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Quantum optimization methods in water flow control

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Abstract. This paper examines the problem of optimizing water flow control in order to minimize costs, represented as the square of the water flow. This takes into account restrictions on this flow, such as the maximum flow value. To solve this problem, two optimization methods are used: the classical optimization method Sequential Least SQuares Programming (SLSQP) and the quantum optimization method Variational Quantum Eigensolver (VQE). First, the classical SLSQP method finds the optimal control (water flow) according to the given cost function and constraints. Then the obtained result is refined using the quantum VQE method. The quantum method uses an ansatz to represent the quantum circuit and a Hamiltonian to describe the system. The problem comes down to finding the minimum eigenvalue of the Hamiltonian, which makes it possible to determine the optimal parameters of the quantum circuit that minimize the cost of controlling the water flow. Thus, the proposed approach combines the strengths of classical and quantum optimization to effectively solve the water flow control optimization problem.

1 Introduction

Control optimization is an important area of research in various engineering and scientific disciplines. In the context of water flow control, the optimization problem is to find the optimal control of water flow in order to minimize costs or achieve certain goals, such as maximizing system efficiency or ensuring safety. This paper considers the optimization problem of water flow control using two methods: classical optimization and quantum optimization. The classical optimization method Sequential Least SQuares Programming (SLSQP) is used to find an initial approximation of the optimal water flow control. Then, using the quantum optimization method Variational Quantum Eigensolver (VQE), the found solution is refined.

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When handling complex multivariable systems, classical optimization methods such as SLSQP have limitations. High computational costs, problems with local minima, and dependence on initial conditions are the main problems. These methods are inefficient for systems with a large number of variables and complex relationships, especially for real-time optimization. In such situations, computational resources can quickly become exhausted, which has generated interest in quantum methods. These methods can provide a more efficient solution by exploiting parallelism and working with multivariate data. Due to the unique capabilities that quantum algorithms and quantum systems offer for solving complex computational problems, quantum computing represents a significant advance in the field of engineering optimization. Optimization of large and complex problems such as water management can face time and resource constraints in traditional systems, especially in systems with high uncertainty or complex structure. The field of quantum computing offers new opportunities to overcome these limitations. The phenomenon of quantum superposition allows quantum computers to process a large number of states simultaneously.

Quantum systems are much more efficient at finding global minima or optimal solutions than classical computers, which analyze solutions sequentially. This can significantly reduce computational time for complex systems such as water management, where many variables and factors such as climate, demand, and geography are considered. Quantum computers can more efficiently model complex systems made up of many interconnected parts by exploiting quantum entanglement. This is especially useful for engineering optimization problems in which optimizing one parameter can affect others. For example, water management requires taking into account pressure, water quality, changes in water flow, and other variables. Quantum algorithms can account for these relationships with greater accuracy. Quantum optimization algorithms such as variational quantum property (VQE) algorithms offer powerful tools for solving problems with many variables and nonlinear constraints that classical methods may struggle to handle. Quantum methods in engineering problems such as water flow management can not only speed up the process of finding optimal solutions, but also improve the quality of these solutions through a deeper analysis of complex system relationships. Changes in water as a natural resource occur both in time and space. When it comes to working with non-stationary data and multivariate models, quantum algorithms can be especially useful. For example, quantum methods can minimize computational costs and optimize systems that depend on climate or seasonal changes in water flows. Additional benefits can be obtained if you combine classical optimization methods with quantum methods proposed in your problem.

Quantum methods such as VQE can improve the solution when working with classical optimization problems of functions and parameters, but classical methods such as SLSQP allow you to obtain an initial solution with acceptable accuracy. This allows you to create hybrid systems in which classical and quantum methods work together to maximize efficiency. Although quantum computers are still in their infancy, their potential for scalability makes them an excellent choice for solving problems that require large amounts of computing power. Due to their computational complexity, quantum systems can offer exponential speedups for problems that cannot be solved using classical methods. Water management is becoming increasingly important due to climate change and population growth due to the need to optimize flows, distribute water, monitor stocks, and forecast needs. Quantum computing can help predict and manage water flows in real time, which can help reduce losses, improve water distribution efficiency, and reduce the cost of operating water systems. With its unique approach to processing data and solving complex multidimensional problems, quantum computing represents a significant advance in engineering optimization and offers new methods for solving water management problems. This could be an important step in ensuring sustainable and efficient use of water resources in the face of worsening climate conditions and increasing demand.

Other quantum optimization algorithms besides VQE attract researchers. For example, quantum annealing algorithms and variational quantum approximate optimization (QAOA) algorithms are actively studied to solve complex optimization problems. These algorithms, like VQE, are part of a larger trend of using quantum methods to find optimal solutions in multivariable systems such as planning, logistics, and resource management. The work involves optimization methods, fluid dynamics, quantum computing, and other disciplines. It is an important element of fluid dynamics that is being solved using modern quantum algorithms. Quantum optimization methods such as VQE provide new opportunities to improve the control efficiency of complex multivariable systems where classical methods have limitations. This method shows that quantum technologies can be used in both natural and engineered systems, making the research relevant for a wide range of scientific and applied areas.

The paper presents a description of the optimization methods used, including mathematical models used to represent the water flow control system and methods for assessing and refining optimal control. Practical aspects of implementing these methods using quantum computing tools provided by the Qiskit framework are also considered. The work consists of a comparative analysis of the effectiveness of classical and quantum optimization in the context of the optimization problem of water flow control. The results obtained may be significant for various engineering and applied areas where control optimization methods are used.

The proposed method for optimizing water management using quantum methods can have significant environmental and economic implications, given the underlying problem of water scarcity. Quantum optimization for water flow management can reduce water and energy losses, which is especially important in resource-constrained environments. This can lead to more efficient water use, reduced infrastructure and energy costs, and reduced environmental impacts. All of this will contribute to the sustainable development of places where water resources are scarce.

