PRECONDITIONED BLOCK ENCODINGS FOR QUANTUM LINEAR SYSTEMS

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ABSTRACT

Quantum linear system solvers like the Quantum Singular Value Transformation (QSVT) require a block encoding of the system matrix A within a unitary operator U_A . Unfortunately, block encoding often results in significant subnormalisation and increase in the matrix's effective condition number κ . affecting the efficiency of solvers. Matrix preconditioning is a well-established classical technique to reduce κ by multiplying A by a preconditioner P. Here, we study quantum preconditioning for block encodings. We consider four preconditioners and two encoding approaches: (a) separately encoding A and its preconditioner P, followed by quantum multiplication, and (b) classically multiplying A and P before encoding the product in U_{PA} . Their impact on subnormalisation factors and condition number κ are analysed using practical matrices from Computational Fluid Dynamics (CFD). Our results show that (a) quantum multiplication introduces excessive subnormalisation factors, negating improvements in κ . We study preamplified quantum multiplication to reduce subnormalisation. Conversely, we see that (b) encoding of the classical product can significantly improve the effective condition number using the Sparse Approximate Inverse preconditioner with infill. Further, we introduce a new matrix filtering technique that reduces the circuit depth without adversely affecting the matrix solution. We apply these methods to reduce the number of QSVT phase factors by a factor of 25 for an example CFD matrix of size 1024x1024.

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1 Introduction

Many engineering applications, such as Computational Fluid Dynamics (CFD), adopt a predictor-corrector approach, where the predictor step involves the solution of a large system of linear equations. This step is generally the most time-consuming part of the solver, where a quantum speed-up could be impactful. The system is expressed as the matrix equation

$$Ax = b (1)$$

where $A \in \mathbb{R}^{N \times N}$ and $x, b \in \mathbb{R}^N$. Typically, A has sparsity, s, where s does not depend on N.

Direct classical solvers, such as Lower-Upper decomposition, have time complexity $O(N^3)$. These follow a prescribed sequence of steps that do not depend on the matrix condition number, κ , of the matrix. Classical iterative methods, such as the family of Krylov subspace methods [1, 2] are far more efficient. For example, the Conjugate Gradient (CG) method has time complexity $O(Ns\sqrt{\kappa}\log(1/\epsilon))$ where ϵ is the precision of the solution. For non-symmetric matrices, the CG-Squared method scales with $O(\kappa)$ and later variants, such as Bi-CGSTAB [3], can recover the $O(\sqrt{\kappa})$ scaling with a higher prefactor.

Quantum Linear Equation Solvers (QLES) can offer complexity advantages over classical solvers. The first QLES is the HHL algorithm [4] with time complexity $O(\log(N)s^2\kappa^2/\epsilon)$). Later, Linear Combination of Unitaries [5] and Quantum Singular Value Transform (QSVT) [6, 7] techniques improved the query complexity to $O(\kappa \log(\kappa/\epsilon))$, an exponential improvement in precision, ϵ . Finally, the discrete adiabatic (DA) method [8] achieves provably optimal

query complexity of $O(\kappa \log(1/\epsilon))$. It is important to note that these quantum algorithms require assumptions on I/O to be effective [9], such as efficient block encoding circuits for loading matrices in QSVT.

For second-order elliptic problems, such as the pressure-correction equations considered here, κ scales with $O(N^{2/d})$ where d is the dimension of the domain [10]. Hence, in 2-dimensions, CG scales with $O(N^{3/2}s\log(1/\epsilon))$ and, the query complexity of QSVT is $O(N\log(N/\epsilon))$. Hence, although the quantum solvers have worse scaling with κ than, say, CG they can deliver a quantum speed-up, provided sufficiently efficient block encodings are available.

Classical CG methods are prone to loss of precision that can lead to divisions by near-zero numbers. The GMRES method [11] addresses this, but needs to store search vectors of length N over which it can minimise the search error. This consumes computer memory and most implementations of GMRES truncate the search to a small number of vectors. However, most iterative classical methods solve the preconditioned system

$$PAx = Pb \tag{2}$$

where P is the preconditioning matrix such that, ideally, $\kappa(PA) \ll \kappa(A)$. This reduces the dependence on the condition number and also makes the solver more stable.

