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Variational Quantum Eigen-Decomposition Preconditioning Method for Solving Computational Mechanics Problems

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ABSTRACT

Recently, quantum computing emerged as a paradigm for solving systems of linear equations. However, large condition numbers significantly increase the computational complexity of quantum linear equation solvers. In this work, a new quantum preconditioning approach called variational quantum eigen-decomposition (VQED) is proposed, where the preconditioner is defined as a weighted projector onto the subspace spanned by the eigenvectors of a matrix. A variational quantum algorithm with projection-based deflation is performed to calculate eigenvalue-eigenvector pairs for constructing the preconditioner. The proposed VQED method is used with quantum singular value transformation to solve linear systems for mechanics examples. It is demonstrated that the VQED can reduce the condition numbers to as low as 1.03, which is a significant improvement over the original condition number.

Keywords

Quantum linear system algorithm, Preconditioning, Variational quantum algorithm, Quantum singular value transformation, Quantum scientific computing.

1 INTRODUCTION

Most differential equations in computational mechanics problems can be numerically linearlized and solved as systems of linear equations. Given a coefficient matrix A and a vector $\mathbf{b}$, the goal is to obtain the solution vector $\mathbf{x}$ such that $A\mathbf{x} = \mathbf{b}$. However, solving very large linear systems is still computationally expensive when high-fidelity solutions for complex systems are desirable.

Recently, quantum computing emerged as an alternative paradigm for scientific computing, where qubits encode information and quantum phenomena of superposition and entanglement are utilized for computation. Particularly, several quantum linear system algorithms have been proposed. The first algorithm is the Harrow-Hassidim-Lloyd (HHL) algorithm [Har09], where the quantum linear systems problem is formulated as the eigenvalue problem, and the inverse quantum Fourier transform is utilized for phase estimation to obtain the eigenvalues. In the variational quantum linear solver [Bra23], a variational quantum circuit is constructed to minimize the residue. Classical optimization is used to find the optimal parameters. The third approach is utilizing quantum singular value transformation (QSVT) [Gil19, Mar21] to obtain the inverse of the coefficient matrix, which is approximated with the Chebyshev expansion. Although the computational advantages of quantum linear solvers over classical counterparts were shown, the accuracy and efficiency of these quantum methods are sensitively dependent on the condition number of the matrix. Large condition numbers significantly increase the computational complexity of these algorithms, which is quadratically dependent on the condition number (e.g., $\mathcal{O}(\kappa^2/\varepsilon)$ for HHL algorithm with condition number κ and target level of error ε). Therefore, reducing the condition number is necessary to improve the accuracy of the solution given the available computer resources.

Preconditioning is an effective numerical approach to reduce the condition numbers of matrices and improve the numerical accuracy in classical linear equation solvers. In this process, a preconditioner matrix M transforms the original linear system into $MA\mathbf{x} = M\mathbf{b}$. M is chosen so that the condition number of MA is much smaller than the condition number of A. Different preconditioning methods have been developed for numerical solvers on classical computers. However, very limited work has been done for quantum preconditioning, which is to obtain M with quantum algorithms. One approach is to implement the classical sparse approximate inverse method on a quantum computer [Cla13]. In this method, a preconditioner approximates the inverse of the coefficient matrix as $M \approx A^{-1}$. Each row of the preconditioner is obtained by solving a linear system with the vector on the right-hand side formed with an identity element. However, the preconditioning in [Cla13] relies on a quantum oracle without providing the details of implementation. Another approach is the quantum circulant preconditioner [Sha18]. The inverse of Toeplitz matrix is proved to be the optimal circulant preconditioner that makes the preconditioned coefficient matrix close to the identity matrix. The circulant preconditioner is easily implemented using quantum Fourier transform. A third method is the fast inverse method [Ton21], where the original matrix is decomposed into a sum of fast-invertible and perturbation matrices. The preconditioner is the inverse of the fast-invertible matrix, which is block-encoded in the QSVT circuit to solve the linear system. The norm of the fast-invertible matrix is much larger than the norm of the perturbation matrix so that the preconditioner is approximately equal to the identity. However, the method is not generalizable since the fast-invertible matrix is assumed to be non-singular, Hermitian, and unitarily diagonalizable.