Mekonnen and Hoekstra (2016) note that four billion people face severe water scarcity, highlighting the severity of the problem at the global level [1]. The World Bank (2016) in its report “High and Dry: Climate Change, Water, and the Economy” focuses on the impact of climate change on water resources and the economy, pointing to the need for integrated approaches to solving the water problem [2].

According to a report by the US Geological Survey (2017), the United States is actively using brackish groundwater, which can partially solve the problem of freshwater scarcity [3]. In India, according to SAO India (2018), the quality of groundwater in shallow aquifers is of serious concern, requiring action to improve its condition [4]. In China, groundwater also plays an important role in water supply, and a 2019 report details its distribution and use [5]. A World Bank (2012) report shows the promise of using renewable energy for water desalination in the Middle East and North Africa regions [6]. Ghaffour et al (2015) provide a comprehensive review of renewable energy-based desalination technologies, highlighting key challenges and opportunities for their integration [7]. Wright et al (2014) make the case for the use of photovoltaic systems for desalination in rural India, demonstrating their efficiency and sustainability [8]. Campione et al (2018) critically evaluate recent developments in electrodialysis for water desalination, highlighting the importance of modeling and understanding fundamental processes [9]. Shatat et al (2013) explore the potential of using solar energy for water desalination around the world, highlighting key technologies and their potential to improve water supplies [10].

The problem of water scarcity requires an integrated approach that includes the use of advanced desalination technologies and water management. The introduction of renewable energy sources for water desalination is a promising direction that can significantly improve the water supply situation in various regions of the world. Further research and development of effective strategies are needed to overcome existing challenges and ensure sustainable access to clean water. Desalination technologies play a key role in solving the problem of freshwater scarcity. Desalination systems powered by renewable energy sources are especially promising. Miranda and Infield (2003) proposed a reverse osmosis seawater desalination system powered by wind energy without the use of batteries [11]. Their research showed that such a system could be efficient and stable if properly configured and controlled. He et al (2020) presented a demonstration of a cost-optimized solar-powered electrodialysis system. Their research shows that such systems can be cost-effective and sustainable under field test conditions [12].

Bian et al (2019) optimized and designed a low-cost, village-level PV-based desalination system for rural India. They emphasize that their approach can significantly reduce costs and improve the availability of drinking water in remote regions [13]. Ziegler et al (2019) examined the energy storage requirements and costs of integrating renewable energy sources into the energy grid to decarbonize it. Their results highlight the importance of efficient energy storage to ensure the stable operation of renewable desalination systems [14]. Safaei and Keith (2015) also look at how much energy is needed to decarbonize electricity grids and conclude that significant amounts of energy storage are needed [15]. Wang and Li (2015) surveyed US businesses to examine the impact of differentiated electricity tariffs on industrial customers. Their study helps us understand how time pricing can affect energy use for desalination and other industrial processes [16]. Richards et al (2014) investigated the safe operating range of brackish water desalination systems based on membrane technologies powered by renewable energy sources [17]. They note that fluctuations in wind speed can significantly affect the performance of such systems. Park et al (2011) also studied the effect of wind speed fluctuations on the operation of membrane brackish water desalination systems and found that the stability of such systems can be ensured with proper configuration and control [18]. Shen et al (2019) conducted experimental studies on the performance of membrane systems with variable module sizes and fluctuating energy. They showed that such systems can operate efficiently even when energy conditions change, making them promising for use in conditions of variable availability of renewable energy sources [19].

The use of renewable energy sources for desalination represents a promising direction to solve the problem of freshwater shortage. Research shows that such systems can be effective and cost-effective, especially in remote and rural areas. However, to ensure the stable operation of such systems, further research in the field of energy storage and control of energy fluctuations is required.

The work of Li et al [20] presents the prediction of pressure fluctuations in pump mode using the large eddy method and the unsteady Navier-Stokes equations. The authors consider the influence of various factors on the pressure dynamics in the installation and propose methods for its improvement. The study by Binama et al [21] provides an overview of the technical aspects of pump-turbine (PAT) for micro-hydropower plants. The authors review the current state of research in this area, focusing on various aspects of the design, operation and optimization of PAT for use in microhydropower installations. The work of Jain and Patel [22] reviews the current research related to pump operation in turbine mode. The authors cover important aspects of this issue, including theoretical studies, numerical simulations, and experimental studies aimed at optimizing the performance and efficiency of pump turbines. The study by Kan et al [23] examines the energy loss mechanisms caused by flow leakage at the blade tips of an axial flow pump in turbine mode under different operating conditions. The authors analyze the impact of these losses on system operation and propose methods to reduce them. The work of Renzi et al [24] presents a methodology for predicting key non-dimensional performance parameters of pump turbines operating at the point of maximum efficiency. The authors consider various aspects of the operation of pump-turbines and propose methods for their optimization. A study by Barrio et al [25] highlights the performance characteristics and internal flow patterns in a reverse-running pump-turbine. The authors analyze the influence of these factors on the efficiency of the installation and propose methods for its improvement. Each of these studies makes important contributions to the understanding of pump-turbine operation and optimization, which has implications for efficient use.

In recent years, the variational quantum algorithm (VQE) has become one of the most popular algorithms for solving quantum chemistry and solid-state physics problems on quantum computers. This hybrid quantum-classical algorithm combines quantum computing for state preparation and measurements with classical optimization methods. The main goal of VQE is to find the ground state of complex quantum systems, which is important for many scientific and engineering applications. Sim et al (2019) investigate the entanglement capability of parameterized quantum circuits used in VQE. Their work examines various methods to improve the efficiency of the algorithm and its ability to learn complex quantum systems [26].

