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OPTIMIZING QUANTUM ALGORITHMS FOR SOLVING THE POISSON EQUATION

Abstract: Contemporary quantum computers open up novel possibilities for tackling intricate problems, encompassing quantum system modeling and solving partial differential equations (PDEs). This paper explores the optimization of quantum algorithms aimed at resolving PDEs, presenting a significant challenge within the realm of computational science. The work delves into the application of the Variational Quantum Eigensolver (VQE) for addressing equations such as Poisson's equation. It employs a Hamiltonian constructed using a modified Feynman-Kitaev formalism for a VQE, which represents a quantum system and encapsulates information pertaining to the classical system. By optimizing the parameters of the quantum circuit that implements this Hamiltonian, it becomes feasible to achieve minimization, which corresponds to the solution of the original classical system. The modification optimizes quantum circuits by minimizing the cost function associated with the VQE. The efficacy of this approach is demonstrated through the illustrative example of solving the Poisson equation. The prospects for its application to the integration of more generalized PDEs are discussed in detail. This study provides an in-depth analysis of the potential advantages of quantum algorithms in the domain of numerical solutions for the Poisson equation and emphasizes the significance of continued research in this direction. By leveraging quantum computing capabilities, the development of more efficient methodologies for solving these equations is possible, which could significantly transform current computational practices. The findings of this work underscore not only the practical advantages but also the transformative potential of quantum computing in addressing complex PDEs. Moreover, the results obtained highlight the critical need for ongoing research to refine these techniques and extend their applicability to a broader class of PDEs, ultimately paving the way for advancements in various scientific and engineering domains.

Keywords: partial differential equation, poisson equation, quantum computing, variational quantum eigensolver, optimization

Introduction

In recent years, the field of quantum computing has garnered significant attention due to its potential for solving complex computational problems more efficiently than classical computers. One area of particular interest is the application of quantum algorithms to solve partial differential equations (PDEs), which have widespread applications in various domains, including structural mechanics [1]. PDEs are ubiquitous in modeling physical phenomena and are essential tools in understanding and predicting the behavior of systems governed by these equations. However, as [1] highlights, the computational complexity of solving PDEs increases exponentially with the dimensionality and resolution of the problem, making it challenging for classical computers to tackle large-scale or high-precision PDE problems.

This paper makes a significant contribution by focusing on the optimization of the Variational Quantum Eigensolver (VQE) for solving the Poisson equation. The motivation for this research arises from the limitations of classical computational methods in handling the complexity of high-dimensional PDE problems. By leveraging quantum computing, we aim to develop more efficient methodologies for solving these equations.

Early efforts in quantum algorithms for PDEs focused on the Harrow-Hassidim-Lloyd (HHL) algorithm [2], which demonstrated successful applications to the Poisson equation using central difference approximations and simulations. Concurrently, researchers explored alternative quantum algorithms tailored for the Poisson equation, employing techniques like the Plouffe binary expansion method [3] and demonstrating their efficiency on quantum virtual computing platforms.

More recently, Variational Quantum Algorithms (VQAs) have emerged as a promising avenue for tackling PDEs on near-term quantum devices. These algorithms optimize parameterized quantum circuits to approximate solutions, effectively mitigating the limitations imposed by finite qubit counts and noise inherent in current quantum hardware [4, 5]. Given the wide-ranging potential of variational quantum algorithms in PDE resolution, their utilization for addressing the specific challenge of solving the Poisson equation warrants special consideration. The Poisson equation, extensively employed across physics and engineering domains, serves as a significant benchmark for showcasing the capabilities of quantum computing.

An initial quantum algorithm for the approximate solution of Poisson's equation was introduced in [6], demonstrating exponential speedup over classical algorithms while overcoming the "curse of dimensionality". In [7], a variant of VQA was introduced, featuring a novel decomposition approach wherein the data matrix is expressed as a sum of tensor products of simple operators. This method achieved an accuracy level of 0.99%, validated through numerical methods. In [8], an optimized VQA was presented for solving the Poisson equation, which required a small number of quantum measurements, regardless of the problem size, by defining the total potential energy as an expectation of observables decomposed into a linear combination of Pauli operators. In [9], an approach that used CRZ rotations to reduce the number of required qubits and gates was used, demonstrating low error rates and faster solution times compared to classical methods. In [10], to optimize VQA, a method was used involving the decomposition of the coefficient matrix A into a minimal number of Hermitian, one-sparse, and self-inverse operators, which significantly reduces the number of measurements and circuit complexity.

