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Hayato Ushijima-Mwesigwa
Fujitsu Laboratories of America

Ruslan Shaydulin
Clemson University

Christian F.A. Negre
Los Alamos National Laboratory

Susan M. Mniszewski
Los Alamos National Laboratory

Yuri Alexeev
Argonne National Laboratory

See next page for additional authors

Authors
Hayato Ushijima-Mwesigwa, Ruslan Shaydulin, Christian F.A. Negre, Susan M. Mniszewski, Yuri Alexeev, and Ilya Safro

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HAYATO USHIJIMA-MWESIGWA[*†‡], Fujitsu Laboratories of America, Inc.
RUSLAN SHAYDULIN[*†], School of Computing, Clemson University
CHRISTIAN F. A. NEGRE, Theoretical Division, Los Alamos National Laboratory
SUSAN M. MNISZEWSKI, Computer, Computational, & Statistical Sciences Division, Los Alamos National Laboratory
YURI ALEXEEV, Computational Science and Leadership Computing Divisions, Argonne National Laboratory
ILYA SAFRO[†], School of Computing, Clemson University

Emerging quantum processors provide an opportunity to explore new approaches for solving traditional problems in the Post Moore's law supercomputing era. However, the limited number of qubits makes it infeasible to tackle massive real-world datasets directly in the near future, leading to new challenges in utilizing these quantum processors for practical purposes. Hybrid quantum-classical algorithms that leverage both quantum and classical types of devices are considered as one of the main strategies to apply quantum computing to large-scale problems. In this paper, we advocate the use of multilevel frameworks for combinatorial optimization as a promising general paradigm for designing hybrid quantum-classical algorithms. In order to demonstrate this approach, we apply this method to two well-known combinatorial optimization problems, namely, the Graph Partitioning Problem, and the Community Detection Problem. We develop hybrid multilevel solvers with quantum local search on D-Wave's quantum annealer and IBM's gate-model based quantum processor. We carry out experiments on graphs that are orders of magnitudes larger than the current quantum hardware size and observe results comparable to state-of-the-art solvers.
Reproducibility: Our code and data are available at [1]

CCS Concepts: • **Mathematics of computing → Graph algorithms**; *Combinatorial optimization*; • **Hardware → Quantum computation**.

Additional Key Words and Phrases: NISQ, Quantum Annealing, Graph Partitioning, Modularity, Community Detection

1 INTRODUCTION

Across different domains, computational optimization problems that model large-scale complex systems often introduce a major obstacle to solvers even if tackled with high-performance computing systems. There are several reasons for this, including but not limited to a large number of variables and even larger number of interactions, and dimensionality required to describe each variable or interaction, and time slices. The combinatorial and mixed integer optimization problems introduce additional layers of complexity with integer variables often making the problem NP-hard (e.g., in cases of non-linearity and non-convexity). A common practical approach to solve these problems is to use iterative

[*]Both authors contributed equally to this work.
[†]Corresponding authors.
[‡]Work on this paper was in part performed while the author was affiliated with Clemson University.

Authors' addresses: Hayato Ushijima-Mwesigwa, hayato@us.fujitsu.com, Fujitsu Laboratories of America, Inc. Sunnyvale, CA, 94085; Ruslan Shaydulin, rshaydu@g.clemson.edu, School of Computing, Clemson University, Clemson, SC, 29634; Christian F. A. Negre, Theoretical Division, Los Alamos National Laboratory, Los Alamos, NM, 87545, cnegre@lanl.gov; Susan M. Mniszewski, Computer, Computational, & Statistical Sciences Division, Los Alamos National Laboratory, Los Alamos, NM, 87545, smm@lanl.gov; Yuri Alexeev, Computational Science and Leadership Computing Divisions, Argonne National Laboratory, Argonne, IL, 60439; Ilya Safro, isafro@clemson.edu, School of Computing, Clemson University, Clemson, SC, 29634.

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methods. The iterative methods, while being composed with completely different algorithmic principles, share a common property: several fast improvement iterations followed by a long tail of slow improvement iterations [27, 63]. Typically, in such iterative algorithms, solving a large-scale system with respect to the first-order interaction laws per iteration advances the solution towards a local attraction basin at each iteration, which often appears to be false with respect to the global optimal solution. In other words, local methods tend to converge to a false local optimum, which often corresponds to the solution of lower quality than the true global optimum [23]. Moreover, in some cases, another problem may exist within each iteration – the algorithms used to solve them are not necessarily exact. To accelerate the solvers at each iteration various heuristics, parallelization-friendly methods, and ad-hoc tricks are employed, which often reduce the quality of the solution.

In this paper, we take steps towards building more robust solvers for mid- to large-scale combinatorial optimization problems by fusing two areas whose simultaneous application is only beginning to be explored, namely, quantum computing and multiscale methods. Recent advances in quantum computing provide a new approach for algorithm development for many combinatorial optimization problems. However, Noisy Intermediate Scale Quantum (NISQ) devices are widely expected to be limited to a few hundred, and for certain sparse architectures up to a few thousands qubits. The current state of quantum computing theory and engineering suggests moderately optimistic expectations. In particular, it is believed that in the near future, we will witness relatively robust architectures with much less noise. This would allow algorithms like the Quantum Approximate Optimization Algorithm (QAOA) and Quantum Annealing (QA) to be run on hardware with limited error correction. Given the realistic level of precision and, in the case of QAOA, ansatz depth, these algorithms are prime candidates for demonstrating Quantum Advantage, that is solving a computationally hard problem (such as NP-hard) faster than classical state-of-the-art algorithms. Such algorithms are our first building block.

The multiscale optimization method is our second building block. These methods have been developed to cope with large-scale problems by introducing an approach to avoid entering false local attraction basins (local optima), a complementary method to stochastic and multi-start strategies that help to escape it if trapped. Because of historical reasons, on graph problems, they have been termed *multilevel* (rather than multiscale), which we will use here. The multilevel (or multiscale) methods have a long history of breakthrough results in many different optimization problems [10, 13, 16, 18, 20, 25, 31, 32, 43, 44, 46–49, 52, 53] and have been implemented on a variety of hardware architectures. The success of multilevel methods for optimization problems supports our optimism about proposed ideas.

There is no unique prescription on how to design multilevel algorithms, but the main idea behind them is to "*think globally while acting locally*" on a hierarchy of coarse representations of the original large-scale optimization problem. A multilevel algorithm therefore begins by constructing such a hierarchy of progressively smaller (coarser) representations of the original problem. The goal of the next coarser level in this hierarchy is to approximate the current level problem with a coarser one that has fewer degrees of freedom and thus can be solved more effectively. When the coarse problem is solved, its solution is projected back to the finer level and further refined, a stage that is called uncoarsening. As a result of such a strategy, the multilevel framework is often able to significantly improve the running time and solution quality of optimization methods. The quality of multilevel algorithms in large part depends on that of the optimization solvers applied at all stages of the multilevel framework. In many cases, these locally acting optimization solvers are either heuristics that get stuck in a local optimum or exact solvers applied on a small number of variables (i.e., on subproblems). In both cases, the quality of a global solution can significantly suffer depending on the quality of the solution from the local solver. The optimization algorithms running on the NISQ devices that may replace such local solvers are expected to be a critical missing component to achieve a game changing breakthrough in multilevel methods for combinatorial optimization.