In this work, a new quantum preconditioning approach, variational quantum eigen-decomposition (VQED), is proposed. The preconditioner is defined as a weighted projector onto the subspace spanned by the eigenvectors of the coefficient matrix. The eigenvectors are constructed recursively. A trial state is projected onto the subspace spanned by the previously calculated eigenvectors to determine a new orthogonal eigenvector. The proposed preconditioning approach can be integrated with different quantum linear equation solvers. Here, QSVT is used to demonstrate its capability.

In the remainder of the paper, the proposed VQED preconditioning method is described in Section 2. Experimental settings and evaluation criteria are introduced in Section 3. The method is demonstrated with two mechanics examples in Section 4. The results are summarized and future extensions are discussed in Section 5.

2 PROPOSED VARIATIONAL QUANTUM EIGEN-DECOMPOSITION PRECONDITIONER

Let $A \in \mathbb{C}^{n\times n}$ be a positive semi-definite Hermitian matrix representing a physical or engineering system, such as a stiffness matrix in structural mechanics. A can be decomposed as

$$A = \sum_{i=1}^{r} \lambda_i \left|u_i\right\rangle \left\langle u_i\right|, \tag{1}$$

where λ_i's are non-negative eigenvalues and $|u_i\rangle$'s are orthonormal eigenvectors.

Eigen-decomposition

Preconditioning is achieved by constructing a preconditioner M such that $MA \approx I$. MA is subsequently used in quantum linear solvers to improve the accuracy of the solutions.

In VQED, the preconditioner is iteratively calculated in a subspace spanned by the eigenvectors of A. When A is singular, a lower-rank approximation of M is obtained as

$$M_k = \sum_{i=1}^{k} \frac{1}{\lambda_i} \left|u_i\right\rangle \left\langle u_i\right|, \tag{2}$$

where $k < r$. Then, we define

$$M_k A \approx \sum_{i=1}^{k} \left|u_i\right\rangle \left\langle u_i\right| \tag{3}$$

as a projector onto the span of eigenvectors with the k smallest eigenvalues. The condition number of Eq. (3) could be reduced when higher-order eigenvectors are iteratively added to expand the subspace of M_k. When A is non-singular, $M_k A$ cannot be approximated as the identity. Instead, it is necessary to construct the complete eigenspace as

$$M = \sum_{i=1}^{r} \frac{1}{\lambda_i} \left|u_i\right\rangle \left\langle u_i\right| \tag{4}$$

so that $M = A^{-1}$.

Variational Eigenvector Computation

In the VQED method, a variational quantum algorithm [Per14] is used to iteratively extract eigenvectors of A with the k smallest eigenvalues in increasing order, similar to the deflation technique [Hig19].

The variational circuit is constructed based on the Pauli basis. A parameterized hardware efficient ansatz [Kan17] is used to prepare a quantum state $|\psi(\boldsymbol{\theta})\rangle$ from the initial state $|0\rangle^{\otimes n}$, where n is the number of qubits to encode A. The objective is to find a vector of parameters $\boldsymbol{\theta}^*$ so that the parameterized quantum state $|\hat{u}(\boldsymbol{\theta}^*)\rangle$ is equivalent to an eigenvector $|u_k\rangle$. To calculate each $|u_k\rangle$, $\boldsymbol{\theta}$ is optimized so that $|\hat{u}(\boldsymbol{\theta})\rangle$ is orthogonal to the previously obtained eigenvectors. For $|\hat{u}(\boldsymbol{\theta})\rangle$, $\boldsymbol{\theta}$ is omitted to $|\hat{u}\rangle$ in the following when it is clear in the context.

The variational quantum algorithm is first applied to obtain

$$\boldsymbol{\theta}^* = \underset{\boldsymbol{\theta}}{\arg\min} \operatorname{Re}\left[\langle \psi(\boldsymbol{\theta})| A \,|\psi(\boldsymbol{\theta})\rangle\right] \tag{5}$$

such that $|\psi(\boldsymbol{\theta}^*)\rangle = |\hat{u}_1\rangle$ and $\hat{\lambda}_1 = \langle \hat{u}_1| A \,|\hat{u}_1\rangle$.