In the realm of exploring challenges related to solving PDEs, notably the Poisson equation, on quantum computers, a thorough comprehension of the limitations and hurdles faced by VQA is paramount. In [11], an extensive examination of VQA's performance in the context of Poisson equation resolution is conducted, shedding light on crucial aspects that constrain the current capabilities of quantum computing. Noteworthy findings include error detection even in noise-free quantum computing environments, trade-offs in estimating expected values, and

the considerable expense associated with gradient estimation, which significantly impacts solution accuracy and efficiency. These challenges underscore the imperative to optimize variational quantum algorithms to enhance their performance and achieve improved convergence in PDE resolution. Optimization of VQA entails devising novel strategies for error reduction, enhancing methods for expected value and gradient estimation, and exploring more efficient approaches for selecting and fine-tuning algorithm parameters.

In [12], an analysis of key methods for optimizing VQE was made in the context of comparing their effectiveness. Diverse optimization strategies have been proposed for enhancing VQA performance. In [13], a novel method for executing the sine transform was developed, optimizing the algorithm by reducing circuit depth from n^2 to n. Quantum gate threshold errors were determined to ensure circuit output accuracy above 90%. Additionally, in [14], quantum parametric circuit parameter optimization using Estimation Distribution Algorithms (EDA) within VQA was explored. Results revealed statistically significant enhancements in minimizing the cost function compared to conventional optimizers, particularly with a low number of layers. Furthermore, in [15], the impact of error reduction strategies on VQA was examined. VAQEM presents a dynamically adaptable approach to error mitigation within VQA, tailored for real-world quantum machines with noise. VAQEM showcased notable accuracy improvements in various applications on IBM quantum machines.

Regarding VQE, optimization strategies for enhancing its performance can be categorized based on specific stages of the algorithm, including initialization, parameter configuration, measurement, and others. In [16], the focus is on VQE initialization. Authors introduce a method named Variational Tensor Network Eigensolver (VTNE), which optimizes VQE initialization through classical simulation of quantum circuits using tensor networks, particularly matrix product states (MPS) with bounded link sizes. This pre-optimization technique aims to address challenges like barren plateaus, optimization in noisy conditions, and slow convergence commonly encountered in Noisy Intermediate-Scale Quantum (NISQ) devices. In [17], a strategy known as Qubit Reduction via Z2 Symmetries was investigated to enhance qubit efficiency and convergence rates. This method capitalizes on a qubit reduction scheme that exploits Z2 symmetries of Hamiltonians, a concept previously introduced by Bravyi et al. The approach effectively minimizes the total number of qubits required, thereby reducing qubit manipulations prone to errors. In [18], a tailored VQE kernel was devised, integrating prior knowledge of quantum circuits. Specifically, it aligns the functions of the map kernel with the VQE constraint and introduces a novel data collection feature called Expected Maximum Improvement in Confident Regions (EMICoRe). This feature optimizes by targeting parameters in regions of interest, effectively learning these areas as periodic observations. Such a strategy enables accurate estimation of the objective function over extensive spatial extents, often with impressive accuracy — sometimes even with minimal data points. The methodology relies on physical principles to refine process optimization. Meanwhile, in [19], the impact of parameter configurations on optimization efficiency was scrutinized. Authors examined how different configurations influence the accuracy of analytically optimized single-qubit gates. They introduced a new metric called configuration cost or C-cost to quantify the disparity in optimization accuracy attributable to statistical errors in measurements. In contrast, [20] introduces a hybrid approach termed "Measurement Simplification", tested across various VQAs including VQE and VQLS. This method simplifies the evaluation of quantum circuits by reducing the complexity of expressions used, leading to significant reductions in computation time and memory requirements.

The application of the HHL algorithm to the Poisson equation problem has found that quantum schemes minimizing the cost function may face optimization difficulties. In this context, a method based on the Feynman-Kitaev formalism using the HHL algorithm and VQE

was proposed to obtain the complete evolution of the system after a single optimization of a well-defined cost function. The Feynman-Kitaev formalism was utilized to represent the Poisson equation as a quantum Hamiltonian, which was then solved using quantum algorithms such as the VQE.