In this paper, we introduce Multilevel Quantum Local Search (ML-QLS), which uses an iterative refinement scheme on NISQ devices within a multilevel framework. ML-QLS extends the Quantum Local Search (QLS) [55, 56] approach to solve larger problems. This work builds on early results using a multilevel framework and the D-Wave quantum Annealer for the Graph Partitioning Problem [61]. We demonstrate the general approach of solving combinatorial optimization problems with NISQ devices in a multilevel framework on two well-known problems as our use cases. In particular, we solve the Graph Partitioning Problem and the Community Detection Problem on graphs up to approximately $29,000$ nodes using subproblem sizes of 20 and 64 that map onto NISQ devices such as IBM Q Poughkeepsie (20 qubits) and D-Wave 2000Q (~2048 qubits). Such graphs are orders of magnitude larger than those solved by state-of-the-art hybrid quantum-classical methods. To implement this approach, we develop a novel efficient subproblem formulation method.

In contrast, some of the authors of this paper have previously developed quantum and quantum-classical algorithms for the Graph Partitioning Problem and the Community Detection Problem for multiple parts (> 2) [33, 60]. These did not use a multilevel approach, instead an *all at once* or concurrent approach was employed.

The rest of paper is organized as follows. In Section 2, we discuss the relevant background on quantum optimization, multilevel methods, and define the problems. In Sections 3 and 4, we discuss the hybrid quantum-classical multilevel algorithm and computational results, respectively. A discussion of the outlook and important open problems that represent major future research directions are presented in Section 5.

2 BACKGROUND

The methods proposed and implemented in this work aim to solve large graph problems by integrating NISQ optimization algorithms into a multilevel scheme. In this section, we provide a brief introduction into all three components: target graph problems (Sec. 2.1), quantum optimization (Sec. 2.2) and multilevel methods (Sec. 2.3)

Many optimization problems discussed in this work are posed in Ising form. The Ising model is a common mathematical abstraction to represent the energy of n discrete spin variables $\sigma_i \in \{-1, 1\}$, $1 \le i \le n$, and interactions J_{ij} between σ_i and σ_j. For each spin variable σ_i, a local field h_i is specified. The energy of a configuration σ is given by the Hamiltonian function:

$$H(\sigma) = \sum_{i,j} J_{ij}\sigma_i\sigma_j + \sum_i h_i\sigma_i, \quad \sigma_i \in \{-1, 1\}. \tag{1}$$

An equivalent mathematical formulation is the Quadratic Unconstrained Binary Optimization (QUBO) problem. The objective of a QUBO problem is to minimize (or maximize) the following function:

$$H(x) = \sum_{i<j} Q_{ij}x_ix_j + \sum_i Q_{ii}x_i, \quad x \in \{0, 1\}.$$

2.1 Problem Definitions

Let $G = (V, E)$ be an undirected graph with vertex set V and edge set E. We denote by n and m the numbers of nodes and edges, respectively. For each node i, define $\mathbb{v}_i \in \mathbb{R}$ as the volume of node i and $A_{ij} \in \mathbb{R}$ as the positive weight of edge (i, j). For a fixed integer k, the *Graph Partitioning Problem* is to find a partition $V_1, \dots, V_k$ of the vertex set V into k parts with equal total node volume such that the total weight of *cut edges* is minimized. A *cut edge* is defined as an edge whose end points are in different partitions. A requirement of equal total sizes of V_i for all i is sometimes referred as *perfectly balanced* graph partitioning, otherwise an imbalancing parameter is usually introduced to allow imbalanced partitions [12]. However, in this work we deal with perfect balancing constraints and limit the number of parts to $k = 2$. In this case we can write the GP problem as the following quadratic program

$$\begin{aligned} \max \quad & \mathbf{s}^T A \mathbf{s} \\ \text{s.t.} \quad & \sum_{i=1}^{n} \mathbb{v}_i s_i = 0 \\ & s_i \in \{-1, 1\},\ i = 1, \ldots, n, \end{aligned} \tag{2}$$

which, as shown in [60], can be reformulated into the following Ising model,

$$\begin{aligned} \max \quad & \mathbf{s}^T (\beta A - \alpha \mathbb{v}\mathbb{v}^T) \mathbf{s} \\ \text{s.t.} \quad & s_i \in \{-1, 1\},\ i = 1, \ldots, n, \end{aligned} \tag{3}$$

for some constants $\alpha, \beta > 0$, where $\mathbb{v}$ is a column vector of volumes such that $(\mathbb{v})_i = \mathbb{v}_i$.

Maximization of modularity is a famous problem in network science where the goal is to find communities in a network through node clustering (also known as modularity clustering) [34]. For the graph G, the problem of Modularity Maximization is to find a partitioning of the vertex set into one or more parts (communities) that maximizes the modularity metric. The modularity matrix is a symmetric matrix given by

$$B_{ij} = A_{ij} - \frac{k_i k_j}{2|E|}, \tag{4}$$

where k_i is the weighted degree of node i, namely, $k_i = \sum_j A_{ij}$. Whereas the modularity is typically defined on unweighted graphs, within the multilevel framework, due to the coarsening of nodes, we primarily work with weighted graphs. It can equivalently be written in matrix-vector notation as

$$B = A - \frac{1}{2|E|} \mathbb{k}\mathbb{k}^T \tag{5}$$

where $\mathbb{k}$ is a vector of weighted degrees of the nodes in the graph. For up to 2 communities, the *Modularity Maximization Problem*, also referred to as the *Community Detection Problem*, can be written in Ising form as follows:

$$\begin{aligned} \max \quad & \frac{1}{4|E|} \mathbf{s}^T \left(A - \frac{1}{2|E|} \mathbb{k}\mathbb{k}^T \right) \mathbf{s} \\ \text{s.t.} \quad & s_i \in \{-1, 1\},\ i = 1, \ldots, n \end{aligned} \tag{6}$$

where the objective value of equation 6, for a given assignment of resulting communities, is referred to as the *modularity*. For more than 2 communities, the Ising formulation of the Community Detection Problem is given in [33].

Note that the above formulation of Modularity Maximization can be viewed as the Graph Partitioning Problem in the Ising model given in equation (3) where the volume of a node is defined as the weighted degree and the penalty constants $\beta = 1, \alpha = \frac{1}{2|E|}$. We exploit this deep duality between the two problems in our implementation.

2.2 Optimization on NISQ devices

In recent years we have seen a number of advances in quantum optimization algorithms that can be run on NISQ devices. Two most prominent ones are the Quantum Approximate Optimization Algorithm (QAOA) and Quantum Annealing (QA), which are inspired by the adiabatic theorem. There are many formulations of the adiabatic theorem (see [6] for a comprehensive review), but all of them stem from the adiabatic approximation formulated by Kato in

1950 [26]. Adiabatic approximation states, roughly, that a system prepared in an eigenstate (e.g. a ground state) of some time-dependent Hamiltonian $H(t)$ will remain in the corresponding eigenstate[1] provided that $H(t)$ is varied "slowly enough". The requirement on the evolution time scales as $O(1/\Delta^2)$ in the worst case [15], where Δ is the minimum eigengap between ground and first excited state of $H(t)$. Adiabatic Quantum Computation (AQC) is quantum Merlin-Arthur (QMA)-complete [6] and is equivalent to gate-based universal quantum computation.

