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Hybrid Quantum-Classical Solver for the Helmholtz Equation

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Abstract

Seismic modeling in the frequency domain relies heavily on the Helmholtz equation; however, solving the resulting linear systems, especially at high frequencies, presents formidable computational challenges. This study investigates the application of the Variational Quantum Eigensolver (VQE), a hybrid quantum-classical algorithm, to solve the one-dimensional Helmholtz equation. By reformulating the problem as an eigenvalue problem, we encode the discretized operator into a parameterized quantum circuit using the `EfficientSU2` ansatz with CX entangling gates. The Hamiltonian is decomposed into Pauli terms and optimized using the L-BFGS-B algorithm. Simulations with 2–4 qubits demonstrate convergence to solutions closely approximating the analytical result. While this study focuses on a simplified one-dimensional case using Noisy Intermediate-Scale Quantum (NISQ) devices, it establishes the feasibility of applying quantum algorithms to Helmholtz-based seismic modeling.

Introduction

The Helmholtz equation plays a fundamental role in seismic applications, where it is used to simulate wavefields in the frequency domain and serves as the foundation for algorithms such as migration and inversion (Claerbout, 1985). However, solving it remains computationally demanding due to the large size of discretized models and the increased difficulty of handling high-frequency components, which lead to challenging linear systems. In light of recent advances in quantum computing, which has shown potential in solving problems in linear regression, optimization, number factoring, and unstructured database search, this study explores the use of the Variational Quantum Eigensolver (VQE) (Peruzzo et al., 2014), a hybrid quantum-classical algorithm designed for Noisy Intermediate-Scale Quantum (NISQ) devices (Preskill, 2018), to address the Helmholtz equation in a simplified one-dimensional setting.

We reformulate the Helmholtz equation as an eigenvalue problem and encode it into a quantum circuit, using parameterized gates to approximate the system's eigenstates and eigenvalues (Liu et al., 2021). The approach is evaluated through numerical simulations and a critical assessment of its performance, focusing on aspects such as ansatz selection and convergence behavior. This work represents an initial step toward the application of quantum computing in wave-based simulations, addressing a simplified one-dimensional scenario. While not intended to solve large-scale problems, the results demonstrate the feasibility of quantum approaches and open new avenues for research in seismic modeling and its applications.

Theory

The One-Dimensional Helmholtz equation

The one-dimensional Helmholtz equation is given by

$$u_{xx}(x,\omega) + k^2 u(x,\omega) = -f(x,\omega), \tag{1}$$

where $u(x)$ is the wavefield in the frequency domain, k is the wavenumber, ω is the angular frequency, and $f(x,\omega) = \delta(x - x_S)A(\omega)$ represents the amplitude of the Fourier transform of the source wavelet injected at position x_S. We consider a spatial domain L discretized into N uniformly spaced grid points with spacing Δx, such that $x_i = i\Delta x$ for $i = 0, \ldots, N-1$. A classical approach for approximating the solution is the finite-difference method, which replaces derivatives with discrete approximations. In this study, the second derivative is approximated using a centered finite-difference stencil, leading to a discretized version of the Helmholtz equation. Rearranging terms yields a tridiagonal linear system of the form $\mathbf{Au} = \mathbf{b}$, where the impedance matrix $\mathbf{A}$ contains the discretized differential operator, and the right-hand side vector $\mathbf{b}$ incorporates the source term. The accuracy of the solution improves with finer grid resolution, though the computational cost increases accordingly. It is important to note that, for our test case, we considered homogeneous Dirichlet boundary conditions, i.e., $u(0) = u(L) = 0$, which allow for the computation of an analytical solution.

Overview of the Variational Quantum Eigensolver (VQE)

The VQE is a hybrid algorithm developed to estimate the ground state energy of a quantum system, described by a Hermitian operator known as the Hamiltonian, H. It leverages the variational principle of quantum mechanics, which states that for any normalized quantum state $|\psi(\theta)\rangle$, the expectation value of the Hamiltonian satisfies $E(\theta) = \langle\psi(\theta)| H |\psi(\theta)\rangle \geq E_0$, where E_0 is the true energy of the ground state. The VQE algorithm minimizes this expectation value with respect to a set of variational parameters θ to approximate the ground state and its corresponding energy. This algorithm consists of several essential components that work together to estimate the ground state energy of a quantum system.