Given that block encoding oracles of $O(\log(N))$ for general purpose matrices remain elusive, it is essential to improve QLES as much as possible to gain a speed-up. In this light, the present paper considers preconditioning for QLES, and improves block encodings with a circuit trimming procedure.

1.1 Previous work

The first investigation of preconditioning a quantum linear equation solver [12] adopted the Sparse Approximate Inverse (SPAI) technique that is popular in classical supercomputing as it solves an independent set of small $n \times d$ least squares problems where n and d depend on the sparsity of the matrix and its approximate inverse. The rows of the preconditioner were calculated independently and a single unitary was used to calculate the elements of PA. The preconditioning was implemented within the HHL algorithm and applied to electromagnetic scattering.

A quantum algorithm for solving a circulant matrix system using a modified HHL solver [13] demonstrated the benefit of being able to express circulant matrices in terms of Quantum Fourier Transforms. Separately, [14] showed how to implement a circulant preconditioner using a modified quantum singular value estimation scheme.

Incomplete Lower Upper (ILU) preconditioning was used by [15] in conjunction with the Variational Quantum Linear Solver. The ILU preconditioner was computed and applied as a classical preprocessing step with VQLS used to solve the preconditioned system.

A fast inversion scheme for preconditioning [16] writes the matrix system as $(A + B)|x\rangle = |b\rangle$ and assumes ||A|| >> ||B||. Rewriting gives:

$$(I + A^{-1}B)|x\rangle = A^{-1}|b\rangle \tag{3}$$

A is fast-invertible if, after rescaling A so that $||A^{-1}||=1$, there is a block-encoding of A^{-1} where the number of oracle queries for A is not dependent on its condition number. Diagonal and 1-sparse matrices can be fast-inverted. Although for general matrices, the scheme requires a classical Singular Value Decomposition to give $A=UDV^{\dagger}$. For normal matrices, U=V and in certain cases V is easily computed, e.g. when V is the Quantum Fourier Transform. A comparison of the SPAI, circulant and fast inversion preconditioners [17] showed significant scaling benefits for fast inversion using an inverse Laplacian preconditioner. The test case focussed on fracture mechanics and split the matrix into $A=\Delta+A_F$, where Δ is the Laplacian of the flow field in the absence of fractures and A_F is the fracture matrix. For the cases studied, the Laplacian has a known eigenvalue decomposition. Classical preconditioning using an inverse Laplacian [18, 19, 20, 21] has demonstrated similar benefits using Krylov subspace iterative solvers.

The likely effect of subnormalisation factors on quantum preconditioning for solving elliptic PDEs was considered by [22]. Instead of either quantum or classical multiplication, the preconditioned matrix PA was formed directly on the classical computer using the multi-level BPX preconditioner [23].

Whilst previous work has provided some practical details on preconditioning quantum linear solvers, none has explicitly considered the practical impact of the subnormalisation factors arising from block encoding. Nor has the difference between the circuit implementations of classical and quantum multiplication of P and A been considered.

1.2 This work

This work investigates matrix preconditioning within the context of block encoding for quantum solvers such as QSVT. We consider the SPAI and circulant preconditioners that have previously been reported and an approximate Toeplitz

preconditioner. For the SPAI and Toeplitz preconditioners we also evaluate the effect of infill. Separately, we apply diagonal scaling as a precursor step. This can be cast in the form of a fast inverse but is a $\mathcal{O}(N)$ operation that is classically efficient.

First, the matrices in questions (preconditioners P, CFD matrix A, or products PA) must be implemented as block encodings amenable to quantum computation, these are shown in Section 2.

Next, in Section 3 we study preconditioning. Many classical methods do not explicitly form the matrices A and P, instead subroutines are called to perform the matrix-vector multiplication. For QLES, the classical overhead of forming PA suggests the analogous approach of multiplying the encoded matrices for A and P rather than encoding PA. For compactness, we use the terms *quantum multiplication* for the separate encoding of P and PA and classical multiplication for pre-multiplication of PA and PA prior to encoding the product PA. We also consider preamplified quantum multiplication (Section 3.3.1), which can improve the figure of merit when multiplying block encodings. Both approaches (classical multiplication and quantum multiplication) are studied and compared: We investigate how the subnormalisation factors associated with the block-encoding of PA, and PA affect the condition number for each of the preconditioners considered.