Our approach employs a Hamiltonian constructed using a modified Feynman-Kitaev formalism, allowing the representation of classical systems in a quantum framework. This enables the optimization of quantum circuits by minimizing the VQE cost function, thus achieving the solution to the original classical system. The modifications introduced in our methodology enhance the performance and accuracy of quantum circuits, reducing computational resources required.

Effective optimization requires strategies that provide a sufficiently accurate solution in an acceptable number of iterations, which is necessary for the practical application of variational algorithms [21]. In this paper, the VQE is applied by adapting it to solve Poisson equations. The approach presented in this paper involves using the Feynman-Kitaev formalism to transform a classical system in the form of a quantum Hamiltonian using quantum operators and states [22]. This allows us to optimize quantum schemes in such a way as to minimize the cost function corresponding to a particular VQE. This paper aims to demonstrate that optimizing quantum algorithms can significantly improve the process of solving VQEs by reducing computational time and enhancing the accuracy of the results.

In summary, this research optimizes quantum algorithms for solving the Poisson equation, demonstrating the practical advantages and transformative potential of quantum computing in addressing complex PDEs. Our findings underscore the importance of continued research in this area, with the aim of applying these techniques to a broader class of PDEs.

Methods and Materials

The sequential workflow commences with the formulation of a PDE problem and the selection of a method to solve it. In this case, the one-dimensional form of the Poisson equation is considered. Subsequently, the Feynman-Kitaev formalism is employed to transform the classical system into a quantum system, thereby enabling the utilization of quantum algorithms for solving PDEs. The sequential operation diagram is illustrated in Fig. 1.
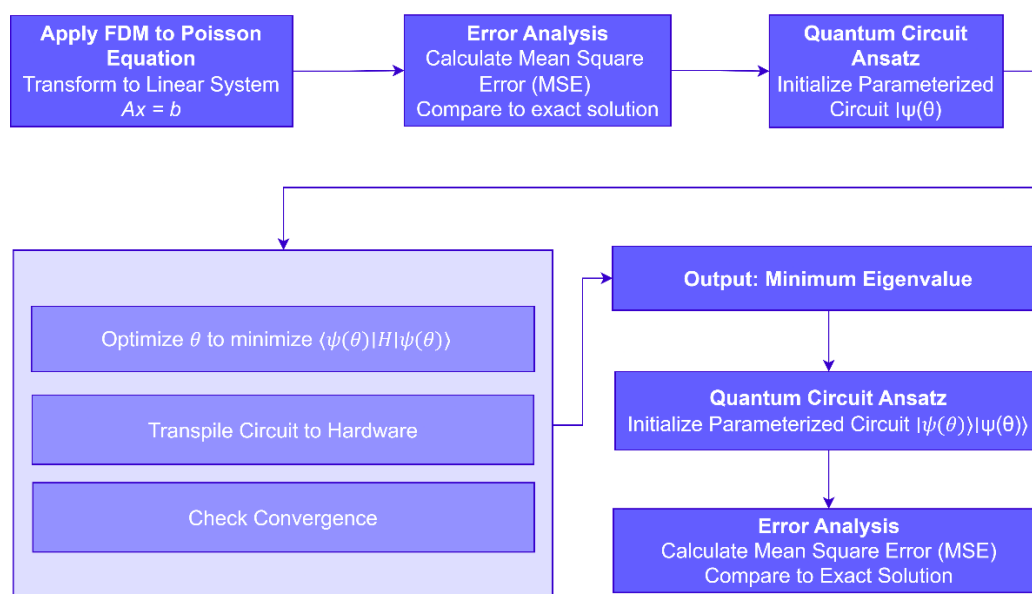

Figure 1. Sequential algorithm optimization scheme

Following this, VQE is adapted and applied to solve PDEs. This method involves the use of a parameterized quantum circuit ansatz, which is a series of quantum gates applied to the initial state of the qubits. The parameters of this quantum circuit are then optimized using the Adam optimizer to identify the minimum eigenvalue of the Hamiltonian, which corresponds to the solution of the PDE. The results obtained from the VQE algorithm are compared with the exact solution of the PDE, and experiments are also conducted on the "ibm_osaka" system from the IBM Quantum platform to evaluate the algorithm's performance in practical settings.

