A Quantum Solver for Multidimensional Partial Differential Equations: Practical Case Studies

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Abstract

Quantum computing is consistently becoming transformational for computational problem-solving. This capability appears particularly suited for numerical solution of multidimensional partial-differential-equations (PDEs). Although many quantum techniques are currently available for solving PDEs, these algorithms, particularly the ones based on variational-quantum-algorithms (VQAs), suffer from low accuracy, high execution times, and low scalability. In this work, we propose an efficient and scalable algorithm targeting multidimensional PDEs. We present two variants of the algorithm, that differ on how the final quantum circuit is generated. While both utilize finite-difference-method (FDM) and classical-to-quantum (C2Q) encoding as the initial steps, the first variant uses numerical-instantiation and the second uses column-by-column-decomposition (CCD) for quantum circuit synthesis. Our proposed algorithm has been validated by various case studies such as Poisson, Heat, Black-Scholes, and Navier-Stokes equations. The results demonstrate better accuracy and scalability with faster execution times compared to VQA-based solvers on noise-free and noisy quantum simulators and promising results on real-quantum-hardware.

Keywords

Classical-to-quantum (C2Q) encoding, column-by-column decomposition (CCD), Poisson equation, Heat equation, Black-Scholes equation, Navier-Stokes equation

1 Introduction and Background

Researchers have been exploring the potential of quantum computation to solve various computationally difficult problems [1]. The use of quantum computing for solving computationally intensive partial differential equations (PDEs), found in domains including engineering, science, mathematics, and finance, is an active area of research [2]. Motivating this interest is the fact that even with the best classical algorithms, solving multidimensional PDEs can be extremely challenging due to the "curse of dimensionality" [3]. Quantum computing can offer significant performance by efficiently solving such classes of problems [4].

Existing quantum techniques for solving PDEs are primarily based on either the Harrow-Hassidim-Lloyd (HHL) algorithm or variational-quantum-algorithms (VQAs) [5]. The HHL algorithm discretizes and transforms PDEs into a linear set of equations using finite difference method (FDM) [6]. Although the HHL algorithm offers exponential speedup over classical techniques for solving linear systems with sparse matrices, it depends on error-corrected quantum systems. This severely limits its use in currently available Noisy-Intermediate-Scale-Quantum (NISQ) devices, which has motivated researchers to investigate various VQA-based methods to solve PDEs [7–10]. VQAs are primarily based on variational-quantum-linear-solvers (VQLS) or variational-quantum-eigensolvers (VQE) [7–10]. However, currently used VQA-based techniques suffer from low scalability, low accuracy, and high execution times.

In this work, we propose a generalized quantum algorithm for solving multidimensional PDEs. We have demonstrated generality through a number of case studies that include Poisson equation, Heat equation, Black-Scholes equation, and Navier-Stokes equation.

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2 Methodology

The proposed algorithm is categorized into two variants: Variant 1 and Variant 2. Variant 1 uses FDM, classical-to-quantum (C2Q) encoding [11], and numerical instantiation [12], while Variant 2 uses FDM, C2Q, and column-by-column decomposition (CCD) [13] [14], see Fig. 1. Using FDM, a PDE is converted into a system of

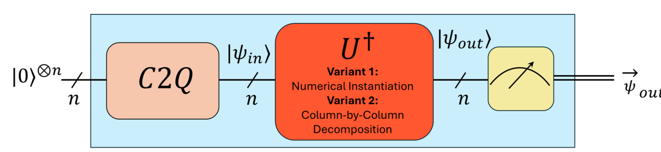


Figure 1: Proposed PDE solver algorithm (a) Variant 1 (b) Variant 2.

linear equations $A\vec{u} = \vec{b}$. The matrix A is preprocessed utilizing polar decomposition to generate the unitary matrix U and the symmetric positive semi-definite matrix P. The matrix P and U are used in $A\vec{u} = \vec{b}$ to obtain $(PU)\vec{u} = \vec{b}$. By rearranging and dividing it by the normalization factor $||P^{-1}\vec{b}||$ we can reduce it to (1).

$$|\psi_{out}\rangle = U^{\dagger} \cdot |\psi_{in}\rangle \text{ , where}$$
$$|\psi_{out}\rangle = \frac{\vec{u}}{\left\|P^{-1}\vec{b}\right\|}, \text{ and } |\psi_{in}\rangle = \frac{P^{-1}\vec{b}}{\left\|P^{-1}\vec{b}\right\|} \quad (1)$$

Using the singular value decomposition (SVD) [15] of matrix $A = W\Sigma V^{\dagger}$, we obtain the matrices $P^{-1} = W\Sigma^{-1}W^{\dagger}$ and $U^{\dagger} = VW^{\dagger}$. Here, W and V are unitary matrices and Σ is a diagonal matrix. Using $P^{-1} = W\Sigma^{-1}W^{\dagger}$ in (1), we obtain $|\psi_{in}\rangle$ as shown in (2) [16].

$$|\psi_{in}\rangle = \frac{W\Sigma^{-1}W^{\dagger}\vec{b}}{\left\|W\Sigma^{-1}W^{\dagger}\vec{b}\right\|} \tag{2}$$

The classical output vector $\overrightarrow{\psi}_{out}$ is obtained by measuring the output quantum state $|\psi_{out}\rangle$, as described in (3) [16]. The solution vector $\vec{u}$ is obtained by using (4) [16].