In Section 4, we introduce a circuit trimming technique that reduces the depth of query oracles used in the block encodings. Although we have used efficient encoding techniques [24] that have low subnormalisation factors and a low number of ancilla qubits, the depth of the query oracles scales with the number of non-zero entries in the matrix. We introduce a double-pass filtering technique that places the entries of the matrix into bins of equal value and show how this can reduce the depth of the query oracle with a minimal effect on the solution accuracy.

Finally, in Section 5 we turn to CFD applications of the methodology presented. Using emulated circuits for CFD matrices ranging from 16×16 to $4,096 \times 4,096$ we provide the first practical circuit level evaluations of preconditioning with QSVT.

2 Matrices and their block encodings

For this study four preconditioners are considered:

- Diagonal scaling, see Appendix A.
- Sparse Approximate Inverse (SPAI), see Appendix B.
- Toeplitz Approximate Inverse (TPAI), see Appendix C.
- Circulant Approximate Inverse (CLAI), see Appendix D.

Whether the matrix A and its preconditioner P are being encoded separately or as a classically computed product, the key factors of an efficient block encoding are the reduction in subnormalisation and circuit depth. In the next Section 2.1, we review the impact of subnormalisation on the effective condition number. Then (Sections 2.2–2.5) we present the different encodings used for the matrices appearing in this work, following those of [24]. Finally, in Section 2.6 we discuss the sparsity/infill of the required matrices, and how they are affected by preconditioning.

2.1 Condition numbers of encoded matrices

Block encoding a matrix $A \in \mathbb{R}^{N \times N}$ with $N = 2^n$ entails creating a unitary operator such that:

$$U_A = \begin{pmatrix} A/s & * \\ * & * \end{pmatrix} \tag{4}$$

where s is the subnormalisation factor [25, 26].

When inverting a matrix using QSVT, it is the subnormalised condition number, κ_s , that dictates the number of phase rotations, where:

$$\kappa_s = \frac{1}{|\lambda_s^{min}|} \tag{5}$$

and λ_s^{min} is the smallest eigenvalue of A/s. If A/s is not diagonalisable, then λ_s^{min} is the smallest singular value.

Note that due to the unitary embedding, it is not the case that $\kappa_s = \lambda_s^{max}/\lambda_s^{min}$. Note, also, that while $\lambda_s^{min} = \lambda^{min}/s$ this does not, in general, mean that $\kappa_s = s\kappa$. However, it does give:

$$\kappa_s = \frac{s}{|\lambda^{min}|} \tag{6}$$

2.2 Diagonal scaling and encoding the original matrix

Whilst we have labelled diagonal scaling as a preconditioner, it is best considered as an $\mathcal{O}(N)$ classical pre-processing operation. It is a necessary step for the Toeplitz and circulant preconditioners. It is also beneficial for encoding A since it sets all the entries along the main diagonal to 1. Whilst this has a marginal effect on the condition number, it usually increases $|\lambda_s^{min}|$.

The diagonal scaled matrix DA provides the reference values for measuring the improvements provided by preconditioning. Since D^{-1} is not a preconditioner in the same sense as the others, we will use A to refer to $D^{-1}A$ in the following unless necessary to avoid confusion.

Since A is a banded diagonal matrix, it uses the encoding method described in Section 2.4. However, we first describe the encoding of Toeplitz matrices as the banded diagonal encoding is a generalisation thereof.

2.3 Toeplitz matrix encoding

The encoding of a Toeplitz matrix has the shortest circuit depth and follows directly from the PREP/UNPREP scheme of [24]. We set their parameter p to $\frac{1}{2}$ which means that the UNPREP operator is the adjoint of the PREP operator, except for negative-valued diagonals where there is a sign difference.

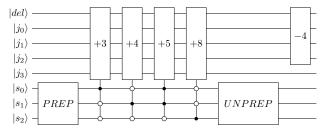


Figure 1: Circuit for encoding a 16x16 pentadiagonal Toeplitz matrix with diagonals at offsets: -4, -1, 0, 1, 4. Negative offsets are super-diagonals, positive offsets are sub-diagonals and 0 is the main diagonal. Strictly, the above circuit has a controlled addition of 0, but this is omitted as it has no effect.