Quantum Annealing is a special case of AQC limited to stochastic Hamiltonians The transverse field Hamiltonian

$$H_M = \sum_i \sigma_i^x \tag{7}$$

is used as the initial Hamiltonian. The final Hamiltonian is a classical Ising model Hamiltonian with the ground state encoding the solution of the original problem:

$$H_C = \sum_{ij} J_{ij} s_i s_j + \sum_i h_i s_i, \quad s_i \in \{-1, +1\}.$$

The evolution of the system starts in the ground state of H_M and it is described by a time-dependent Hamiltonian

$$H(t) = \frac{t}{T} H_C + (1 - \frac{t}{T}) H_M,\ t \in (0, T). \tag{8}$$

QAOA extends the logic of AQC to gate-model quantum computers and can be interpreted as a discrete approximation of the continuous QA schedule, performed by applying two alternating operators:

$$W(\beta_k) = e^{-i\beta_k H_M} \text{ and } V(\gamma_k) = e^{-i\gamma_k H_C}.$$

$W(\beta_k)$ corresponds to evolving the system with Hamiltonian H_M for a period of time β_k and $V(\gamma_k)$ corresponds to evolving H_C for time γ_k. Similarly to QA, the evolution begins in the ground state of H_M, namely $|+\rangle^{\otimes n}$. Alternating operators are applied to produce the state:

$$|\psi(\boldsymbol{\beta}, \boldsymbol{\gamma})\rangle = e^{-i\beta_p H_M} e^{-i\gamma_p H_C} \dots e^{-i\beta_1 H_M} e^{-i\gamma_1 H_C} |+\rangle^{\otimes n} = U(\boldsymbol{\beta}, \boldsymbol{\gamma}) |+\rangle^{\otimes n}. \tag{9}$$

An alternative implementation was proposed, inspired by the success of the Variational Quantum Eigensolver (VQE) [41]. A variational implementation of QAOA combines an ansatz $U(\boldsymbol{\beta}, \boldsymbol{\gamma})$ (that can be different from the alternating operator one described above) and a classical optimizer. A commonly used ansatz is a hardware-efficient ansatz [24], consisting of alternating layers of entangling and rotation gates. The algorithm starts by preparing a trial state by applying the parameterized gates to some initial state: $|\psi(\boldsymbol{\beta}, \boldsymbol{\gamma})\rangle = U(\boldsymbol{\beta}, \boldsymbol{\gamma}) |+\rangle^{\otimes n}$. In the next step, the state $|\psi(\boldsymbol{\beta}, \boldsymbol{\gamma})\rangle$ is measured and the classical optimization algorithm uses the result of the measurement to choose the next set of parameters $\boldsymbol{\beta}, \boldsymbol{\gamma}$. The goal of the classical optimization is to find the parameters $\boldsymbol{\beta}, \boldsymbol{\gamma}$ corresponding to the optimal QAOA "schedule", i.e. the schedule that produces the ground state of the problem Hamiltonian H_C:

$$\boldsymbol{\beta}_*, \boldsymbol{\gamma}_* = \underset{\boldsymbol{\beta}, \boldsymbol{\gamma}}{\arg\min} \langle \psi(\boldsymbol{\beta}, \boldsymbol{\gamma}) | H_C | \psi(\boldsymbol{\beta}, \boldsymbol{\gamma}) \rangle. \tag{10}$$

Both QA and QAOA have been successfully implemented in hardware by a number of companies, universities and national laboratories [5, 14, 35, 37, 38, 42].

[1] A note on terminology: a Hamiltonian H is a Hermitian operator. The spectrum of H corresponds to the potential outcomes if one was to measure the energy of the system described by H. $|\psi\rangle$ is an eigenstate of a system described by Hamiltonian H with energy $\lambda \in \mathbb{R}$ if $H|\psi\rangle = \lambda|\psi\rangle$. In other words, $|\psi\rangle$ is an eigenvector of H with real eigenvalue λ.

2.3 Multilevel Combinatorial Optimization

The goal of the multilevel approach for optimization problems on graphs is to create a hierarchy of coarsened graphs G_0, G_1, ... ,G_k in such a way that the next coarser graph G_{i+1} "approximates" some properties of G_i (that are directly relevant to the optimization problem of interest) but with fewer degrees of freedom. After constructing such a hierarchy, the coarsening is followed by solving the problem on G_k as best as we can (preferably exactly) do and finally uncoarsening the solution back to G_0 through gradual refinement at all levels of the hierarchy, with a refined solution at level $i + 1$ serving as the initial solution at level i. The entire coarsening-uncoarsening process is called a V-cycle. There are other variations of hierarchy levels' coarsening-uncoarsening order, e.g., W- and Full cycles [11]. Fig. 1 presents an outline of a V-cycle.

Typically, when solving problems on graphs in which nodes represent the optimization variables (such as those in the partitioning and Community Detection), having fewer degrees of freedom implies a decreased number of nodes in each next coarser graph $|V_0| > |V_1| > |V_2| > \ldots > |V_k|$.[2] With a smaller number of variables at each level, one can use more sophisticated algorithms at each level. However, it is still not sufficient to solve the original problem as a whole until the coarsening reaches the coarsest level. As a result, at each level, the actual solution is produced by a refinement. Refinement is typically implemented with a decomposition method that uses a previous iteration or a coarser level solution as an initial guess. The multilevel algorithms rely heavily [64] on the quality of refinement solvers for small and local subproblems at all levels of coarseness. Thus, the most straightforward way to use NISQ devices in multilevel frameworks is to iteratively apply them as local solvers to refine a solution inherited from the coarse level. Because the refinement is executed at all levels of coarseness, it is clear that *even a small improvement of a solution at the coarse level*

[2]Note that this does not necessarily imply $|E_0| > |E_1| > |E_2| > \ldots > |E_k|$

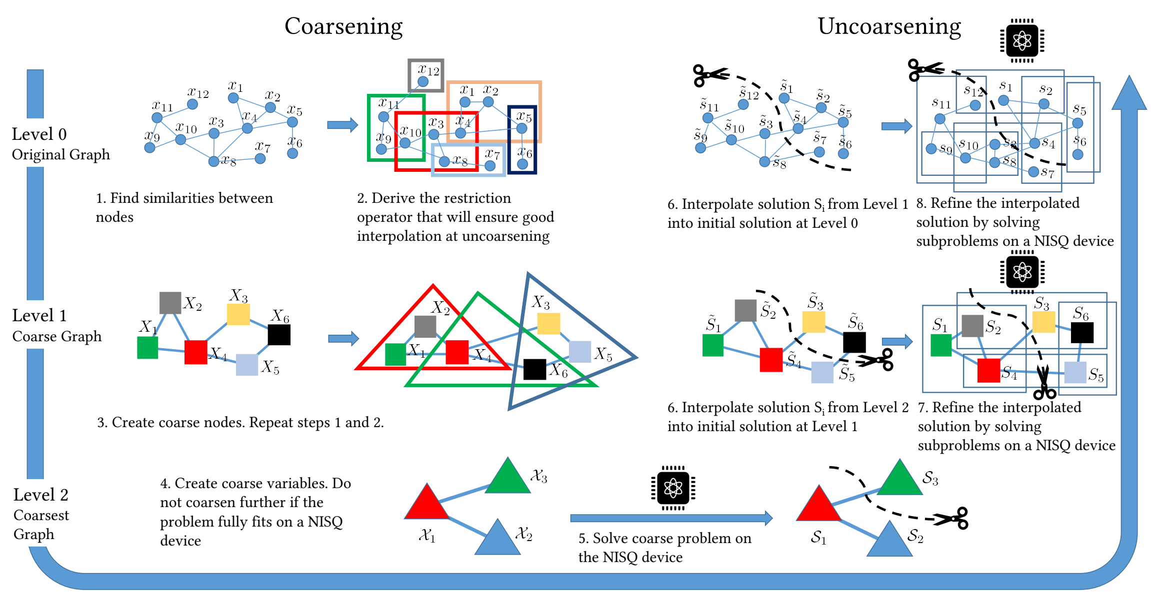


Fig. 1. V-cycle for a graph problem. First, the problem is iteratively coarsened (left). Second, the coarse problem is solved using a NISQ optimization solver (bottom). Finally, the problem is iteratively uncoarsened and the solution is refined using a NISQ solver (right).

may cause a major improvement at the finest scale. Typically, this is the most time-consuming stage of the multilevel process which is expected to be fundamentally better if improved by NISQ devices. Most refinement solvers in multilevel frameworks rely on fast but low-quality heuristics, rather than on the ability to compute an optimal solution. Moreover, in many existing solvers, the number of variables in such local subproblems is comparable with or smaller than the the size of the problems that can be directly embedded on the NISQ devices (see examples in [20, 28, 31]), making them a perfect target for NISQ optimization algorithms. In most multilevel/multiscale/multigrid-based optimization solvers, a refinement consists of covering the domain (or all variables) with *small* subsets of variables (i.e., small subproblems) such that solving a small local problem on a subset improves the global solution for the current level.