Recursively, a projection-based deflation is applied to ensure that the parameterized states are orthogonal to each other. Given the previously computed eigenvectors $\{|\hat{u}_1\rangle, \ldots, |\hat{u}_{k-1}\rangle\}$, the non-normalized vector $\tilde{u}_k$ is calculated as

$$\tilde{u}_k(\boldsymbol{\theta}) = |\psi(\boldsymbol{\theta})\rangle - \sum_{i=1}^{k-1} |\hat{u}_i\rangle \langle \hat{u}_i|\psi(\boldsymbol{\theta})\rangle, \tag{6}$$

which is then normalized to

$$|\hat{u}_k(\boldsymbol{\theta})\rangle = \frac{\tilde{u}_k(\boldsymbol{\theta})}{|\tilde{u}_k(\boldsymbol{\theta})|}. \tag{7}$$

The corresponding eigenvalue is then calculated as

$$\hat{\lambda}_k(\boldsymbol{\theta}) = \mathrm{Re}\left[\langle \hat{u}_k(\boldsymbol{\theta})|A\,|\hat{u}_k(\boldsymbol{\theta})\rangle\right]. \tag{8}$$

The minimum value of Eq. (8) is $\hat{\lambda}_k = \lambda$ when $|\hat{u}_k\rangle = |u_k\rangle$.

After calculating all k eigenvalues and eigenvectors, a spectral preconditioner defined in Eq. (2) is constructed. This matrix, which approximates A^{-1}, is spanned by the computed eigenvectors.

Quantum Singular Value Transformation

The preconditioner M_k can be used in different quantum linear solvers. Here, we use QSVT to demonstrate. QSVT consists of an alternating sequence of block-encoding and projector-controlled phase-shift operations [Mar21]. Suppose that M_kA is decomposed as

$$M_kA = \sum_{i=1}^{r} \sigma_i \,|w_i\rangle\,\langle v_i|, \tag{9}$$

where σ_i is the non-negative real singular value of M_kA, $|w_k\rangle$ is the left singular vector, and $|v_k\rangle$ is the right singular vector. Given a block-encoding of M_kA in a unitary matrix U, the location of the block-encoded matrix can be determined as $M_kA = \Pi_w U \Pi_v$ by the projectors

$$\Pi_w := \sum_{i=1}^{r} |w_i\rangle\,\langle w_i|, \tag{10}$$

and

$$\Pi_v := \sum_{i=1}^{r} |v_i\rangle\,\langle v_i|, \tag{11}$$

which are spanned by its singular vectors. In the projector-controlled phase-shift operations $\Pi_w(\boldsymbol{\phi})$ and $\Pi_v(\boldsymbol{\phi})$, each projection $|w_i\rangle\,\langle w_i|$ in Eq. (10) or $|v_i\rangle\,\langle v_i|$ in Eq. (11) controls a z-rotation applied on an ancilla qubit.

The QSVT sequence depends on the parity of the matrix polynomial. If the parity is odd, then the sequence is defined as

$$\begin{aligned} U_o(\boldsymbol{\phi}) &= \Pi_w(\phi_1)U\left[\prod_{j=1}^{(d-1)/2} \Pi_v(\phi_{2j})U^\dagger \Pi_w(\phi_{2j+1})U\right] \\ &= \begin{bmatrix} \mathscr{P}_o(M_kA) & \cdot \\ \cdot & \cdot \end{bmatrix}, \end{aligned} \tag{12}$$

where

$$\mathscr{P}_o(M_kA) := \sum_{i=1}^{r} \mathscr{P}_o(\sigma_i)\,|w_i\rangle\,\langle v_i| \tag{13}$$

is an odd polynomial. Otherwise, if the parity is even, then the sequence is defined as

$$\begin{aligned} U_e(\boldsymbol{\phi}) &= \left[\prod_{j=1}^{d/2} \Pi_v(\phi_{2j-1})U^\dagger \Pi_w(\phi_{2j})U\right] \\ &= \begin{bmatrix} \mathscr{P}_e(M_kA) & \cdot \\ \cdot & \cdot \end{bmatrix}, \end{aligned} \tag{14}$$

where

$$\mathscr{P}_e(M_kA) := \sum_{i=1}^{r} \mathscr{P}_e(\sigma_i)\,|v_i\rangle\,\langle v_i| \tag{15}$$

is an even polynomial.