Figure 1 gives an overview of the circuit to encode a 16x16 pentadiagonal Toeplitz matrix based on a 4x4 CFD pressure correction equation. Each diagonal has a constant value; these are loaded using the PREP operator. The multiplexed controls then offset each diagonal by a positive amount. Note that there is no offset for the -4 diagonal as a controlled addition of 0 has no effect. After the controlled additions, the final arithmetic operator moves the diagonals to their correct location.

The qubit labels follow [24] where those labelled $|j\rangle$ designate the columns of the matrix, and those labelled $|s\rangle$ designate the diagonals. The $|del\rangle$ qubit is needed so that the encoding creates a 32x32 matrix. This is because when a diagonal is offset, values that move out of the range of the matrix wrap round to the other side. This contaminates the 32x32 matrix but not the upper left 16x16 block.

The subnormalisation factor for PREP/UNPREP encoding is the sum of absolute entries on the diagonal, which is generally lower than the number of diagonals.

2.4 Banded diagonal matrix encoding

Encoding a band diagonal matrix is a straightforward extension of the Toeplitz scheme and is used to encode A and the SPAI preconditioner. Instead of loading a constant value for each diagonal, we must use separate oracles to load the values along each diagonal. To keep the subnormalisation factor as low as possible, the values along each diagonal are scaled to have a maximum value of 1.0. The PREP operator loads the factors needed to scale all the diagonals back to their original values. Since PREP must load a normalised state, the diagonals are not returned to their original values.

Figure 2 shows a schematic of the circuit to encode a 16x16 pentadiagonal matrix. As before, the qubit labels follow [24] where the data loading controlled rotations are applied to the $|d_0\rangle$ qubit. The encoding oracle follows full

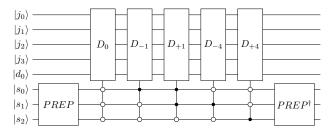


Figure 2: Circuit for encoding a 16x16 pentadiagonal matrix using an LCU to add separately encoded diagonals. Each diagonal encoding operator D_i includes the addition or subtraction of i to give the correct offset from the main diagonal.

matrix encoding [26] but instead of using row-column indexing, diagonal-column indexing is used. Importantly, the subnormalisation factor scales with the number of diagonals rather than with the dimension of the matrix. The operators D_0, D_{-1}, \ldots contain both the data loading oracles and the arithmetic operators to offset the diagonals to the correct position. A negative offset creates a super-diagonal and a positive offset creates a sub-diagonal.

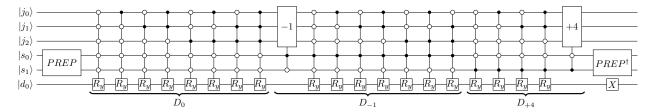


Figure 3: Circuit segment for encoding a banded 8x8 tridiagonal matrix with one super-diagonal offset by 1 from the main diagonal and one sub-diagonal offset by 4 from the main diagonal. Note only 2 PREP qubits are needed to load the 3 diagonals.

Figure 3 shows the circuit segment for loading a banded tridiagonal matrix. The controls on the $|j\rangle$ qubits select the column and the controls on the $|s\rangle$ qubits select the diagonal. By themselves, the controlled rotations create a direct sum of the three diagonal matrices. The controlled subtraction offsets the part of the direct sum containing the super-diagonal by 1. Similarly, the controlled addition offsets the sub-diagonal by 4. The PREP-UNPREP operations scale and mix the diagonals to give the full encoded matrix in the top left corner of the resulting unitary. The X gate after the rotations is required for ARCSIN encoding [27]. Since only the non-zero entries of the matrix are encoded, there is no out of range wrap-around as occurs in the Toeplitz encoding.

In this study, banded diagonal encoding is used to load A and the SPAI preconditioner, and all the classically computed products PA.