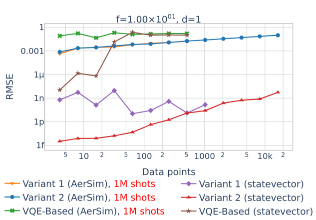
$$\overrightarrow{\psi}_{out} \approx U^{\dagger}|\psi_{in}\rangle \tag{3}$$

$$\vec{u} = \overrightarrow{\psi}_{out}\left\|W\Sigma^{-1}W^{\dagger}\vec{b}\right\| \tag{4}$$

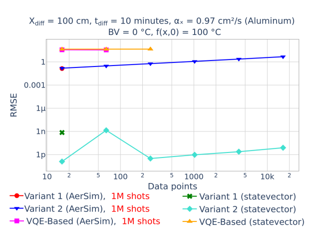
We have demonstrated the generality of our proposed algorithm by using it for solving multidimensional Poisson equation, multidimensional Heat equation, Black-Scholes equation, and Navier-Stokes equation as case studies.

3 Experimental Work

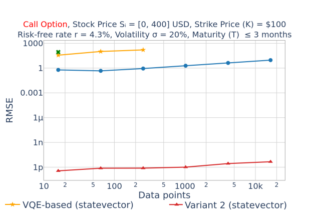
All the experiments were performed at the University of Kansas using a computer cluster node equipped with a 48-core Intel Gold 6342 CPU, three NVIDIA A100 80 GB GPUs (CUDA version 11.7). The accuracy, scalability, and overall execution time of both variants of the proposed algorithm were assessed using noise-free (`statevector simulator`) and noisy (`AerSimulator`) simulators, as well as quantum emulator (`FakeTorino`) and real quantum hardware (`ibm_torino`). In this work, we have used multidimensional Poisson, multidimensional Heat, Black-Scholes, and Navier-Stokes equations, and compared the results obtained by our proposed approach to VQE-based approach. Figures 2 and 3 demonstrate the accuracy, in terms of the root-mean-square-error (RMSE), and the total execution time, respectively, of our proposed algorithm in comparison to VQE-based approaches for various case studies.



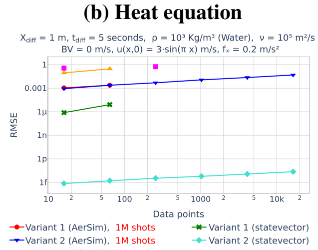
(a) Poisson equation



(b) Heat equation

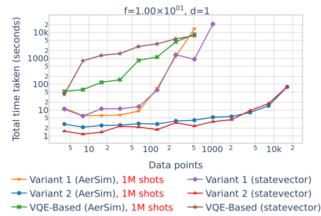


(c) Black-Scholes equation

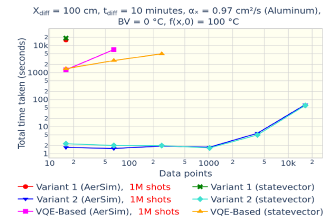


(d) Navier-Stokes equation

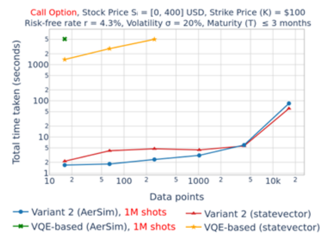
Figure 2: RMSE error in comparison with VQE-based approach for different case studies using noise-free and noisy simulators.



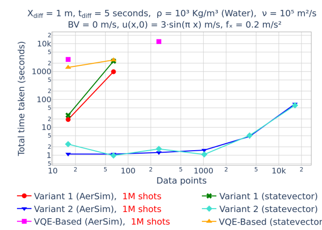
(a) Poisson equation



(b) Heat equation



(c) Black-Scholes equation



(d) Navier-Stokes equation

Figure 3: Total execution time in comparison with VQE-based approach for different case studies using noise-free and noisy simulators.

4 Conclusion

In this work, we present a generalized quantum algorithm with two variants for solving multidimensional partial differential equations (PDEs). As case studies, we have used multidimensional Poisson equation, multidimensional Heat equation, Black-Scholes equation, and Navier-Stokes equation. The experimental results demonstrate favorable performance in terms of accuracy, scalability, and execution time compared to existing PDE solvers based on quantum variational algorithms. This work showcases robust potential of quantum computing for solving multidimensional PDEs.

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