Multilevel Graph Partitioning and Community Detection algorithms are examples of the most successful applications of multilevel algorithms for large graphs, achieving excellent time/quality performance [12]. In this paper, we use the simplest version of coarsening (in order to focus on the hybrid quantum-classical refinement) in which the edges of the fine level graph are collapsed and create coarse level vertices by merging the fine level ones. There are several classes of refinement for both problems but in all of them, at each step a small subset of nodes (or even a singleton) is reassigned with partition (or cluster) that either better optimizes the objective or improves constraints. Some variants of stochastic extensions also exist.

3 METHODS

An iterative improvement scheme is a common approach for solving large scale problems with NISQ devices. Traditionally, this is done by formulating the entire problem in the Ising model or as a QUBO and then solving it using hybrid quantum-classical algorithms (see, for example, "qbsolv" from D-Wave systems [8]). These methods decompose the large QUBO into smaller sub-QUBOs or decrease the number of degrees of freedom to fit the subproblem on the hardware (for example, using a multilevel scheme), and iteratively improve the global solution by solving the small subproblems (sub-QUBOs). One of the main limitations of this approach is the size and density of the original QUBO. For example, in the graph partitioning formulation given by equation 3, the term $\mathbb{v}\mathbb{v}^T$ leads to the formulation of a completely dense $n \times n$ QUBO matrix regardless of whether or not the original graph was sparse. Storing and processing this dense matrix can easily make this method prohibitively computationally expensive even for moderately sized problems. In our implementation of Quantum Local Search (QLS) [56] we circumvent this limitation by developing a novel subproblem formulation of the Graph Partitioning Problem and Modularity Maximization as a QUBO that does not require formulating the entire QUBO.

Another concern is the effectiveness of selection criteria of candidate variables (or nodes) to be included in each subproblem. A common metric used in selecting whether or not a variable is to be included in the subproblem is whether or not changing the variable value would reduce (increase) the objective value for a minimization (maximization) problem. Thus, since computing the change in objective value for a small change in the solution is performed multiple times, it is important to ensure that this computation is efficient. We derive a novel efficient way to compute the change in the objective value of the entire QUBO also without formulating the entire QUBO and thus provide an efficient refinement scheme using current NISQ devices.

We begin by introducing an efficient QUBO subproblem formulation for the Graph Partitioning Problem, and the Community Detection Problem. Then we present an efficient way to compute the gain and change in the objective of the entire QUBO. Finally, we put it all together and outline our algorithm.

3.1 QUBO formulation for subproblems

Let M be an $n \times n$ symmetric matrix that represents the QUBO for a large scale problem such that it is prohibitively expensive to either generate or store M. However, for QLS we need to generate constant-size sub-QUBOs of M which in turn represent subproblems of the original problem. In order to generate a sub-QUBO, let k be the size of the desired sub-QUBO. In other words, the sub-QUBO will have k variables and $n - k$ *fixed variables* that remain invariant for this specific sub-QUBO. We refer to the k variables as *free variables*. Without loss of generality, let the the first k variables of $\mathbf{s}$ be the free variables, then we write $\mathbf{s}$ as

$$\mathbf{s} = \begin{bmatrix} \mathbf{s}_v \\ \mathbf{s}_f \end{bmatrix},$$

where $\mathbf{s}_v$ represents the k free variable terms and $\mathbf{s}_f$ represents the $n - k$ fixed terms. In the next step, M can be represented using block form

$$M = \left[\begin{array}{c|c} M_{vv} & M_{vf} \\ \hline M_{vf}^T & M_{ff} \end{array}\right] \tag{11}$$

such that M_{vv} is a $k \times k$ matrix. Next, we can write $\mathbf{s}^T M \mathbf{s}$ as

$$\mathbf{s}^T M \mathbf{s} = \mathbf{s}_v^T M_{vv} \mathbf{s}_v + \mathbf{s}_v^T (2 M_{vf} \mathbf{s}_f) + \mathbf{s}_f^T M_{ff} \mathbf{s}_f \tag{12}$$

Since $\mathbf{s}_f$ are fixed values, we have $\mathbf{s}_f^T M_{ff} \mathbf{s}_f$ as a constant thus

$$\min\ \mathbf{s}^T M \mathbf{s} = \min\ \mathbf{s}_v^T M_{vv} \mathbf{s}_v + \mathbf{s}_v^T (2 M_{vf} \mathbf{s}_f) \tag{13}$$

From equation (11), we have

$$\mathbb{v}\mathbb{v}^T = \left[\begin{array}{c|c} \mathbb{v}_v \mathbb{v}_v^T & \mathbb{v}_v \mathbb{v}_f^T \\ \hline \mathbb{v}_f \mathbb{v}_v^T & \mathbb{v}_f \mathbb{v}_f^T \end{array}\right] \tag{14}$$

Therefore, from equation (13), we have

$$\min\ \mathbf{s}^T \mathbb{v}\mathbb{v}^T \mathbf{s} = \min\ \mathbf{s}_v^T \mathbb{v}_v \mathbb{v}_v^T \mathbf{s}_v + 2 \mathbf{s}_v^T \mathbb{v}_v \mathbb{v}_f^T \mathbf{s}_f \tag{15}$$

The formulation in (15) is particularly important because it shows that the matrix $\mathbb{v}\mathbb{v}^T$ does not need to be explicitly created at each iteration during refinement. This is a crucial observation because $\mathbb{v}\mathbb{v}^T$ is a completely dense matrix.

As described in Sec. 2.1, the Community Detection Problem is given by

$$\max\ \frac{1}{4|E|} \mathbf{s}^T \left(A - \frac{1}{2|E|} \mathbb{k}\mathbb{k}^T \right) \mathbf{s} \tag{16}$$

or

$$\min\ \mathbf{s}^T\Big(\frac{1}{2|E|}\mathbb{k}\mathbb{k}^T - A\Big)\mathbf{s} \tag{17}$$

and the Graph Partitioning Problem is given by

$$\min\ \mathbf{s}^T\Big(\alpha\mathbb{v}\mathbb{v}^T - \beta A\Big)\mathbf{s}. \tag{18}$$

In the above formulation, modularity clustering can be viewed as the Graph Partitioning Problem in a QUBO model, where the volume of a node is defined as the weighted degree and the penalty constant is $\frac{1}{|E|}$ Therefore, in both cases we can perform a refinement while defining fixed values as

$$\min\ \mathbf{s}^T\Big(\frac{1}{2|E|}\mathbb{k}\mathbb{k}^T - A\Big)\mathbf{s} = \min\ \mathbf{s}_v^T\Big(\frac{1}{2|E|}\mathbb{k}_v\mathbb{k}_v^T\Big)\mathbf{s}_v + \mathbf{s}_v^T\Big(\frac{1}{|E|}\mathbb{k}_v\mathbb{k}_f^T\Big)\mathbf{s}_f - \mathbf{s}^T A\mathbf{s} \tag{19}$$

and

$$\min\ \mathbf{s}^T\Big(\alpha\mathbb{v}\mathbb{v}^T - \beta A\Big)\mathbf{s} = \min\ \mathbf{s}_v^T\Big(\alpha\mathbb{v}_v\mathbb{v}_v^T\Big)\mathbf{s}_v + \mathbf{s}_v^T\Big(2\alpha\mathbb{v}_v\mathbb{v}_f^T\Big)\mathbf{s}_f - \beta\mathbf{s}^T A\mathbf{s} \tag{20}$$

with

$$\min\ -\beta\mathbf{s}^T A\mathbf{s} = \min\ -\beta\mathbf{s}_v^T A_{vv}\mathbf{s}_v - \mathbf{s}_v^T(2\beta A_{vf}\mathbf{s}_f) \tag{21}$$

The formulation in (19) and (20) are particularly important during the refinement step because this implies that the complete dense (and therefore prohibitively large) QUBO or Ising model does not need to be created at each iteration. These formulations also demonstrate a close relationship between the Graph Partitioning Problem and the Community Detection Problem.