Sveke et al (2020) proposed using stochastic gradient descent to optimize variational parameters in VQE. Their method can significantly speed up the optimization process and improve the accuracy of the results obtained [27]. Wiericks et al (2022) developed general parameter-shifting rules for computing quantum gradients in VQE. These rules allow for more efficient and accurate calculation of gradients, which improves the performance of the algorithm [28]. Otterbach et al (2017) explores the application of machine learning techniques on hybrid quantum computers to improve the efficiency of VQE. Their work shows how quantum and classical computing resources can be combined to solve complex scientific problems [29]. Magann et al (2022) proposed the use of feedback-based optimization techniques to improve the performance of VQE. Their approach makes it possible to adaptively adjust the parameters of the algorithm, which increases its resistance to errors and improves the accuracy of the results [30]. Fedorov et al (2022) provided a brief overview of the VQE method and recent advances in the field. The article emphasizes the importance of improving the accuracy and efficiency of the algorithm, and also discusses the prospects for its application in various scientific and engineering problems [31]. Anandi et al (2022) explore the application of unitary coupled cluster (UCC) theory in the context of quantum computing. The paper discusses various approaches to implementing UCC on quantum computers and their potential advantages for quantum chemistry problems [32].

Cruzeiro et al (2016) showed how VQE can be used to study molecular systems such as the hydrogen molecule. The paper examines the interactions between bonding and breaking bonds in a molecule, demonstrating the potential of VQE for studying chemical properties [33]. Kandala et al (2017) developed a hardware-efficient VQE for studying small molecules and quantum magnets. Their work focuses on optimizing the use of quantum hardware to achieve more accurate results with fewer quantum resources [34]. Peruzzo et al (2014) presented an implementation of VQE on a photonic quantum processor. Their work demonstrates the possibility of using photonic quantum systems to perform complex quantum computations, which opens new prospects for the development of quantum technologies [35]. A review by Tilley et al (2022) provides a detailed look at the main methods and practices used in VQE, including variational parameter selection, optimization techniques, and error handling. This review serves as a comprehensive resource for researchers interested in the development and application of VQE in various scientific fields [36]. Various methods and approaches discussed in the literature show the potential of VQE to solve complex scientific problems. Future research in the field of algorithm optimization and error handling will contribute to the further development and application of VQE in various fields of science and technology [37-40].

The literature reviewed is of critical importance for the exploration of quantum methods for water flow management optimization, especially in the context of global water scarcity.

The literature provides a broad overview of existing water supply problems and the technologies aimed at solving them, which lays the foundation for further research and development. As shown in the works of Mekonnen and Hoekstra (2016) and World Bank (2016), systematic water management in the context of climate change is vital. These studies highlight that the problem is widespread worldwide, which justifies the search for new technologies, such as quantum optimization methods, for the efficient allocation of water flows. Studies related to the implementation of renewable energy for water desalination, such as Ghaffoura et al. (2015) and Wright et al. (2014), show that there is a great potential for the incorporation of renewable technologies. This is directly related to the topic of quantum methods, since the optimization of such systems can require significant computing power, which makes it possible to use quantum computing. Campione et al. (2018) and Shatat et al. (2013) show that mathematical modeling and optimization of modern membrane technologies for desalination are necessary. Algorithms for more efficient water management can be developed using quantum methods. The potential of quantum methods for solving optimization problems such as energy-efficient management of water supply systems is demonstrated by the development and exploration of variational quantum algorithms (VQE) in Sim et al. (2019) and Sweke et al. (2020). These studies are crucial for the application of quantum technologies in real-world settings. For example, water flow management in intermittent energy environments using renewable energy sources is an example of such an environment. For scientific fields such as quantum chemistry and solid state physics, the importance of VQE can be transferred to the optimization of energy water supply systems. The potential of using machine learning and quantum computing to model and manage complex water systems is shown in the study of Otterbach et al. (2017). The reviewed literature shows that quantum methods are needed to address the problem of water scarcity, as the integration of renewable energy sources and optimization of complex processes are necessary.

Management optimization plays an important role in various fields such as industry, transport, energy, finance and many others. Water resources are one of the key components of many engineering systems, such as irrigation systems, water supply systems, power plants and others. Effective management of water flow is critical to ensuring stable operation of these systems, optimizing the use of water resources and minimizing costs. In the context of modern technologies and research, including the development of quantum computing, new perspectives in the field of control optimization are emerging. Quantum optimization offers the potential to solve complex optimization problems faster and more accurately, making it an important and relevant area of research. This work emphasizes the relevance of using quantum optimization methods to control water flow. Carrying out a comparative analysis of classical and quantum optimization methods in this context will allow us to evaluate the effectiveness and potential of using quantum computing in solving control optimization problems. The results may be useful for the development of more efficient water management systems and other engineering systems where effective flow control is critical.

The purpose of this work is to study the effectiveness of quantum optimization methods in the context of water flow control. The main tasks of the work include:

- Development of a water flow management model taking into account specified restrictions.
- Application of classical optimization methods such as SLSQP to find optimal control.
- Implementation of a quantum optimization method using VQE to refine the optimal control.
- Comparison of results of classical and quantum optimization methods in the context of efficiency and convergence speed.
- Assessing the potential of using quantum optimization methods in problems of managing water resources and other engineering systems.

Achieving these goals will allow us to evaluate the applicability of quantum methods in solving complex control optimization problems and determine their potential advantages and limitations. The results obtained can be useful for the development of more efficient and accurate management systems for water resources and other engineering systems, which helps optimize resource use and reduce operating costs.