Equations and discretization
The Poisson PDE describes the potential distribution $\varphi(x)$ in a given region, governed by source terms $f(x)$ (1):

$$\tag{1}$$

where p is a function that determines the potential distribution in a given area. The function $f(x)$ represents the sources in this area.

For Dirichlet-type boundary conditions in the region $[a, b]$, where $u(a) - ua$ and $u(b) - ub$, the equation becomes (2):

$$\frac{\partial^2}{\partial x^2} u(x) = f(x), \text{with } u(a) = u_a, u(b) \tag{2}$$

To numerically solve this PDE using the finite difference method, the spatial domain is discretized into a mesh of m grid points with spacing $h - (b - a) / (m - 1)$. The differential operator is approximated by a finite difference operator (3):

$$\frac{\partial^2}{\partial x^2} u(x) \approx \frac{u_{i-1} - 2u_i + u_{i+1}}{h^2} \tag{3}$$

This discretization transforms the Poisson PDE into a system of linear algebraic equations:

$$Ax = b \tag{4}$$

where, A is the coefficient matrix representing the discretized differential operators, x is the vector of unknowns (solution), b is the right-hand side vector containing the boundary conditions and any source terms.

The matrix A arises from the discretization of the Poisson PDE using finite difference method. It encapsulates the coefficients resulting from the discretized differential operators within the computational domain. Solving the linear system $Ax - b$ allows for the determination of the solution vector x, representing the approximate solution to the Poisson equation.

$$A = \begin{bmatrix} -2 & 1 & 0 & \cdots & 0 & 0 & 0 \\ 1 & -2 & 1 & & 0 & 0 & 0 \\ & \vdots & & \ddots & & \vdots & \\ 0 & 0 & 0 & \cdots & 1 & -2 & 1 \\ 0 & 0 & 0 & & 0 & 1 & -2 \end{bmatrix} \tag{5}$$

The vector b complements the coefficient matrix A in (6) and encompasses the boundary conditions, as well as any source terms present in the Poisson equation. Together with the matrix A, vector b forms a system of linear equations representing the discretized Poisson equation. Solving this system yields the numerical solution to the Poisson equation within the specified computational domain.

$$b = \begin{bmatrix} h^2 f_1 - u_a \\ h^2 f \\ \vdots \\ h^2 f_{m-1} \\ h^2 f_m - u_b \end{bmatrix} \tag{6}$$

Quantum Method

Note that the quantum state is mapped onto an exponential grid size. Therefore, the number of quantum resources depends linearly on the number of qubits n, and the discretization error decreases exponentially $O(1/2^n)$. There are several ways to solve this linear system. For long-term applications, the HHL algorithm can be utilized for speedup. On IBM quantum computers, the VQE is considered.

The HHL algorithm is designed to solve systems of linear equations on a quantum computer with exponential acceleration compared to classical methods. It is based on the use of quantum Fourier transform and phase estimation to find solutions, making it particularly useful in quantum linear algebra problems. The VQE algorithm is a hybrid quantum-classical method that is used to find the ground state of a quantum system. VQE minimizes system energy by optimizing parameterized quantum circuits using classical optimization algorithms. The classical part of the algorithm is to iteratively optimize the parameters of the quantum circuit in order to minimize the expected energy value. After each iteration, the quantum computer makes measurements to estimate the current energy value, which is then passed to a classical optimizer. A classical optimizer, such as gradient descent or higher efficiency algorithms, updates the ansatz parameters and feeds them back to the quantum computer for the next round of measurements. This cycle is repeated until the minimum energy value is reached or until the process is stopped by other criteria.

Using VQE in combination with the Feynman-Kitaev formalism allows for efficient representation and evolution of quantum systems, providing a detailed picture of quantum states and their dynamics. The Feynman-Kitaev formalism models the quantum computing process as a sequence of computational steps, making it easier to analyze and improve the algorithm.

The Feynman-Kitaev formalism, also known as the Feynman-Kitaev model, is a conceptual approach to quantum computing that integrates the physical and computational aspects of quantum evolution. The basic idea is to consider the evolution of a quantum system as a sequence of logical operations similar to the steps of a classical computation, and to formalize this evolution as a quantum computational problem. In the Feynman-Kitaev formalism, a quantum algorithm is modeled using a special Hamiltonian that describes the dynamics of the system. This Hamiltonian takes into account both the computational steps of the algorithm and the state of the quantum registers at each moment in time. The evolution of the system is determined by a time parameter, which can be considered as discrete steps of the algorithm. This approach allows us to represent a quantum algorithm as a single quantum process, which simplifies the analysis of its correctness and complexity.