In linear systems problems, the inverse of M_kA with non-zero singular values is defined as

$$(M_kA)^{-1} = \sum_{i=1}^{r} \frac{1}{\sigma_i}\,|v_i\rangle\,\langle w_i|. \tag{16}$$

QSVT method can be utilized to find a polynomial $\mathscr{P}_o(\sigma_i) \approx 1/\sigma_i$ such that

$$(M_kA)^{-1} \approx \sum_{i=1}^{r} \mathscr{P}_o(\sigma_i)\,|v_i\rangle\,\langle w_i|. \tag{17}$$

3 EXPERIMENTS

The quantum preconditioning method is demonstrated with two examples of solid mechanics. The first example is a truss structure, whereas the second example involves a Messerschmitt-Bölkow-Blohm (MBB) beam.

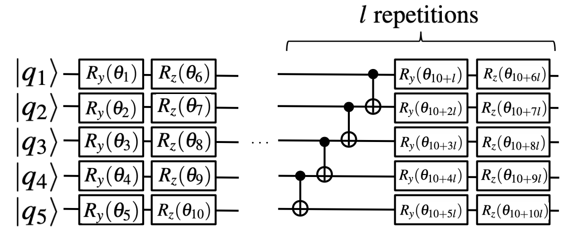

Figure 1: Hardware efficient SU2 ansatz used to compute eigenvalues and eigenvectors of A for VQED.

The proposed preconditioner was tested on systems of 32 linear equations derived from the partial differential equations. Eigenstates were prepared using hardware efficient SU2 circuit in Figure 1 with l repeated layers. With this circuit, M was constructed by preparing 32 eigenvalue-eigenvector pairs. The optimization is performed using the classical sequential least squares programming (SLSQP) algorithm [Kra88]. 200 iterations were performed to calculate each eigenstate. Condition numbers of MA were computed for ten values of l ranging from one to ten. A total of 5 random seeds were tested for each value of l.

Two metrics are used to assess the performance of the VQED method. The first metric is the fidelity of the calculated solution. The fidelity is defined as

$$F = |\,\langle x_c|x_q\rangle\,|^2, \tag{18}$$

where $|x_c\rangle$ and $|x_q\rangle$ are the actual and estimated solutions, respectively. The second metric is the relative error of the calculated solution compared to the classical solution. This metric is defined as

$$\delta = \frac{z_q - z_c}{z_c}, \tag{19}$$

where z_c and z_q are displacements from $|x_c\rangle$ and $|x_q\rangle$, respectively.

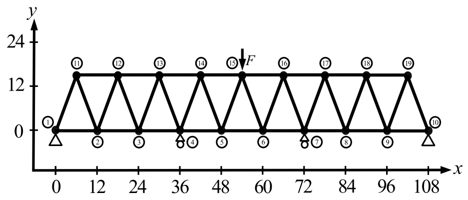

Figure 2: Truss structure

4 RESULTS

Truss Structure

The truss structure is illustrated in Figure 2, where the x- and y-axes indicate spatial coordinates in inches. The truss consists of 19 nodes and 35 members. Each element has a cross-sectional area of 8.5 in^2 and elastic modulus of 29,000 ksi. For the boundary conditions, two pin supports are located at nodes 1 and 10. Two roller supports are located at nodes 4 and 7. A downward point load of 5,500 kips is applied at node 15.

Table 1: Condition number of MA for the truss structure with different circuit depths and ansatz-random seeds.