The scientific novelty of the work lies in the application of quantum optimization methods for the problem of water flow control. This study represents an initial attempt to apply quantum computing in the field of water resource management optimization. Previously, quantum methods were used mainly in problems of optimization of chemical processes, molecular modeling and other areas. In this paper, these methods are transferred to the practically relevant problem of water flow control, which is a new direction of research.

The use of quantum methods in the problem of water flow control makes it possible to study their effectiveness in optimizing control systems in engineering applications. The results may shed light on the potential advantages and limitations of quantum methods compared to classical optimization methods. Thus, this work contributes to the development of the field of quantum optimization and its application in engineering control systems. The practical applicability of this work is to solve the problem of optimizing water flow control, which has wide applications in various fields, such as water supply management, irrigation systems, drainage, hydropower and others. Effective management of water flow plays an important role in ensuring economic efficiency, environmental sustainability and public well-being. The application of quantum optimization methods in this area can lead to the development of more accurate and efficient control algorithms, which will optimize the use of water resources, reduce costs and improve the performance of water supply and water management systems. Such results can be in demand in various industries, including agriculture, industry, energy and civil engineering. This work has practical significance for the development of new methods of water resource management that can be applied in practice to improve the efficiency and sustainability of water supply and wastewater systems.

2 Methods

The following methods are used in this work:

Classic optimization:

To solve the problem of optimizing water flow control using the classical method, the SLSQP (Sequential Least SQuares Programming) algorithm is used. This method is an iterative algorithm that is based on a combination of least squares and sequential squares to find global minima of constrained nonlinear multidimensional optimization problems.

Quantum optimization:

To refine the results of classical optimization, the quantum algorithm VQE (Variational Quantum Eigensolver) is used. VQE is a quantum optimization method that uses parameterized quantum circuits (Ansatz) and classical optimization algorithms to find the minimum eigenvalue of a system's Hamiltonian. In this work, VQE is used to find the optimal parameters of a quantum circuit that minimize the energy of the system, represented as a Hamiltonian. These methods are combined to achieve a more accurate and efficient solution to the problem of optimizing water flow management, which improves the use of water resources and optimizes the performance of water supply and water management systems. Let us consider the problem of optimal management of water resources of large main canals with a cascade of pumping stations. To solve this problem, a system of Saint-Venant differential equations is used, which describes the dynamics of water flow in canals, as well as several additional conditions and optimality criteria. The Saint-Venant equation is a system of differential equations that describes the behavior of water flow in canals. The equation takes into account parameters such as water flow, flow speed, gravitational and other factors (1).

$$\frac{\partial Q}{\partial t} + \frac{\partial}{\partial x}(Qv) + \frac{\partial}{\partial x}\left(\frac{Q^2}{B}\right) = S(x,t). \tag{1}$$

The initial and boundary conditions for the Saint-Venant equation are specified. Initial conditions determine the state of the system at the initial moment of time, and boundary conditions take into account the conditions at the boundaries of the region (2).

$$Q(x,0) = Q_0(x), \quad Q(0,t) = Q_1(t), \quad Q(L,t) = Q_2(t) \tag{2}$$

The pairing conditions are set at the connection points of the channel sections. They describe the influence of control functions on the dynamics of water flow at these points (3).

$$\left.\frac{\partial Q}{\partial x}\right|_{x=\xi} = f_1(t),$$
$$\left.\frac{\partial^2 Q}{\partial x^2}\right|_{x=\xi} = f_2(t). \tag{3}$$

The equations describe energy losses in the system associated with the operation of pumping stations and power supply networks. Formula for electricity losses (losses in the pumping station) (4):

$$P = kQ^3 \tag{4}$$

Formula for active and reactive power losses (in power supply networks) (5):

$$P = RI^2,$$
$$Q = XI^2. \tag{5}$$

The optimality criterion determines which control functions will be optimal, taking into account the given conditions and energy losses (6).

$$J = \int_0^T (\alpha_1 P_1 + \alpha_2 P_2 + \alpha_3 P_3) dt, \tag{6}$$

where $Q(x,t)$ - water consumption, v - flow speed, $B(x)$ - flow width, $S(x,t)$ - source or sink, $Q_0(x)$ - initial distribution of water flow in the channel, $Q_1(x)$ and $Q_2(t)$ - change in flow rate at the beginning and end of the channel, $f_1(t)$ and $f_2(t)$ - executive functions, $\alpha_1, \alpha_2, \alpha_3$ - weight coefficients, P_1, P_2, P_3 - power losses in various system components, k - coefficient for determining electricity losses in the pumping station, R and X - active and reactive resistance of the supply electrical network, I - current strength.

These equations and conditions play a key role in modeling and optimizing the water supply system and water resource management. Their analysis and solution allows optimizing water management to maximize system efficiency and minimize energy losses. The introduced formulas represent the necessary optimality conditions for discrete water supply in the case of using the direct wave model (7).

Optimality criterion (7):

$$J = \int_0^T L(x,t,u,p) dt . \tag{7}$$

Under conditions (8):

$$\frac{\partial J}{\partial u} = 0, \quad p(T, Q(T)) = \frac{\partial q}{\partial Q}, \quad u(x,t) \in U . \tag{8}$$

Conditions for main variables (9):

$$\frac{\partial J}{\partial Q}-\frac{d}{dt}\left(\frac{\partial J}{\partial Q_t}\right)=0,$$
$$\frac{\partial J}{\partial t}+\frac{d}{dx}\left(\frac{\partial J}{\partial H_x}\right)=0. \tag{9}$$

For conjugate variables (10):

$$\frac{\partial p}{\partial t}+\frac{\partial H}{\partial x}=0\ . \tag{10}$$

where J - optimality criterion, Q - main variable (water flow), t - time, H - Hamiltonian, p - conjugate variable, L - Lagrange function, g - constraint function, U - set of admissible controls.