The essence of the formalism is that each state of a quantum system can be associated with a specific computation step. For example, if a quantum algorithm consists of a sequence of elementary operations (gates), then each intermediate state of the system will correspond to a certain set of operations performed. The Hamiltonian in this case models the transitions between these states, ensuring the correct execution of the algorithm. Integrating the HHL and VQE algorithms with the Feynman-Kitaev formalism provides a powerful tool for solving complex quantum mechanics and optimization problems, as the formalism allows for efficient

representation and analysis of quantum computing processes, facilitating the synthesis and improvement of algorithms.

To solve the Poisson equation using a quantum approach, we need to map the classical linear system $Ax - b$ into a Hamiltonian operator H that can be handled by a quantum computer. This mapping is achieved through the following steps:

$$H = A\dagger(I - |b\rangle\langle b|)A \tag{7}$$

where, $A\dagger$ represents the conjugate transpose (Hermitian adjoint) of the matrix A obtained from the finite difference discretization. I is the identity operator, and $|b\rangle$ is the vector b (the source term) encoded as a quantum state.

To understand how this Hamiltonian formulation works, we can substitute the solution $|x\rangle$ (the desired potential x as a quantum state) and observe:

$$H|x\rangle = A\dagger(I - |b\rangle\langle b|)A|x\rangle = A\dagger(I - |b\rangle\langle b|)|b\rangle = 0|x\rangle \tag{8}$$

This shows that the Hamiltonian H annihilates the solution state $|x\rangle$, meaning that $|x\rangle$ is an eigenstate of H with eigenvalue 0. Therefore, by finding the ground state (lowest energy eigenstate) of H, we can obtain the solution $|x\rangle$ to the original linear system $Ax = b$, which corresponds to the solution of the Poisson equation.

The solution is encoded in the ground state H with eigenvalue 0. Hamiltonian can be constructed by using Poisson equation and transforming it into the corresponding Hamiltonian. The VQE algorithm is then used to optimize the parameters of the quantum circuit to find the minimum eigenvalue of this Hamiltonian, which will be a solution to Poisson equation.

The COBYLA (Constrained Optimization by Linear Approximations) optimizer is chosen for this paper due to its suitability for NISQ devices. COBYLA is a derivative-free optimizer that performs well under conditions where gradient information is not reliable or available. Its robustness against noise and simplicity in implementation make it an attractive choice for optimizing quantum circuits on current quantum hardware platforms. Specifically, for solving the Poisson equation, COBYLA's ability to handle noise and its efficiency in finding the minimum eigenvalue of the Hamiltonian are crucial for achieving accurate results.

While the COBYLA optimizer is advantageous for its simplicity and robustness, it also has limitations. As a derivative-free method, COBYLA may require a large number of function evaluations to converge, which can be computationally expensive. Additionally, its performance can vary based on the problem's complexity and the quantum device's characteristics. For the Poisson equation, these factors are particularly important because the accuracy of the solution is highly dependent on the optimizer's efficiency.

Results

This section elaborates on the specific quantum computational techniques employed to address the Poisson equation, focusing on the configuration and optimization of a parameterized quantum circuit.

The quantum approach to solving the Poisson equation involves leveraging a parameterized ansatz, a sequence of quantum gates applied to the initial qubit state to efficiently tackle the associated linear system problem. For this study, the EfficientSU2 ansatz is adopted, comprising layers of single-qubit rotation gates and two-qubit CNOT gates. Single-qubit rotations manipulate qubit state amplitudes, while CNOT gates establish entanglement between qubits.