Repetitions (l)	Best Seed	Condition Number
1	4	21.0823
2	1	11.6798
3	2	7.8683
4	4	3.9361
5	2	1.5099
6	1	1.0936
7	**1**	**1.0052**
8	4	1.0050
9	3	1.0045
10	0	1.0049

The VQED method was used to reduce the condition number of MA. The results are shown in Table 1, where the best choice is $l = 7$, where the condition number of MA has been significantly reduced to 1.0052 without further increasing the circuit depth. This is significantly smaller than 71.49, which is the original condition number of A.

The convergence plot of 32 eigenvalues for the truss structure with ansatz depth of seven and random seed of one is plotted in Figure 3. For all eigenvalues, convergence was clearly observed after 200 iterations. Using the minimum eigenvalues and corresponding eigenvectors, the fidelity and $L2$ error for the solution generated from QSVT were 1.0000 and 0.0033, respectively. Overall, the VQED method can effectively generate the very accurate solution to the linear system.

The surface plots for x- and y-displacements in the truss structure are visualized in Figure 4. The surfaces from the proposed algorithm and classical linear solver are nearly identical. Nodes with displacements close to zero are omitted. Overall, most of the truss structure displacements from QSVT are close to the displacements from the classical linear solver.

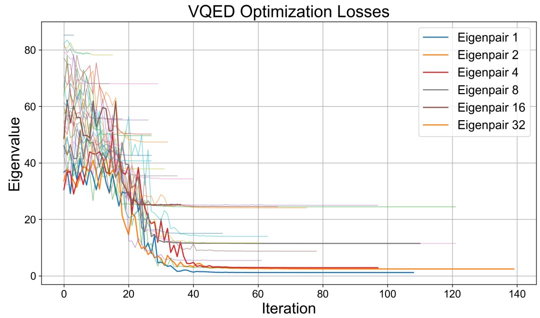

Figure 3: Convergence plot of 32 eigenvalues for the truss structure.

MBB Beam

The MBB beam is shown in Figure 5. The beam is divided into a 4×3 rectangular grid of elements. The side length of each square element is 2 in. The left edge of the beam is supported by four roller supports, whereas the bottom edge is supported by two pin supports. A downwards point load of 3,500 kips is applied at node 17.

Table 2: Condition number of MA for the MBB beam with different circuit depths and ansatz-random seeds.

Repetitions (l)	Best Seed	Condition Number
1	0	21.3801
2	3	15.8670
3	0	9.3430
4	1	4.2713
5	0	1.9161
6	**1**	**1.0278**
7	0	1.0235
8	3	1.0174
9	4	1.0138
10	4	1.0129

Similarly, the sensitivity of VQED with respect to the circuit depth was performed. The calculated condition numbers of MA are shown in Table 2, where the best choice is $l = 6$ with the condition number of 1.0278. This is significantly smaller than the original condition number of A, which is 101.85.

Figure 6 shows the convergence behavior of 32 eigenvalues. It is observed that 31 out of 32 eigenvalues are able to converge within 200 iterations. With the calculated eigenvalues and corresponding eigenvectors, the fidelity and $L2$ error of the solution from QSVT are 0.9994 and 0.0254, respectively.