2.5 Circulant matrix encoding

From Equation (36) in Appendix D, the circulant preconditioner must load $F\Lambda^{-1}F^{\dagger}$ where F is the Fourier transform. The diagonal matrix of inverse eigenvalues, Λ^{-1} , can be computed from Equation (35) and can be encoded using diagonal encoding. The resulting circuit including the product with A is shown in Figure 4

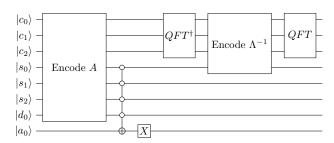


Figure 4: Circuit for encoding $C^{-1}A$ for an 8x8 pentadiagonal matrix.

2.6 Matrix infill

Although the inverse of a sparse matrix is not, itself, sparse, the default for many preconditioners is to impose the same sparsity pattern on P as the original matrix A. This limits the effectiveness of the preconditioning but is often necessary due to computational limits. An alternative is for the preconditioner to use *infill* where P is allowed to have more non-zeros than A. This is discussed in Appendix B and illustrated in Figure 12. For banded diagonal matrices, the infill procedure introduces additional diagonals. The infill algorithm can be repeated with each repetition giving a better approximation to A^{-1} at the expense of adding more diagonals.

	TPAI			SPAI			
Infill levels	$\operatorname{diag}(P)$	diag(PA)	diag(P)	diag(PA)	non-zero $diag(PA)$		
0	5	13	5	13	9		
1	11	23	13	25	13		
2	17	33	25	41	17		
3	23	43	41	61	21		

Table 1: Number of banded diagonals in P and the classical product PA for different infill levels with the TPAI and SPAI preconditioners. The final column shows the number of diagonals that have non-zero entries.

Table 1 shows the number of diagonals with infill levels from zero to three for P and the classical product PA using the TPAI and SPAI preconditioners. Note that CLAI generates a dense matrix for which infill is not relevant. As described in Appendix B and Appendix C, the preconditioners use different infill strategies with SPAI adding more diagonals per infill operation.

An unexpected feature of SPAI is that a number of diagonals in the product PA consist entirely of zeros to within the precision of the arithmetic. The is a result of exactly solving each reduced system as described in Appendix B.1. For SPAI with three levels of infill, performing quantum multiplication requires encoding two banded matrices with 5 and 41 diagonals. Whereas, classical multiplication encodes a single banded matrix with 21 diagonals. Of course, the latter has a high classical pre-processing cost to compute PA prior to encoding.

Although the TPAI reduced system is also solved exactly, the initial approximation of A as a Toeplitz matrix means PA has no diagonals with zero values.

3 Preconditioning

As a test case for preconditioning, we use CFD pressure correction matrices for the flow in a lid-driven cavity taken from the open source **qc-cfd** 3 repository. The CFD meshes range from 4×4 to 64×64 cells. The corresponding pressure correction matrices have dimensions ranging from 16×16 to $4,096 \times 4,096$ and are each extracted from the non-linear solver after 100 outer iterations.

	DS	CLAI	TPAI	SPAI	Section	Figure
Classical	√	✓	✓	✓	§3.1	§5
Quantum multiplication		\checkmark	\checkmark	\checkmark	§3.2, §3.3	§6, §7
Classical multiplication			\checkmark	\checkmark	§3.4	§ 8

Table 2: Results presented in this section. DS = Diagonal scaling. CLAI, TPAI, SPAI = Circulant, Toeplitz and Sparse Approximate Inverse respectively.

We study the impact of preconditioning on subnormalisation and subnormalised condition number, where Table 2 gives an overview of the scenarios considered. Firstly, the preconditioners are evaluated exactly as they would be used by a classical solver (Section 3.1). Then we study the subnormalisation factors for each preconditioner (Section 3.2), required for preconditioning by quantum multiplication. In Sections 3.3 and 3.4, we study preconditioning with the quantum multiplication and classical multiplication approaches, respectively. For preconditioning by classical multiplication, only TPAI and SPAI are considered as the CLAI preconditioner produces a dense matrix that would require excessive

³https://github.com/rolls-royce/qc-cfd/tree/main/2D-Cavity-Matrices

classical computing resources. The effects of preconditioning on both subnormalisation factors and condition numbers are considered.

As mentioned above diagonal scaling is a preprocessing method used by all the preconditioners. It is included in the classical section only to show the small effect it has. The SPAI and TPAI results include infill up to three levels. All matrices are scaled to have $||A||_{max} = 1$ prior to block encoding.