The ansatz's depth, governed by a depth parameter, determines how many times each layer repeats, enhancing the qubit state's complexity and solution capability. Fig. 2 illustrates the quantum circuit.
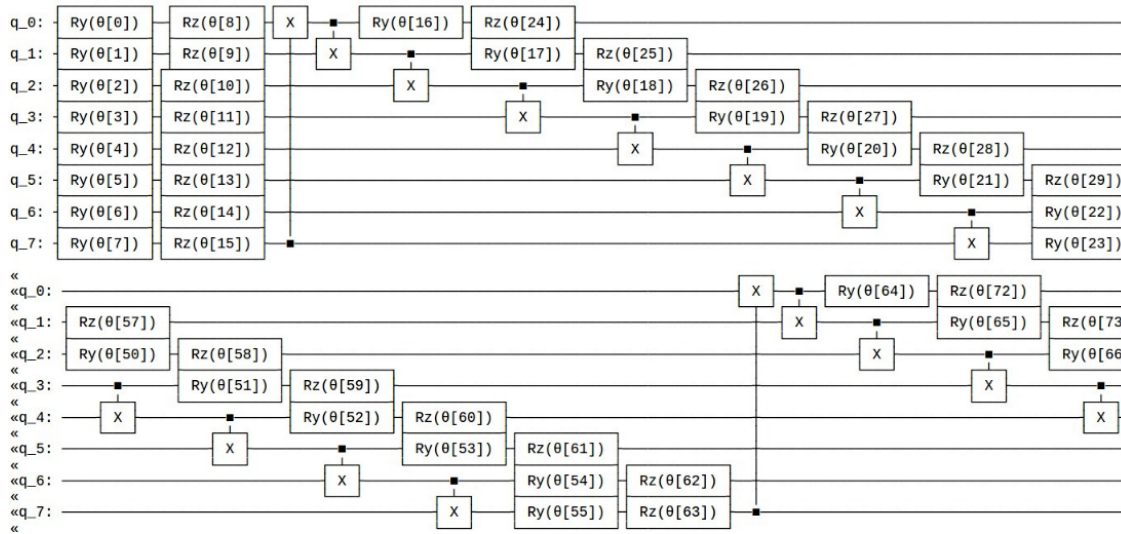
Figure 2. Quantum circuit for numerical solution of Poisson's equation

To optimize the ansatz, transpilation is employed. Transpilation involves rewriting the input circuit to match a specific quantum device's topology and/or optimizing it for performance in noisy quantum systems. In this study, transpilation with optimization level 3 is utilized, incorporating various techniques like gate reduction and operation order optimization to enhance the quantum circuit's performance.

Consequently, the quantum scheme employs single-qubit rotation and two-qubit CNOT gates to prepare the qubit state best suited for solving the classical linear system. The VQE object integrates parameters such as ansatz, optimizer, and quantum instance, facilitating quantum computation of the Hamiltonian's minimum eigenvalue. This energy value and the corresponding qubit state are stored for subsequent analysis.

The most optimal outcome obtained during the optimization process is retained for further scrutiny. Executing the quantum circuit across diverse quantum devices yields performance insights. Each optimization iteration provides details on the energy value discovered and the best result achieved thus far.

Fig. 3 compares the classical and quantum solutions obtained from the 8-qubit VQE with COBYLA for solving the Poisson equation across boundary conditions from 0.0 to 1.0. While the solutions converge at the extremes, the quantum approach exhibits an irregular profile with multiple local extrema, deviating significantly from the distinct U-shaped classical solution in the intermediate boundary region. This suggests the quantum algorithm may offer an alternative solution with accuracy advantages over the classical method for certain boundary conditions.
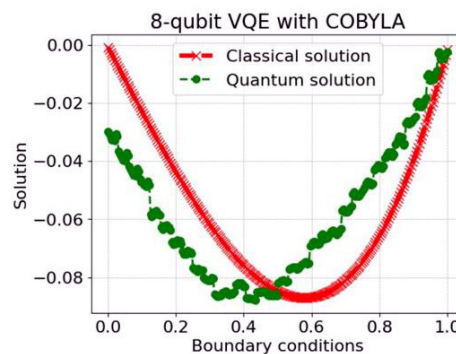

Figure 3. VQE results for 8 qubits, using the COBYLA optimizer

Increasing the number of qubits augments the dimensionality of the state space of the quantum system, intensifying the complexity of the problem and subsequently impacting the error rate and execution time of the algorithm. The COBYLA optimizer demonstrates promising performance under these conditions.

After executing the VQE algorithm and obtaining the quantum solution, the mean square error (MSE) between the quantum solution and the exact solution is computed. The MSE serves as an indicator of the accuracy of the obtained quantum solution relative to the exact solution. It is calculated as the mean of the squares of the differences between each element of the quantum solution vector and the exact solution.

Finally, the Poisson equation was tested using VQE on quantum simulator and real quantum hardware using the "ibm_osaka" system from the IBM Quantum platform.