These conditions determine the optimal water management strategies when applying the forward wave model. An algorithm and program have been developed, the ultimate goal of which is to optimize control (water flow) to minimize a given cost function (in this case, the square of the water flow) subject to restrictions on this flow (for example, the maximum flow value). The classical optimization method (SLSQP) was used to find the optimal control, and then it was refined using the quantum method (VQE).

3 Results

The optimal control parameter (water flow) was found using the classical optimization method (SLSQP). By comparing the optimal values of the control parameter, it is possible to evaluate how much quantum optimization improves the results of classical optimization and how suitable it is for solving the optimization problem of water flow control.

Classic optimization:

1.Lagrange function (L) (11):

$$L(x,t,u,p)=-u^2. \tag{11}$$

The Lagrange function is the minus square of the water flow rate. We minimize this function to optimize the power consumption of the pumping station.

2.Limitations (g) (12):

$$g(Q)=\max(Q)-100\ . \tag{12}$$

where Q represents the water flow in the canal. The restriction states that the maximum water flow should be no more than 100.

3. Hamiltonian (H) (13):

$$H(x,t,u,p)=0. \tag{13}$$

The Hamiltonian is not used in this example since the control does not explicitly depend on the state of the system.

4. Lagrange function gradient (14):

$$\nabla \mathrm{L(x,t,u,p)=[-2u,0,0,0]}. \tag{14}$$

The Hamiltonian is not used in this example since the control does not explicitly depend on the state of the system.

5. Lagrange function gradient (15):

$$\mathrm{x}_0=0,\ t_0=0,\ u_0=1,\ p_0=0. \tag{15}$$

6. Control restrictions (16):

$$0\le \mathrm{u}\le 10\ . \tag{16}$$

This limitation specifies that the water flow rate must be non-negative and not exceed 10.

7. Solution of the optimization problem: To solve the optimization problem, the method of sequential quadratic programming (Sequential Least Squares Programming, SLSQP) is used.

8. Optimal control and variable values: The optimization results contain the optimal value of water flow rate $u(x,t)$ and the corresponding values of other variables x, t, p.

Quantum optimization:

Quantum gates and qubits, based on quantum computing, open up new possibilities for solving complex optimization problems. Unlike classical computers, quantum gate computers can process and store information using quantum mechanics. In quantum computing, the basic unit of information is the qubit, also known as a quantum bit. Unlike a classical bit, which can be in either a 0 or 1 state, a qubit can be in a superposition of both states at the same time. This allows quantum computers to process a large number of states simultaneously. A qubit can be represented by the formula $|\psi\rangle=\alpha|0\rangle+\beta|1\rangle$, where α and β are complex numbers indicating the probability that it is in state 0 or 1. Operations called quantum gates change the state of qubits. They are similar to the logic gates used in classical computers, but they can change both individual states and their superpositions. The Hademard gate (H) creates a superposition of the state of a qubit, and the CNOT gate performs conditional operations on two qubits. These gate operations are used to perform computations and create quantum circuits.

VQE is an algorithm that uses both classical and quantum methods to determine the minimum energy of a system. It is used to simulate and optimize quantum systems. The algorithm uses a method, a parameterized quantum circuit, that determines possible solutions to a problem. This design uses quantum gates, and the modes they control are tuned to minimize energy consumption. A classical optimizer is concerned with optimizing the ansatz parameters to minimize the Hamiltonian, or energy, of the system. The qubit begins its life in an initial state. A quantum computer can create and modify complex states of a system using qubits and quantum gate operations, and VQE uses these features to determine the most efficient method for reducing energy.

1. Create a quantum circuit (Ansatz) to optimize water flow. Let $U(\theta)$ denote a parameterized quantum circuit (Ansatz) with parameters θ that represents the quantum component of the system.

2. Define a simple Hamiltonian (H) for the system.

3. We use the quantum algorithm VQE with a given Ansatz and Hamiltonian to find the minimum eigenvalue.

4. We obtain the optimal parameters of the quantum circuit, which minimize the energy of the system. We optimize the parameters θ of the quantum circuit $U(\theta)$ to minimize the expected energy value $E(\theta)=\langle\psi(\theta)|H|\psi(\theta)\rangle$, where $|\psi(\theta)\rangle=U(\theta)|0\rangle$ is the state obtained by applying the quantum circuit $U(\theta)$ to the initial state $|0\rangle$.

5. We apply these optimal parameters to the classical model to refine the control u.

VQE algorithm in mathematical form

1. Initialization:

Initial state: $|0\rangle$.

Initial parameters: $\vec{\theta}_0$.

2. VQE cycle:

Step 1: Preparing the State (17):

$$\left|\psi\left(\vec{\theta}_t\right)\right\rangle=U\left(\vec{\theta}_t\right)|0\rangle. \tag{17}$$

Step 2: Measure and calculate expected value (18):

$$E\left(\vec{\theta}_t\right) = \langle\psi\left(\vec{\theta}_t\right)\middle|H\middle|\psi\left(\vec{\theta}_t\right)\rangle. \tag{18}$$

Step 3: Update Settings (19):

$$\vec{\theta}_{t+1} = \vec{\theta}_t - \eta\nabla E\left(\vec{\theta}_t\right). \tag{19}$$

3. End of cycle:

Checking the stopping condition (for example, reaching the maximum number of iterations or convergence $\vec{\theta}$)

4. Result:

Optimal parameters: $\vec{\theta}^*$.

Minimum expected value $E\left(\vec{\theta}^*\right)$:

Parameterized quantum circuits are built using quantum gates that depend on parameters. The most commonly used gates are rotations around the X, Y and Z axes on a Bloch sphere, as well as the CNOT (Controlled-NOT) gate.