3.2 Efficient Evaluation of the Objective

In order to select the free variables for the subproblem, we need to be able to efficiently compute the change of the objective function by moving one node from one part to another. In other words, for each vertex v, we need to efficiently compute the *gain* which is the decrease (or increase) in the edge-cut together with penalty if v is moved to the other part.

For a symmetric matrix M, the change in the value $Q = \mathbf{s}^T M\mathbf{s}$ by flipping a single variable s_i corresponding to the node i is given by

$$\Delta Q(i) = 2(\sum_{j\in C_1} M_{ij} - \sum_{j\in C_2} M_{ij}) \tag{22}$$

where C_1 and C_2 correspond to all variables with $s_i = -1$ and $s_i = 1$ respectively. Next, we define

$$deg(v, C) := \sum_{j\in C} A_{vj};\quad Deg(C) := \sum_{i\in C} k_i;\quad Vol(C) := \sum_{i\in C}\mathbb{v}_i$$

then

$$2(\sum_{j\in C_1} A_{ij} - \sum_{j\in C_2} A_{ij}) = 2deg(v_i, C_1) - 2deg(v_i, C_2)$$

and finally

$$\begin{aligned} 2(\sum_{j\in C_1}(\mathbb{v}\mathbb{v}^T)_{ij} - \sum_{j\in C_2}(\mathbb{v}\mathbb{v}^T)_{ij}) &= 2\Big(\mathbb{v}_i\sum_{j\in C_1, i\neq j}\mathbb{v}_j - \mathbb{v}_i\sum_{j\in C_2}\mathbb{v}_j\Big) \\ &= 2\mathbb{v}_i\big(Vol(C_1\backslash i) - Vol(C_2)\big) \end{aligned}$$

where we assume that $i \in C_1$. This expression can be computed in $O(1)$ time.

In the same way

$$
\begin{aligned}
2(\sum_{j\in C_1}(\mathbb{k}\mathbb{k}^T)_{ij} - \sum_{j\in C_2}(\mathbb{k}\mathbb{k}^T)_{ij}) &= 2\Big(k_i \sum_{j\in C_1, i\neq j} k_j - k_i \sum_{j\in C_2} k_j\Big) \\
&= 2k_i\big(Deg(C_1\backslash i) - Deg(C_2)\big)
\end{aligned}
$$

can also be computed in $O(1)$ time given $Deg(C_1)$ and $Deg(C_2)$, where $Deg(C_i)$ represents the sum of weighted degrees of nodes in community i.

Therefore, the change in modularity is given by

$$
\Delta Q(i) = \frac{k_i}{|E|}\big(Deg(C_1\backslash i) - Deg(C_2)\big) - 2\Big(deg(v_i, C_1) - deg(v_i, C_2)\Big) \tag{23}
$$

and change in edge-cut together with penalty value is given by

$$
\Delta Q(i) = 2\alpha \mathbb{v}_i\big(Vol(C_1\backslash i) - Vol(C_2)\big)) - 2\beta\Big(deg(v_i, C_1) - deg(v_i, C_2)\Big) \tag{24}
$$

For each node i, both expressions (23) and (24) can be computed in $O(k_i)$ time, where k_i is the unweighted degree of i.

At no point during the algorithm should the complete QUBO matrix be formulated. This also applies to the process of evaluating a given solution. In other words, evaluating the modularity for the Community Detection Problem or edge-cut together with penalty term for the Graph Partitioning Problem should be done in $O(1)$ time and space. The term is

$$
\mathbf{s}^T \mathbb{v}\mathbb{v}^T \mathbf{s} = \big(Vol(C_1) - Vol(C_2)\big)^2
$$

where as

$$
\mathbf{s}^T A\mathbf{s} = 2(|E| - 2cut).
$$

Therefore,

$$
\mathbf{s}^T(\alpha\mathbb{v}\mathbb{v}^T - \beta A)\mathbf{s} = \alpha\Big(Vol(C_1) - Vol(C_2)\Big)^2 - 2\beta(|E| - 2cut) \tag{25}
$$

and

$$
\mathbf{s}^T\Big(\frac{1}{2|E|}\mathbb{k}\mathbb{k}^T - A\Big)\mathbf{s} = \frac{1}{2|E|}\Big(Deg(C_1) - Deg(C_2)\Big)^2 - 2(|E| - 2cut) \tag{26}
$$

where equations (25) and (26) give the formulations for computing the modularity and edge-cut with corresponding penalty value respectively without creating the QUBO matrix.

3.3 Algorithm Overview

Now we can combine the building blocks described in the previous two subsections. Let $G = (V, E)$ be the problem graph. ML-QLS begins by coarsening the problem graph. During the coarsening stage, for some integer k, a hierarchy of coarsened graphs $G = G_0, G_1, \ldots, G_k$ is constructed. In this work, we used the coarsening tools implemented in KaHIP Graph Partitioning package [51]. We used the coarsening implementation that is performed using maximum weight matching with "expansion^{*2}" metric as described in [22]. The maximum edge matching is found using the Global Path Algorithm [22]. In the next step, a QUBO is formulated for the smallest graph G_k and solved on the quantum device. If $|V_k|$ is greater than the hardware size[3], QLS [56] with a random initialization is used to solve for G_k. Then, the solution is iteratively projected onto finer levels and refined using QLS. The algorithm overview is presented in Alg. 1.

[3]more specifically, greater than the maximum number of variables in a problem that can be embedded on the device

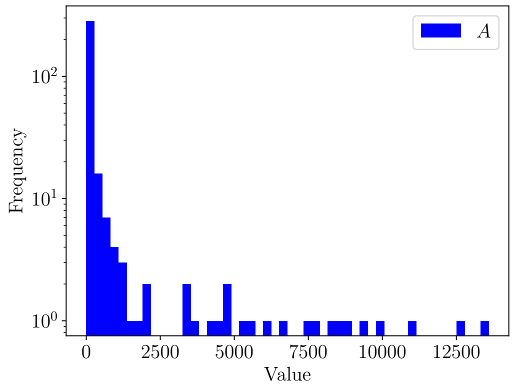
Algorithm 1 Multilevel Quantum Local Search

```
function ML-QLS(G, problem_type)
    if problem_type is modularity then
        G = UpdateWeights(G)
    G_0, G_1, ..., G_k = KaHIPCoarsen(G)
    if |V_k| ≤HardwareSize then
        // solve directly
        QUBO = FormulateQUBO(G_k)
        solution = SolveSubproblem(QUBO)
    else
        // use QLS
        initial_solution = RandomSolution(G_k)
        solution = RefineSolution(G_k, initial_solution)
    for G_i in G_{k-1}, G_{k-2}, ..., G_0 do
        projected_solution = ProjectSolution(solution, G_i, G_{i+1})
        solution = RefineSolution(G_i, projected_solution)
    return solution
function RefineSolution(G_i, projected_solution)
    solution = projected_solution
    while not converged do
        ΔQ = ComputeGains(G_i, solution)
        X = HighestGainNodes(ΔQ)
        QUBO = FormulateQUBO(X)
        // using IBM UQC or D-Wave QA
        candidate = SolveSubproblem(QUBO)
        if candidate > solution then
            solution = candidate
    return solution
```