The given results, in Table 1, contain the results of hardware experiments with quantum devices, where COBYLA optimizer was used for each device, and MSE between the quantum solution and the exact solution was calculated.

Table 1. Results of experiments with quantum devices using the COBYLA optimizer

Quantum devices	Optimizer	MSE
ibmq_qasm_simulator	COBYLA	0.00042
ibm_osaka	COBYLA	0.00164

These results allow us to compare the performance of VQE solutions of Poisson's equation optimized with COBYLA on different devices.

Discussion

This study highlights the challenges encountered when employing quantum algorithms, such as VQE, to solve PDE equations, particularly the Poisson equation. To address these challenges, a method utilizing the Feynman-Kitaev formalism in conjunction with the HHL and VQE algorithms was proposed. This approach enables the complete evolution of the system post-unit cost function optimization.

In this paper, adaptations of VQE algorithms were utilized for Poisson equation resolution. Leveraging the Feynman-Kitaev formalism facilitated the transformation of classical systems into quantum counterparts, enabling quantum circuit optimization to minimize the appropriate cost function for specific problems. The objective was to showcase how optimizing quantum algorithms can significantly enhance the PDE-solving process by reducing computational time and enhancing result accuracy.

Nevertheless, this approach faces several limitations. Limited access to quantum devices poses significant challenges for conducting extensive experiments. Additionally, the choice of optimizer for a VQE algorithm is critical to its performance. COBYLA's ability to operate without gradient information aligns well with the characteristics of quantum hardware, making it a practical choice for optimizing quantum circuits in the presence of noise. While COBYLA demonstrated promising results in this study (Fig 3.), further exploration of alternative optimizers tailored for specific quantum hardware configurations may yield insights into improving performance under varying conditions.

The results presented in Table 1 highlight the performance variations of VQE solutions across different quantum devices. Specifically, MSE values revealed significant insights into the accuracy and reliability of the quantum solutions. For instance, the MSE for the "ibmq_qasm_simulator" was remarkably low at 0.00042, indicating a high level of precision in the quantum solutions produced. This suggests that the simulator's environment, being ideal and noise-free, allows for a more accurate execution of quantum algorithms. Conversely, the MSE for "ibm_osaka" was higher at 0.00164, reflecting a noticeable discrepancy in performance. This

increased error can be attributed to hardware-specific factors and the noise levels inherent to the physical quantum device. The difference in MSE values between the "ibmq_qasm_simulator" and "ibm_osaka" highlights the impact of quantum hardware noise and imperfections on the accuracy of VQE solutions. These findings underscore the necessity for continued research into optimizing quantum algorithms for specific applications, as the MSE values indicate the accuracy and reliability of the quantum solutions relative to exact solutions.

Further research and development in this domain hold promise for devising more efficient methods for PDE resolution using quantum computing, thereby unlocking new avenues in various scientific and engineering disciplines.

Conclusion

This study delved into optimizing quantum algorithms for solving PDEs, with a focus on the Poisson equation. While applying the HHL algorithm to the Poisson equation, it became evident that quantum schemes aimed at minimizing the cost function could encounter optimization challenges. In response, a method based on the Feynman-Kitaev formalism, integrating the HHL algorithm and VQE, was proposed.

Successfully adapting VQE to address Poisson's equations involved leveraging the Feynman-Kitaev formalism to transition classical systems into quantum ones. This adaptation facilitated the optimization of quantum circuits to minimize the cost function relevant to the Poisson equation, demonstrating the approach's applicability to numerically solving the Poisson equation on a quantum platform.

Experiments utilized the COBYLA optimizer in conjunction with the VQE algorithm on various quantum devices. The performance of the VQE algorithm was evaluated using both a quantum simulator and real quantum hardware. Specifically, the experiments conducted on the «ibm_osaka» system from the IBM Quantum platform yielded mean square error (MSE) values of 0.00042 on the «ibmq_qasm_simulator» and 0.00164 on the «ibm_osaka» device. These results highlight the crucial role of the optimizer in determining the accuracy and convergence speed of the VQE algorithm.

These findings lead to the conclusion that optimizing quantum algorithms holds significant potential for enhancing the solution process of partial differential equations. This enhancement could lead to reduced computation time and improved result accuracy. Continued exploration in this field may yield more efficient methodologies for resolving PDEs via quantum computation.

Acknowledgment

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