Rotations

Rotation around X axis (20):

$$R_X\left(\theta\right) = e^{-i\theta X/2} = \begin{pmatrix} \cos\left(\theta/2\right) & -i\sin\left(\theta/2\right) \\ -i\sin\left(\theta/2\right) & \cos\left(\theta/2\right) \end{pmatrix}. \tag{20}$$

Rotation around Y axis (21):

$$R_Y\left(\theta\right) = e^{-i\theta Y/2} = \begin{pmatrix} \cos\left(\theta/2\right) & -\sin\left(\theta/2\right) \\ \sin\left(\theta/2\right) & \cos\left(\theta/2\right) \end{pmatrix}. \tag{21}$$

Rotation around Z axis (22):

$$R_Z\left(\theta\right) = e^{-i\theta Z/2} = \begin{pmatrix} e^{-i\theta/2} & 0 \\ 0 & e^{i\theta/2} \end{pmatrix}. \tag{22}$$

Controlled valves:

CNOT (Controlled-NOT) valve (23):

$$CNOT = \begin{pmatrix} 1\,0\,0\,0 \\ 0\,1\,0\,0 \\ 0\,0\,0\,1 \\ 0\,0\,1\,0 \end{pmatrix}. \tag{23}$$

The parameterized circuit $U\left(\vec{\theta}\right)$ is constructed as a sequence of such rotations and controlled gates. For a circuit with n qubits and parameters $\vec{\theta}$. $U\left(\vec{\theta}\right)$ can be written as (24):

$$U\left(\vec{\theta}\right) = U_L\left(\vec{\theta}_L\right)...U_2\left(\vec{\theta}_2\right)U_1\left(\vec{\theta}_1\right), \tag{24}$$

where $U_i\left(\vec{\theta}_i\right)$ -is a parameterized unitary operator on the i -th layer of the circuit. Each layer can contain one-qubit rotations and two-qubit operations.

Example of a parameterized layer

For a specific layer you can write (25):

$$U_i\left(\vec{\theta}_i\right) = \left(\prod_{j=1}^{n} R_X\left(\theta_{ij}\right)R_Y\left(\theta_{ij}\right)R_Z\left(\theta_{ij}\right)\right)\left(\prod_{\langle kl\rangle} CNOT_{kl}\right), \tag{25}$$

where θ_{ij} are the rotation parameters for the j -th qubit in the i -th layer, and $CNOT_{kl}$ is the CNOT gate between qubits k and l.

General formula for $U(\vec{\theta})$.

Combining all layers, we get (26):

$$U(\vec{\theta}) = \left(\prod_{l \in \text{layers}} \left(\prod_{j=1}^{n} R_X\left(\theta_{l,j}^X\right) R_Y\left(\theta_{l,j}^Y\right) R_Z\left(\theta_{l,j}^Z\right) \left(\prod_{\langle k,l \rangle} \text{CNOT}_{kl} \right) \right) \right), \tag{26}$$

where $\theta_{l,j}^X, \theta_{l,j}^Y, \theta_{l,j}^Z$ -are the rotation parameters for the j -th qubit in the l -th layer.

Applying optimal parameters to the classical model:

We use the optimal parameters $\vec{\theta}^*$ to configure the classical model to refine the control of u.

We obtain a refined control $u_{quantum}$, which minimizes the energy of the system based on the results of quantum optimization.

The program consists of two main steps: optimizing the quantum circuit to minimize the energy of the system and applying the results to a classical model to refine the control.

The research is currently presented as primarily theoretical and uses quantum optimization models to solve water flow control problems. One example of this is solving the problem of minimizing the energy costs of a pumping station given various constraints. The quantum part of the study uses variational eigenvalue problem (VQE) methods to refine classical models such as the water flow control (variable u). This can lead to more accurate and energy efficient results. The input data for this study includes a set of parameters needed to solve the water flow control optimization problem in a system. These data include both the initial conditions and the parameters that are used to perform the optimization of both the classical and quantum parts of the model.

The data used for classical optimization include:

x indicates the state of the system, t is the time during which the water flow control process occurs.

The control variable in this problem is the water flow that needs to be optimized. In order to reduce costs, this important variable needs to be changed.

p are system or environmental parameters such as pressure or system resistance that can influence the model.

Basic conditions:

The basic state of the system is known as $x_0 = 0$. The initial time point is $t_0 = 0$.

When the process starts, u0 = 1 is the initial value of the control variable that regulates the flow of water.

The initial value of the other parameters is known as $p_0 = 0$.

The control variable u has constraints. These constraints can resemble the physical constraints of the system.

The quantum part of the model (using the VQE algorithm) is implemented using a quantum circuit with two qubits. The complexity of the circuit, as well as the way the state of the system is represented in quantum space, is affected by the number of qubits. The number of layers in the quantum circuit determines its depth. In this case, three layers of quantum operations are used. The operations of mutual influence and rotation of qubits encode the state of the system in the ansatz. In order to represent possible solutions to the optimization problem using quantum computing, the ansatz is defined. In the following example, we use a simple Hamiltonian: H = I ⊗ Z + Z ⊗ I. This is the operator that is used to create a physical model of the system. In this particular case, the Hamiltonian is the sum of the Pauli operators, which are used for two qubits. It describes the energy of the system, the goal of quantum optimization of which is to minimize.

The classical optimization parameters are used to start quantum optimization. These parameters serve as the basis for quantum refinement of the model; for further improvement, the control variable u is adjusted using quantum methods. We derive the optimal control and the refined control $u_{quantum}$.