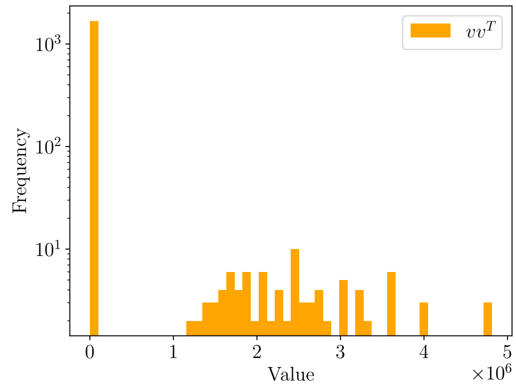
For the Graph Partitioning Problem, the initial weight of each node is one by definition, therefore coarsening of the nodes keeps the total node volume constant at each coarsening level. For the Community Detection Problem, the initial weight of each node is set to the degree of the node. This ensures that the size of the graph (total number of weighted edges) is also kept constant at each level. Note that Graph Partitioning is defined with respect to total node volume ($|V|$), while modularity is defined with respect to the size ($|E|$, the total number of weighted edges) of the graph.

3.4 Addressing the Limited Precision of the Hardware

One of the subproblem solvers we used in this work is Quantum Annealing, which we ran on the LANL D-Wave 2000Q machine. The D-Wave 2000Q is an analog quantum annealer with limited precision. In this work, we used a simple coarsening that constructs coarser graphs by aggregating nodes at a finer level to become a single node at the coarser level (i.e. many nodes on the finer level are merged into one node at the coarser level, with the volume of the new node set to be the sum of the volumes of the nodes on the coarser level). This causes the precision required to describe the node volumes and edge weights for coarser graphs to increase dramatically, especially for the large scale problems. Thus, a QUBO describing the coarsest graph could require significantly more precision to represent compared to the finest graph. For example, in Graph Partitioning where the QUBO problem to be minimized is $A - \alpha \mathbb{v}\mathbb{v}^T$, the range of values in the matrix A increase at a different rate than the range of values in the matrix $\mathbb{v}\mathbb{v}^T$ during the coarsening process,



(a) Edge weights of the coarsest graph SSS12.



(b) Entries of the matrix $\mathbb{v}\mathbb{v}^T$.

Fig. 2. In Figure 2a, the maximum value is approximately 13×10^3.In Figure 2b, the maximum value is approximately 5×10^6 and minimum value 1. A naive scaling of QUBO matrix $A - \mathbb{v}\mathbb{v}^T$ can result in values that are too large to be handled by the quantum annealer due to its limited precision. Such values of A are ignored, leading to random balanced partitions.

increasing the precision required to describe the overall QUBO formed at each level (see an example on Fig. 2a). Thus, if the QUBO $A - \alpha\mathbb{v}\mathbb{v}^T$ is directly scaled to accommodate the limited precision of the device, the quality of the results can suffer. In our experiments, we observe that directly scaling the QUBO returned feasible, but low quality solutions. In order to overcome this challenge, for the problems solved on the D-Wave device, we first scaled the matrices A and $\alpha\mathbb{v}\mathbb{v}^T$ separately, and then formed the QUBO to be optimized. This approach then resulted in achieving results with high quality solutions on the D-Wave device.

4 EXPERIMENTS AND RESULTS

Implementation. The general framework for ML-QLS is implemented in Python 3.7 with NetworkX [19] for network operations. We have used the coarsening algorithms available in the KaHIP Graph Partitioning package [51] which are implemented in C++. The code for the general ML-QLS framework is available on GitHub [1].

Systems. The refinement algorithms presented in this work require access to NISQ devices capable of solving problems formulated in the Ising model. To this end, we have used the D-Wave 2000Q quantum annealer located at Los Alamos National Laboratory, as well as IBM's Poughkeepsie 20 qubit quantum computer available on the Oak Ridge National Laboratory IBM Q hub network together with the high-performance simulator, IBM Qiskit Aer Simulator [7]. However, our framework is modular and can easily be extended to utilize other novel quantum computing architectures as they become available.

The D-Wave 2000Q is the state-of-the-art quantum annealer at this time. It has up to 2048 qubits which are laid out in a special graph structure known as a Chimera graph. The Chimera graph is sparse, thus the device has sparse connectivity. Fully connected graphs as dense problems need to be embedded onto the device, which leads to the maximum size of 64 variables. We have used the embedding algorithm described in [9] to calculate a complete embedding of the 64 variable problem. We found this embedding only once and reused it during our experiments. We utilized D-Wave's

Solver API (SAPI) which is implemented in Python 2.7, to interact with the system. The D-Wave system is intrinsically a stochastic system, where solutions are sampled from a distribution corresponding to the lowest energy state. For each subproblem, the best solution out of 10,000 samples is returned. The annealing time for each call to the D-Wave system was set to 20 microseconds.

In order to solve problems formulated in the Ising model on IBM's Poughkeepsie quantum computer and simulator, we implemented QAOA using the SBPLX [45] optimizer to find the optimal variational parameters. We allowed 2000 iterations for SBPLX to find optimal parameters for QAOA run on the simulator and 250 iterations for QAOA on the device. Due to the limitations of NISQ devices available in IBM Q hub network [54], we used the RYRZ variational form [3] (also known as a hardware-efficient ansatz) as the ansatz for our QAOA implementation. For the experiments run on IBM quantum device Poughkeepsie, we perform the variational parameter optimization on the simulator locally and run QAOA on the device via the IBM Q Experience cloud API. This is done due to the job queue limitations provided via the IBM Q Experience. However, we expect to be able to run QAOA variational parameter optimization fully on a device as more devices are becoming available on the cloud. We have used GNU Parallel [59] for the large-scale numerical experiments performed on the quantum simulator.

Considering the fact that solutions from the NISQ devices and simulator do not provide optimality guarantees, we have also solved various subproblems formulated in the Ising model using the solver Gurobi [36] together with modeling package Pyomo [21]. The results using Gurobi as a solver for each subporblem are denoted as "Optimal" in our plots to highlight the point that each subproblem was solved and proven to be optimal.

Instances. A summary of the graphs used in the experimentes together with their properties is presented in Table 1. For the Graph Partitioning Problem, we evaluate ML-QLS on five graphs, four of which are drawn from The Graph Partitioning Archive [58] (`4elt`, `bcsstk30`, `cti` and `data`) and one from the set of hard to partition graphs (`vsp_msc10848_300sep_100in_1Kout`, denoted in figures as `SSS12`) [49]. For the Modularity Maximization Problem, we evaluate ML-QLS on six graphs. The graphs `roadNet-PA-20k` and `opsahl-powergrid` are real-world networks from the KONECT dataset [29]. Graphs `msc23052` and `finan512-10k` are taken from the graph archive presented in [50]. The graphs `finan512-10k` and `roadNet-PA-20k` are reduced to 10,000 and 20,000 nodes respectively by performing a breadth-first search from the median degree node. Note that due to the high diameter of these networks and their structure (portfolio optimization problem and road network), this preserves their structural properties. `GirvanNewman` is a synthetic graph generated using the model introduced by Girvan and Newman (GN) [17]. The graph `lancichinetti1` is a synthetic graph generated using a generalization of the GN model that allows for heterogeneity in the distributions of node degree and community size, introduced by Lancichinetti et al. [30]. Table 2 shows the parameters used to generate the synthetic graphs.