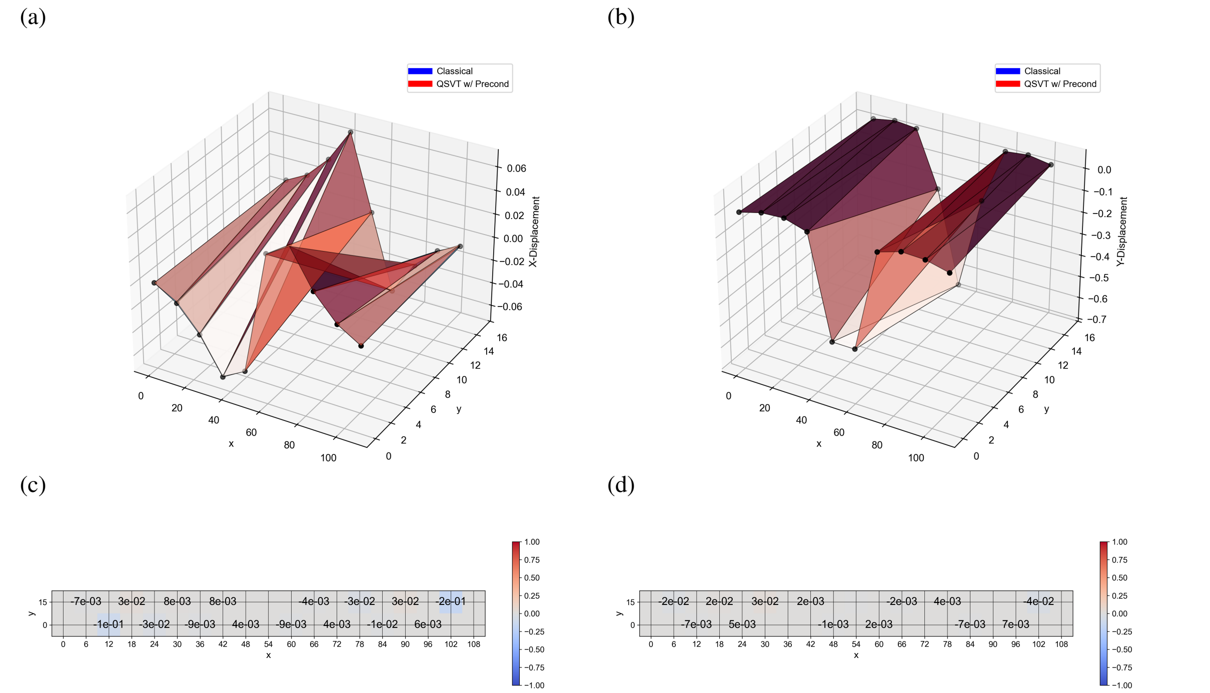

Figure 4: Surface plots of (a) x-displacements and (b) y-displacements, and relative errors for (c) x-displacements and (d) y-displacements for the truss structure. Nodes with displacements close to zero are omitted for visual clarity.

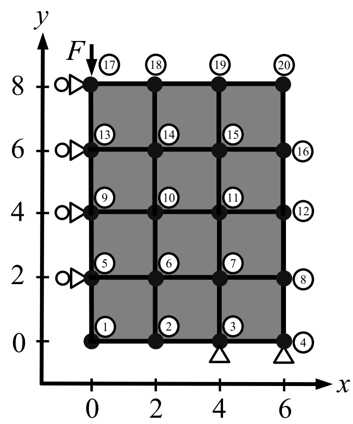

Figure 5: MBB beam

In the displacement surfaces shown in Figure 7, the estimated displacements calculated with the quantum algorithm deviate from theoretical values by relative errors ranging from 0% to 29%. It is observed that the free nodes have larger relative errors for both x- and y-displacements than the constrained nodes. In addition, the boundary condition and the external load cause the beam to move more freely in the vertical direction. As a result, the relative error tends to be larger for x-displacements than y-displacements. Although the largest relative error is 29%, the displacement surfaces for both classical and QSVT methods are very similar.

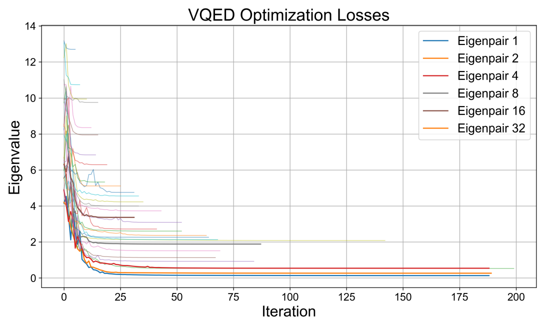

Figure 6: Convergence plot of 32 eigenvalues for the MBB beam.

5 CONCLUDING REMARKS

In this paper, a VQED preconditioning method is proposed as a quantum preconditioning method. A spectral preconditioner M_k is constructed from variationally computed eigenvalues and eigenvectors of a Hermitian matrix A. This spectral preconditioner can reduce the condition number of A, which, in turn, improves accuracy of solving linear systems. The VQED method can be used for Hermitian matrices of low-rank.