The process begins with the *Hamiltonian encoding*, where the system's Hamiltonian H is expressed as a sum of tensor products of Pauli operators, $H = \sum_j c_j P_j$, where each P_j represents a tensor product of Pauli matrices (I, X, Y, Z) acting on different qubits, and each coefficient $c_j \in \mathbb{R}$. This decomposition is critical because quantum computers can efficiently evaluate expectation values only when the operators are written in this form. An *ansatz* is then selected, which is a parameterized quantum state $|\psi(\theta)\rangle$, created by applying a quantum circuit $U(\theta)$ to an initial state, typically the all-zero state $|0\rangle^{\otimes n}$, resulting in $|\psi(\theta)\rangle = U(\theta)|0\rangle$. The ansatz circuit typically includes layers of parameterized single-qubit rotations and entangling gates. Its structure directly impacts the expressiveness and efficiency of the algorithm. Common ansatz choices include hardware-efficient designs, the Unitary Coupled Cluster (UCC) method for quantum chemistry, and problem-specific constructions (de Jesus et al., 2025).

Following state preparation, the *expectation values* of each term in the Hamiltonian are measured individually on a quantum device. The total energy is given by $E(\theta) = \sum_j c_j \langle\psi(\theta)| P_j |\psi(\theta)\rangle$. Due to the probabilistic nature of quantum measurement, this step requires multiple repetitions to estimate the energy accurately. Finally, a *classical optimization* routine is used to adjust the parameters θ in order to minimize the estimated energy. The goal is to find optimal parameters $\theta^* = \arg\min_\theta E(\theta)$. Both gradient-free methods, such as COBYLA and Nelder-Mead, and gradient-based methods, such as L-BFGS-B and Adam, are commonly used, depending on the characteristics of the optimization landscape.

The optimization is terminated once the energy change between iterations falls below a predefined threshold or the maximum number of iterations is reached. The final parameters θ^* define the approximate ground state, and the corresponding energy $E(\theta^*)$ serves as the estimate of the lowest eigenvalue of H. However, several computational challenges must be considered. Deeper quantum circuits can represent more complex states, but may suffer from increased noise and optimization difficulty. Another challenge is the barren blateau (McClean et al., 2018), when the energy landscape may become flat in high-dimensional spaces, making gradients vanish and optimization inefficient.

Additionally, quantum measurements are inherently probabilistic and introduce sampling noise. To mitigate these statistical errors, it is necessary to employ sufficient sampling strategies or apply error mitigation techniques.

Results

We analyze the VQE approach for solving the one-dimensional Helmholtz equation as an eigenvalue problem. In this setting, the spatial domain is defined as $L = 1.0\,\mathrm{m}$ and discretized according to the number of qubits q, such that the number of grid points is $N = 2^q$. We consider a wavenumber $k = 5.0\,\mathrm{m}^{-1}$ and assume a real-valued system in which the right-hand side vector $\mathbf{b}$ is defined by a sinusoidal source term $f(x) = -\sin(2\pi x)$. To solve the problem using VQE, we adopt the `EfficientSU2` ansatz available in the Qiskit library. For the classical optimization within the VQE loop, we employ the L-BFGS-B algorithm, which provided the best approximation results among several tested methods. The VQE solution is compared against the analytical solution, i.e., $u(x) = \sin(2\pi x)/(k^2 - 4\pi^2)$, and the numerical solution obtained using the `linalg.solve` function from the NumPy library, which solves the linear system resulting from the discretized Helmholtz equation (equivalent to the quantum formulation but solved classically). The accuracy is assessed using the root mean square error (RMSE), taking the analytical solution as reference.

