parameters are set to reproduce the proper connectivity in the graph, through r_b .

¹<https://pulser.readthedocs.io>

BBQ-mIS algorithm: Given a graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$, with \mathcal{V} as the set of vertices, $n = |\mathcal{V}|$, and \mathcal{E} as the set of undirected edges the goal is to find a feasible coloring that assigns colors to vertices such that connected vertices have distinct colors. A *graph coloring* (GC) problem arises when the focus is on achieving a feasible coloring of \mathcal{G} while minimizing the number of colors, referred to as the chromatic number of \mathcal{G} .

An initial insight is that an *MIS* solution is a viable color assignment since independent vertices within the *MIS* can be colored uniformly. Moreover, quantum systems’ probabilistic nature requires multiple measurements, thus the outcome of the quantum *MIS* solver results in a histogram of potential color assignments. Then recalling the definition of *maximal Independent Set* (*mIS*), an independent set that is not properly contained in another independent set of \mathcal{G} , we can apply Th.1 to restrict our solutions space investigation to *mIS*s as colors.

Theorem 1 (Optimal graph coloring) *Every graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ has an optimal coloring in which (at least) one of the colors is a maximal independent set.*

Hence, we can set up an effective minimization of colors for a *GC* problem. **BBQ-mIS** algorithm relies on a Branch&Bound (BB) approach that branches on *mIS* solutions and considers as bounds the lower bounds on the chromatic number. It operates outside the *MIS* quantum solver and considers all solutions from its measurements. Then, it branches over induced sub-graphs by removing all vertices in one of the parent node’s *mIS*. The BB tree starts at the root with the graph \mathcal{G} to be colored. The optimization proceeds to retrieve the best coloring found so far, ultimately yielding the **BBQ-mIS** solution with the fewest required colors.

For the evaluation of our algorithms, we constructed a dataset comprising 120 unit-disk graph samples, each having a varying number of vertices n within the set $\{10, 11, 12, 13, 14, 15\}$. Specifically, there are 20 samples corresponding to each possible value of n . The *GEAN model* detailed in [3] is employed to derive the unit-disk feasible representation for each graph. **BBQ-mIS** consistently and effectively addresses graph coloring problems for all graph samples in our dataset, achieving optimal colorings with the minimum number of colors. The benchmark solutions are provided by the exact solver *Gurobi*.

The current findings exhibit promising outcomes in addressing the GC problem using **BBQ-mIS**. However, there are potential avenues for further enhancement and broader assessment.

One prospect involves exploring the Quantum Adiabatic Algorithm (QAA) as an alternative to the QAOA approach for solving the Maximum Independent Set problem, thus significantly reducing quantum resource usage. Additionally, evaluating emulated results against simulations on actual quantum hardware can establish the method’s robustness in the presence of noise. Finally, these hybrid quantum-classical algorithms, initially designed for GC problems, may serve as inspiration for developing methods focused on conserving qubits for other combinatorial optimization challenges.

References

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