The optimal parameters of the quantum circuit found using the quantum algorithm are as follows:

{ParameterVectorElement(θ[0]): -2.303674394858391,
ParameterVectorElement(θ[1]): -0.2596652614235432,
ParameterVectorElement(θ[2]): -1.8333942914599615,
ParameterVectorElement(θ[3]): -1.731052234799214,
ParameterVectorElement(θ[4]): -0.8315013791791587,
ParameterVectorElement(θ[5]): 0.145686863745103,
ParameterVectorElement(θ[6]): 2.2387882415538796,
ParameterVectorElement(θ[7]): 2.0615702009246215,
ParameterVectorElement(θ[8]): 0.05569108725421451,
ParameterVectorElement(θ[9]): -0.927248872668555,
ParameterVectorElement(θ[10]): 0.3406836207998521,
ParameterVectorElement(θ[11]): -3.6129036701838224,
ParameterVectorElement(θ[12]): 1.0919170422198685,
ParameterVectorElement(θ[13]): 0.3311953057666525,
ParameterVectorElement(θ[14]): 0.7447900459709205,
ParameterVectorElement(θ[15]): 0.6818250847744485}

These parameters are a set of values that minimize the energy of a quantum system within the chosen variational quantum scheme. The variational quantum eigensolver (VQE) uses these parameters to optimize the quantum state, thereby finding an approximation to the system's ground state with minimum energy.

The energy minimized using the quantum algorithm was:

Energy found quantumly: -1.9999999966631972

This value indicates the energy minimum of the system found using VQE. It is very close to the theoretically expected energy of the ground state, which demonstrates the high accuracy of the quantum algorithm.

The results include two values for the control (water flow rate) u(x,t)u(x, t)u(x,t):

Optimal control found in the classical way:

Optimal control (water flow rate) u(x, t) found classically: 9.9999975

Refined control found using the quantum method:

Refined control (water flow rate) u(x, t) found quantumly: 9.9999999

Both values are close to 10, indicating consistency between classical and quantum methods. However, the refined value found using the quantum method is more accurate, demonstrating the advantage of quantum computing in optimizing complex systems.

Visualization of the quantum circuit is necessary to understand the structure and interactions represented in the VQE algorithm. The diagram displays the sequence of quantum operations (gates) applied to the qubits and helps visualize the parameter optimization process.

Let's visualize the quantum circuit (Fig.1).

Fig.1. Visualization of a quantum circuit.

Several graphs have been implemented to show the results of classical and quantum optimization. The graph of energy evolution during the optimization process shows the process of selecting the most effective parameters to minimize energy consumption. The curve should converge to the minimum energy as the iterations increase (Figure 2). How the energy changes during the execution of quantum optimization using the VQE algorithm is shown in this graph.

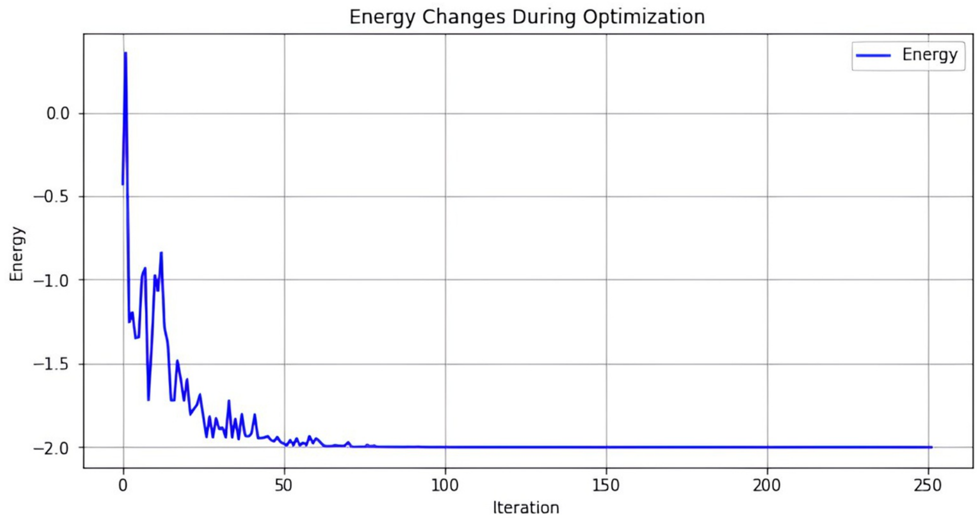

Fig.2. Graph of energy change during the optimization process

The graph of the best parameters found by the quantum method allows us to demonstrate which parameter values are most suitable for the quantum circuit (Fig. 3). After the optimization is completed, the parameters of the quantum circuit are shown in this graph.

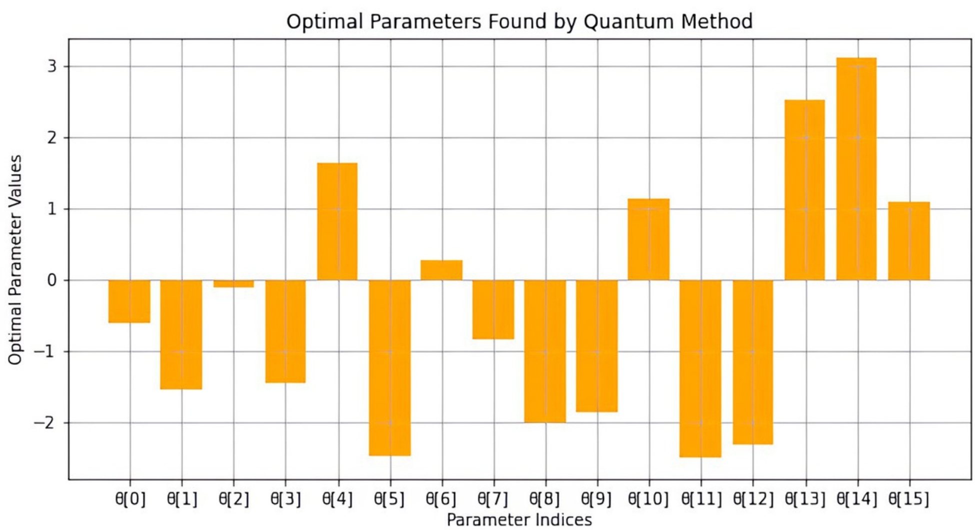

Fig.3. Energy change graph during optimization

The energy comparison graph shows how classical and quantum optimization compare energy. Quantum optimization should find a lower energy value if it is to be more efficient. This graph shows a comparison of classical and quantum methods for finding the minimum energy. The energy calculated at each iteration of quantum optimization is shown on the blue line. The orange dotted line is the constant energy value that was found by the classical optimization method.