3.1 Classical preconditioning

For comparison, we present the purely classical effect that preconditioning has on the matrix condition number. Note that this does not require any encoding, it is a simple matrix-matrix multiplication, and there is no equivalent of a subnormalisation factor.

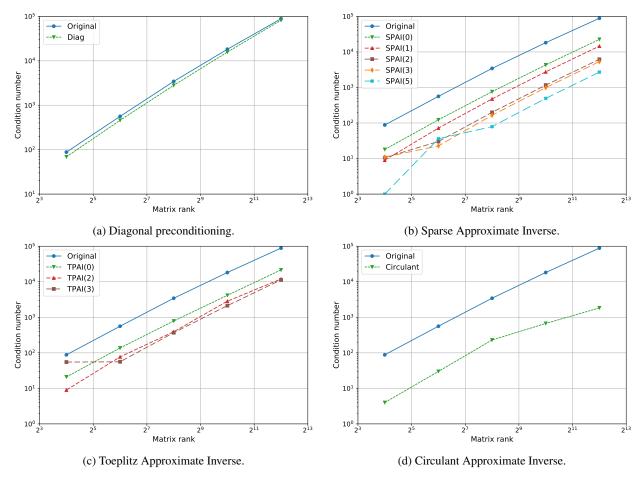


Figure 5: Classical preconditioning - condition numbers for PA as used by a classical algorithm. Computed using simple matrix-matrix multiplication. Numbers in brackets indicate levels of infill.

Figure 5 shows the effect of the four preconditioners on the condition numbers of the CFD matrix. As anticipated, diagonal scaling has little benefit by itself. There is some erratic behaviour for SPAI and TPAI with higher levels of infill on the coarser meshes which is due to the small matrix size. For larger meshes, there is an increasing benefit of more levels of infill. TPAI shows an initial improvement without infill but only a marginal improvement thereafter. There is no option to use infill with CLAI. However, it performs as well as SPAI with 3 levels of infill for the larger matrices.

3.2 Subnormalisation factors of preconditioners

We first consider the subnormalisation factors for encoding the preconditioner P. From Figure 6a we can see that the subnormalisation factor for A is approximately s=2 for all meshes. This is due to the mass conservation equation

being used to construct the pressure correction matrix, where for each row the diagonal entry is the negative of the sum of the off diagonal entries. The small difference from 2 is due to the fact that each diagonal is scaled by $1/||D||_{max}$ prior to encoding. The locations of the maximal entries can occur on different rows of the matrix and, hence, s=2 is lower bound if all the maxima occur on the same row. However, this is small effect that reduces on the finer meshes.

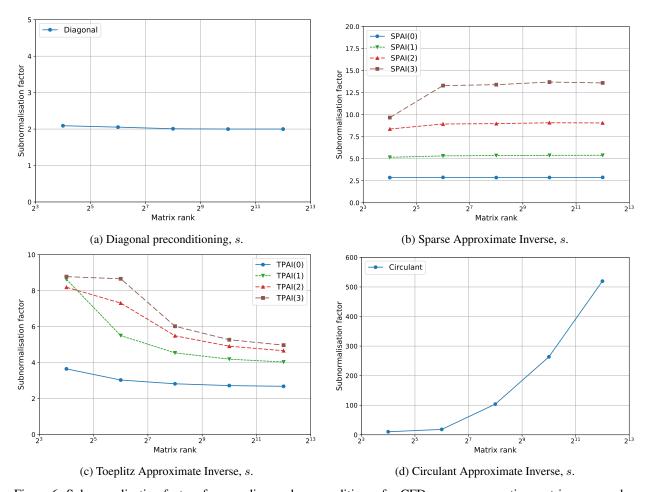


Figure 6: Subnormalisation factors for encoding each preconditioner for CFD pressure correction matrices on meshes ranging from 4×4 to 64×64 cells. Numbers in brackets indicate levels of infill.

The first observation is the striking difference between the values of *s* for the SPAI and TPAI preconditioners, Figure 6b and Figure 6c, as the level of infill is increased. This is largely due to the difference in the way each preconditioner adds infill. The numbers of diagonals added for each level of infill are compared in Table 1. These are independent of the CFD mesh size except for the two smallest cases. The difference in subnormalisation factors is largely attributable to the difference in the number of diagonals. This is not a pro-rata increase as it is the maximum entry along each diagonal that sets the PREP coefficients.