Experimental Setup. Our experiments are performed in order to compare the solutions from ML-QLS with those of high-quality classical solvers, and the best known results, if available. For the Graph Partitioning Problem, the results are compared to those produced by KaHIP [51] which is a state-of-the-art multilevel Graph Partitioning solver. The best known results are taken at The Graph Partitioning Archive [58] where applicable. In order to make our approach more comparable to KaHIP, we follow the user guide [4], and use the `kaffpaE` version of the solver with the option `--mh_enable_kabapE` for high quality refinement for perfectly balanced parts. We use the option `--preconfiguration=fast` to ensure results are compared with a single V-cycle. Our results (cut values) are normalized with either the best known value when applicable or by the smallest cut value found by any of the solvers used.

Network name	$\lvert V\rvert$	$\lvert E\rvert$	d_{avg}	d_{max}
SSS12	21996	1221028	111.02	722
4elt	15606	45878	5.88	10
bcsstk30	28924	1007284	69.65	218
cti	16840	48232	5.73	6
data	2851	15093	10.59	17
roadNet-PA-20k	20000	26935	2.69	7
opsahl-powergrid	4941	6594	2.67	19
msc23052	5722	103391	36.14	125
finan512-10k	10000	28098	5.62	54

Table 1. Properties of the networks used to evaluate ML-QLS. d_{avg} is average degree, d_{max} is maximum degree

Network name	$\lvert V\rvert$	$\lvert E\rvert$	d_{avg}	d_{max}	γ	β	μ
GirvanNewman	10,000	75,000	15.0	15	1	1	0.1
lancichinetti1	10,000	76,133	15.22	50	2	1	0.1

Table 2. Properties of synthetic networks used in the Modularity evaluation. d_{avg} is average degree, d_{max} is maximum degree, γ is the exponent for the degree distribution, β is the exponent for the community size distribution and μ is the mixing parameter. For a detailed discussion of the parameters the reader is referred to Ref. [30]

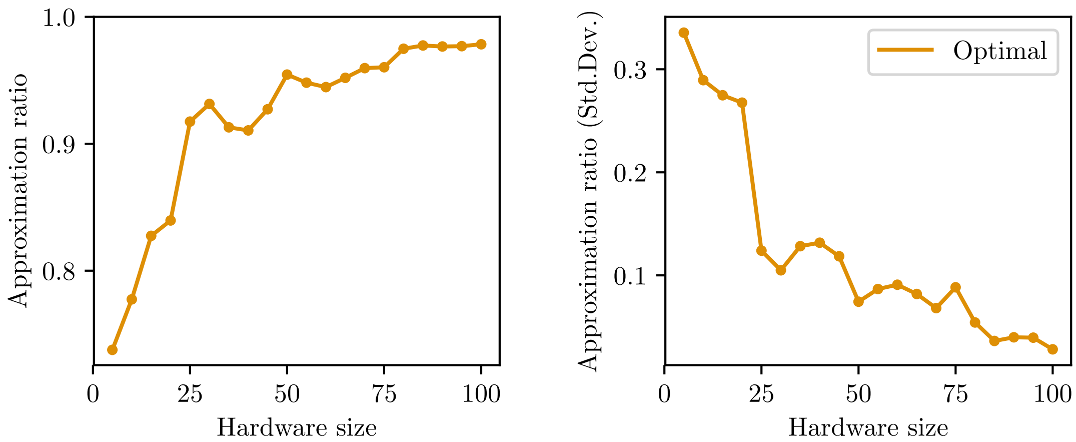
Network name	Best modularity
finan512-10k	0.499
GirvanNewman	0.459
lancichinetti1	0.452
msc23052	0.499
opsahl-powergrid	0.497
roadNet-PA-20k	0.499

Table 3. Highest modularity value found by all methods for a given problem. The highest possible modularity value for at most 2 communities is 0.5.

For the Modularity Maximization Problem, we compare our solutions using ML-QLS with two classical clustering methods, Asynchronous Fluid Communities [39] (implemented in NetworkX [19]) and Spectral Clustering [57, 62] (implemented in Scikit-learn [40]). Note that even though these methods solve the same problem (namely, Community Detection or clustering), they do not explicitly maximize modularity. Therefore, it is unfair to directly compare the modularity of the solution produced by them to ML-QLS, which is explicitly maximizing modularity. However, they provide a useful baseline. Moreover, since the maximum possible modularity for at most 2 communities is 0.5, the best solutions found by all methods are no more than 1%–10% away from the optimal (see Table 3)

The experimental results are presented in Figure 4. We have made all raw result data available on Github [2]. For each problem and method (except for QAOA on IBM Q Poughkeepsie quantum computer, labeled "QAOA (IBMQ Poughkeepsie)" in Figure 4), we perform ten runs of a single V-cycle with different seeds. For "QAOA (IBMQ Poughkeepsie)", we perform just one run per each problem due to the limited access to quantum hardware.

Observations. We observe that ML-QLS is capable of achieving results close to the best ones found by other solvers for all problems. For Graph Partitioning, Figure 4 shows significant variability in the quality of the solution across



(a) Mean

(b) Standard deviation

Fig. 3. Modularity (Approximation ratio) as the function of the size of the subproblem (hardware size). The performance is projected using Gurobi as the subproblem solver and allowing it to solve each subproblem to optimality. The top plot presents the mean approximation ratio averaged over the entire benchmark. The bottom plot presents the standard deviation. As the hardware size increases, the quality of the solution found by ML-QLS improves.

different solvers and problem instances. This effect is also observed for the state-of-the-art Graph Partitioning solver KaHIP, when run for a single V-cycle. This is partially due to the fact that we normalize the objectives to make them directly comparable. For example, for the graph `4elt` the best known cut value presented in The Graph Partitioning Archive [58] is 139. Therefore, an *absolute* difference of 28 edges in cut obtained by a solver translates into a 20% *relative* difference presented in Figure 4. However, the same *absolute* difference of 28 edges would translate into $\approx 0.44\%$ for the graph `bcsstk30` (best known cut 6394). The graph `SSS12` is specifically designed to be hard for traditional Graph Partitioning frameworks [49]. This explains the high variation in the performance of KaHIP on it.

It is worth noting that QAOA on the IBM quantum computers (see "QAOA (IBM Q Poughkeepsie)" in Figure 4) takes more iterations to converge to a solution compared to D-Wave. This is partially due to the fact that we perform the QAOA variational parameter optimization on the simulator and only run once with the optimized parameters on the device. As a result, the learned variational parameters do not include the noise profile of the device, limiting the quality of subproblem solutions. As devices become more easily available, we expect to be able to run full variational parameter optimization on the quantum hardware.

To project the performance improvements for future hardware, we simulate the performance of ML-QLS as a function of hardware (subproblem) size shown in Figure 3. As the subproblem size increases, the average quality of the solution found by ML-QLS improves and variation in results decreases. This shows that performance of ML-QLS can be improved as larger size quantum devices and better quantum optimization routines are developed.