Table 1 presents a comparison of the errors obtained from the numerical solution and the VQE for different numbers of qubits. For 2 and 3 qubits, both methods yield similar and relatively low errors, with VQE slightly outperforming the classical method at 3 qubits. However, for 4 qubits, the VQE error increases, and this trend continues at 5 qubits, where both methods show significantly larger errors. These results indicate that the performance of VQE is sensitive to system size and emphasize the need for improved ansatz design and optimization strategies as the number of qubits increases. Figure 1 illustrates the solution of the one-dimensional Helmholtz equation using three approaches: analytical, numerical, and VQE. For small quantum systems, specifically those involving up to 3 qubits, the VQE solution shows reasonable agreement with the analytical result. This degradation in performance is primarily attributed to a phenomenon known as the barren plateau. In this regime, the gradients of the cost function vanish exponentially with the system size, making the optimization landscape flat and hindering the training of variational quantum circuits. Although limited in scalability, these results demonstrate that quantum algorithms can be applied to differential equations in low-dimensional cases, serving as a proof of concept for future developments.

Table 1: Comparison of errors for numerical and VQE solutions.

Parameter	Grid points	Numerical	VQE
2 qubits	4	0.250	0.250
3 qubits	8	0.212	0.192
4 qubits	16	0.216	0.268
5 qubits	32	2.688	2.792

Conclusions

This study presented a novel application of the VQE to approximate the solution of the one-dimensional Helmholtz equation, a fundamental problem in seismic modeling. By reformulating the problem as an eigenvalue problem and implementing it within a hybrid quantum-classical framework, we demonstrated the feasibility of using quantum computing tools, specifically the VQE algorithm with the `EfficientSU2` ansatz, for Helmholtz-based modeling. The results obtained for systems with 2 to 4 qubits showed good agreement with the analytical solution, indicating that quantum algorithms can capture the essential behavior of physical systems. Importantly, this work also highlights some of the

limitations of the current generation of quantum algorithms, such as increased errors for larger qubit counts and sensitivity to the choice of ansatz and optimizer.

Despite these challenges, this initial exploration reinforces the potential of quantum computing in geophysical applications and opens up new research directions. These include investigating more expressive circuit architectures, improving optimization strategies, and scaling to higher-dimensional seismic problems. As quantum hardware continues to develop, these methods may serve as viable alternatives or complements to classical numerical approaches in seismic modeling.

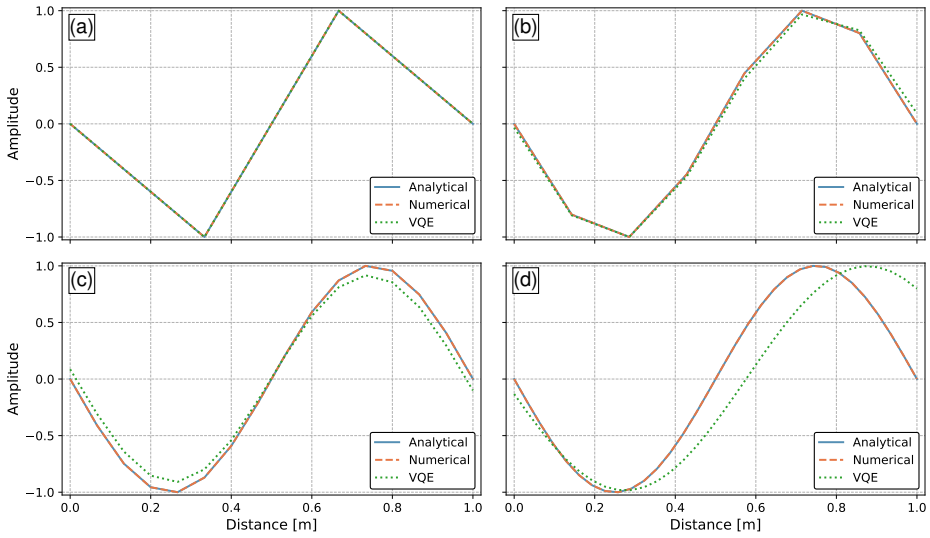

Figure 1: Comparison of the solutions to the one-dimensional Helmholtz equation using (a) 2, (b) 3, (c) 4, and (d) 5 qubits.

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