The VQED method was used to reduce the condition numbers of the stiffness matrices for a truss structure and a MBB beam. It was demonstrated that the VQED can reduce the both condition numbers below 1.03,

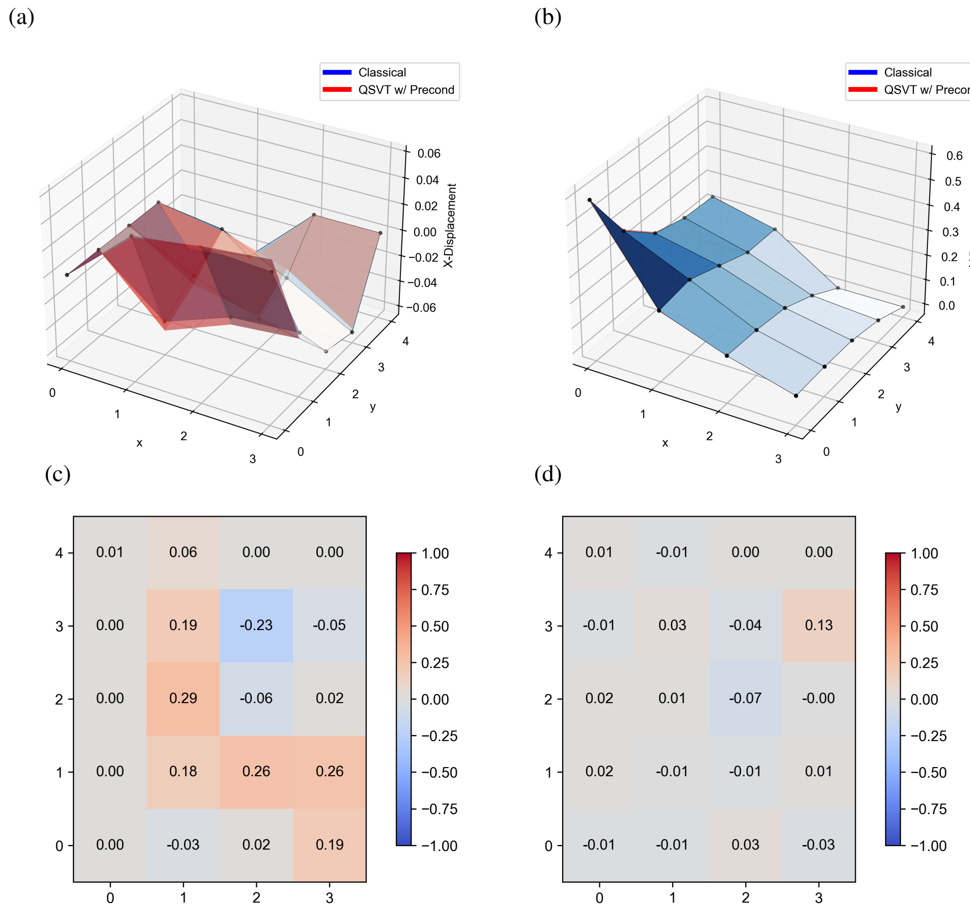

Figure 7: Surface plots of (a) x-displacements and (b) y-displacements, and relative errors for (c) x-displacements and (d) y-displacements for the MBB beam.

which are significant improvements over the original condition numbers. When QSVT is used for the preconditioned linear systems, the estimated displacements achieve very good accuracy and are very close to the results from the classical linear solver.

In the proposed method, classical projection-based deflation is used to generate the orthogonal eigenvectors. Future work will focus on imposing the orthogonality condition with a quantum computational framework. The orthogonality condition can be implemented in quantum computers either by introducing overlap penalty terms in the cost function, implementing a projector with controlled-state preparation, or defining a generalized eigenvalue problem with diagonalization.

The new preconditioning method was tested with classically reconstructed eigenvalues and eigenvectors computed with the VQED method. Future work will also focus on implementing a single quantum computational framework that integrates both VQED and QSVT. The degree d of an odd polynomial for matrix inversion is dependent on the condition number κ such that $d = \mathcal{O}[\kappa \log(\kappa/\varepsilon)]$. To reduce the computational expenses of solving linear systems, the preconditioner must be optimized with VQED before block-encoding it into unitary operators in QSVT.

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