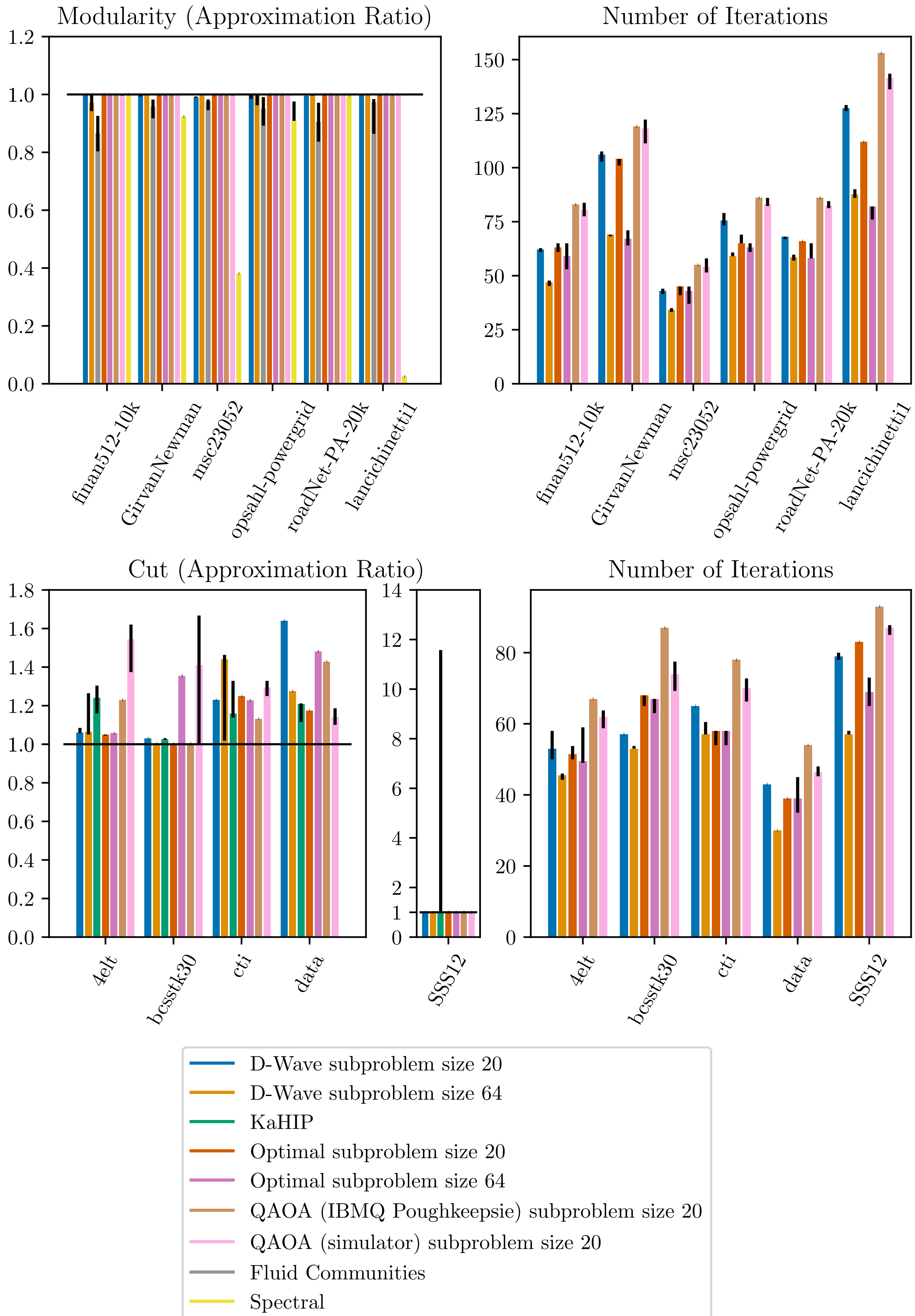


Fig. 4. Quality of the solution and the number of iterations for all problems and solvers. The height of the bars is the median over 10 seeds. Error bars (black) are 25th and 75th percentiles. For the objective function (Cut or Modularity) all results are normalized by the best solution found by any solver (for Graph Partitioning this includes the best known cuts from The Graph Partitioning Archive [58]). Number of iterations is the number of calls to the subproblem solver (ML-QLS only).

5 OPEN PROBLEMS AND DISCUSSION

Revising (un)coarsening operators in anticipation of the new class of high-quality refinement solvers is the first major open problem. The majority of multilevel algorithms for combinatorial optimization problems are inspired by the idea of "thinking globally while acting locally". However, there is a crucial difference between these algorithms for combinatorial problems and such methods as multigrid for continuous problems or multiscale PDE-based optimization. In multigrid (e.g., for systems of linear equations), a relaxation at the uncoarsening stage is convergent [10], and in most cases assumes an optimal solution (up to some tolerance) for a subset of relaxed variables given other variables are invariant (i.e., a fixed solution for those variables that are not in the optimized subset). Examples include easily parallelizable Jacobi relaxation, as well as hard to parallelize Gauss-Seidel relaxation in which most variables are typically optimized sequentially, and many more. Both coarsening and uncoarsening operators (also known as the restriction, and prolongation in multigrid) assume this convergence which in the end provides guarantees for the entire multilevel framework. However, for the *combinatorial* multilevel solvers, the integer variables make this assumption practically impossible, even for subproblems containing tens of variables optimized simultaneously. With the development of noiseless NISQ devices, we can assume that in our hands will be extremely fast heuristics to produce nearly (if hypothetically not completely) optimal solutions for combinatorial optimization problems of up to several hundreds variables. In order to use the multilevel paradigm correctly, there will be a critical need to revise (un)coarsening operators that take this feature into account because (to the best of our knowledge) all existing versions of coarsening operators do not consider optimality of the refinement. Moreover, most existing multilevel frameworks exhibit more emphasis on computational speedup rather than on the quality of the solution to better approximate the fine problem.

The second problem is not unique to multilevel methods but to most decomposition based approaches. Even if quantum devices become fully developed and become more accessible for the broad scientific community, they will still remain more expensive than regular CPU based devices. The decomposition approaches split the problem into many small local subproblems, while multilevel methods may need even more of them because solving subproblems is required at all levels of coarseness. Thus, there is a critical need in developing an extremely fast routing classifier for a subproblem that will decide whether solving a particular subproblem on the NISQ device will be beneficial in comparison to the CPU.

6 CONCLUSION

Current Noisy Intermediate-Scale Quantum (NISQ) devices are limited in the number of qubits and can therefore only be used to directly solve combinatorial optimization problems that exhibit a limited number of variables. In order to overcome this limitation, in this work we have proposed the multilevel computational framework for solving large-scale combinatorial problems on NISQ devices. We demonstrate this approach on two well-known combinatorial optimization problems, the Graph Partitioning Problem, and the Community Detection Problem, and perform experiments on the 20 qubit IBM gate-model quantum computer, and the 2048 qubit D-Wave 2000Q quantum annealer. In order to implement an efficient iterative refinement scheme using the NISQ devices, we have developed novel techniques for efficiently formulating and evaluating sub-QUBOs without explicitly constructing the entire QUBO of the large-scale problem, which in many cases can be a dense matrix that makes it computationally expensive to store and process. In our experiments, for the Graph Partitioning Problem, five graphs were chosen such that the smallest graph had 2851 nodes while the largest had 28924 nodes, while for the Community Detection Problem, the smallest graph had 4941 nodes and largest had 10,000 nodes. For both problems, for comparison purposes, we run one V-cycle of the multilevel framework with the different NISQ devices multiple times and compared the results to the state-of-art methods. Our experimental results give comparable results to the state-of-the-art methods and for some cases we were able to get the best-known results. This work therefore provides an important stepping stone to demonstrating practical Quantum Advantage. As the capabilities of NISQ devices increase, we are hopeful that similar methods can provide a path to adoption of quantum computers for a variety of business and scientific applications.

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