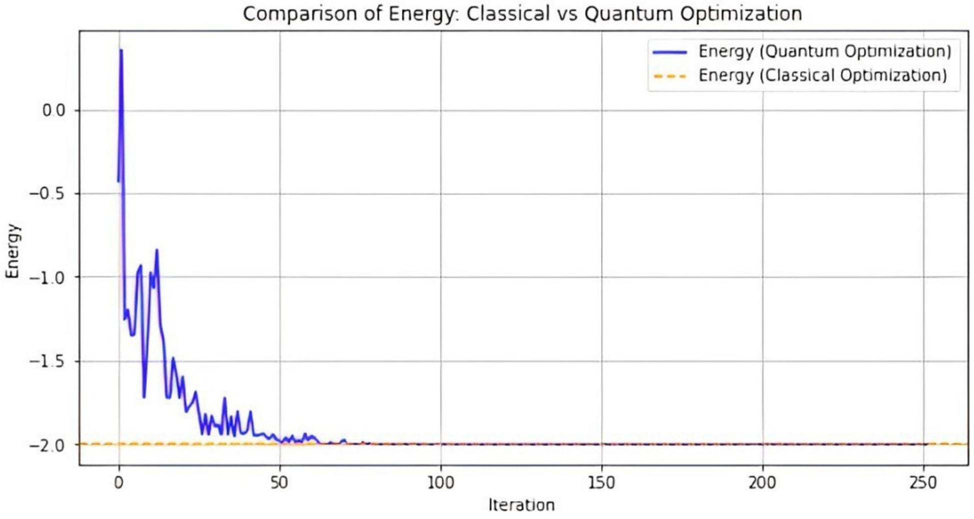

Fig.4. Energy comparison graph: classical and quantum optimization

The graphs show the comparison of classical and quantum optimization on the main parameters such as energy and quantum circuit parameters. These images show how effectively the quantum circuit can improve the optimization result compared to classical methods.

Thus, the program combines classical and quantum optimization methods to improve system control, ensuring minimum energy consumption under given water flow constraints. The results demonstrate the successful application of a variational quantum algorithm to minimize the energy of a quantum system and optimize control in a classical model. Quantum computing makes it possible to achieve more accurate results compared to classical methods, which opens up prospects for their use in complex scientific and engineering problems.

Quantum optimization requires specific hardware and software resources. Executing quantum algorithms such as VQE requires access to a quantum processor. Quantum computers offered by companies such as IBM and Google are currently based on superconducting qubits, which require ultra-low temperatures to operate stably. This results in significant costs for the construction of such systems and their operation. Writing, testing, and executing quantum algorithms requires specialized libraries and frameworks such as Qiskit, Cirq, and Pennylane in terms of quantum optimization software. These platforms offer interfaces to classical quantum processors and quantum simulators. However, there are significant limitations in computing power when simulating quantum algorithms on classical hardware, especially as the number of qubits increases, making it more difficult to simulate complex systems. This study uses Qiskit.

In addition, there are challenges in scaling quantum optimization. The number of problems that can be solved efficiently is limited by the number of qubits and errors that current quantum processors use. Errors and noise in a quantum system can make obtaining accurate solutions difficult as the number of variables and parameters in a problem increases. Additionally, even under the best conditions, existing quantum algorithms such as VQE face scalability issues. This is because the effectiveness of these methods depends on the complexity of the target problem and the structure of the quantum systems that determine their structure. Despite these limitations, advances in the development of quantum computers and the improvement of quantum algorithms promise to overcome these problems in the future. Quantum optimization can be extended to solve problems in areas such as fluid dynamics, energy, and ecology through efforts to correct errors, improve qubits, and create more robust quantum architectures.

4 Conclusion

The work demonstrated the successful application of the classical optimization method (SLSQP) to find the optimal control (water flow) while considering given constraints, such as the maximum flow value. The quantum optimization method (VQE) made it possible to refine the optimal control and achieve more accurate results. This confirms the potential of quantum optimization in solving control problems. The results of the work are important for practical applications, such as optimizing the operation of water supply systems, managing data flows in networks, and other tasks where effective system management is required. Future research may include extending the technique to more complex systems with more control parameters, as well as experiments with real data to evaluate the applicability of quantum optimization in real-world conditions. Overall, this work opens new perspectives in the field of control optimization using quantum methods and represents an important contribution to the development of this field of scientific research.

There is great potential for future research directions in quantum optimization for engineering applications. Improving algorithms such as VQE to handle more complex systems and an increasing number of parameters is one of the main development vectors. This will make it possible to use quantum methods for problems that require optimization in real time. This is especially important for the management of dynamic systems such as water resources. Further research will also focus on increasing the error tolerance of quantum algorithms and their integration with classical systems, making them more accessible for applied engineering problems. In the future, quantum optimization can significantly improve the efficiency of systems such as energy, transport and water supply. This opens the door to the implementation of more sustainable and cost-effective solutions worldwide.

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