Another difference is that for each level of infill, the subnormalisation factors for TPAI reduce as the mesh size increases. Whereas, for SPAI, ignoring the smaller meshes, s is broadly constant as the mesh size increases. This is due to the need to approximate A as a Toeplitz matrix in order to compute the TPAI preconditioner. This adds infill to A which is significant on the smaller meshes but has a diminishing effect as the mesh size increases.

The second observation is that for the circulant preconditioner, s rises rapidly with the size of the matrix. This is due to the fact that as the mesh size increases, the cell dimensions become smaller and the lowest eigenvalue reduces. The increase in s is driven entirely by the need to scale Λ^{-1} so that $||\Lambda^{-1}||_{max} = 1$. There is no subnormalisation factor associated with the quantum Fourier transforms.

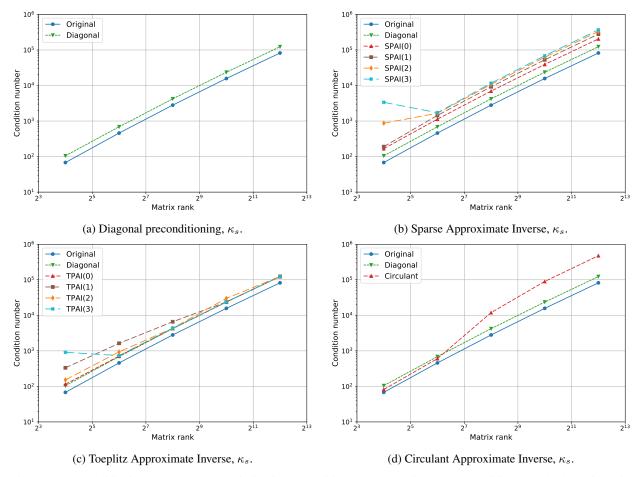


Figure 7: Preconditioning by quantum multiplication - condition numbers using all preconditioners. The blue line with circles (Original) gives the classical condition numbers (κ) of A without preconditioning. The green line with inverted triangles (Diagonal) gives the quantum condition numbers (κ_s) for the encoded matrix U_A without preconditioning. Numbers in brackets indicate levels of infill.

3.3 Preconditioning by quantum multiplication

The first approach to preconditioning is to separately encode A and its preconditioner, P, and then multiply the block encoded matrices on the quantum computer. From a circuit depth perspective, this is attractive as the Toeplitz and circulant preconditioners have efficient circuit implementations. However, the usual method [28] to quantum multiplication of matrices does result in the subnormalisation factors of A and P being multiplied.

Figure 7 shows the resulting values of κ_s for QSVT from Equation (5). All figures have two reference lines. The blue line labelled 'Original' is the classically computed condition number after diagonal scaling. Results below this line are better than a classical solver without preconditioning. The green line labelled 'Diagonal' is the block encoding of the original matrix. Results below this are better that a quantum solver without preconditioning.

As shown, none of the preconditioners reduce κ_s below the unpreconditioned value. For SPAI, Figure 7b, the benefit of increasing infill cannot overcome the increase in subnormalisation factor. All of the SPAI results are worse than not doing preconditioning. TPAI, Figure 7c, fares a little better due to the lower subnormalisation factors but it, too, offers no benefit over not doing preconditioning. CLAI, Figure 7d, performs the worst except for the smallest matrices due to the rapid increase in subnormalisation factor.

3.3.1 Preamplified quantum multiplication

Let U_A and U_P be block encoding circuits of A and P with subnormalisations α and β , respectively. Then [28] constructs a block encoding of AP with subnormalisation $\alpha\beta$ and 1 query to U_A and U_P each. The figure of merit [24]

of the resulting block encoding is the product of subnormalisation and circuit cost

$$\alpha\beta \cdot (\text{gates}(U_A) + \text{gates}(U_P)).$$
 (7)

This figure of merit, and not the gate count of the block encoding alone, determines the total cost of matrix inversion and other quantum algorithms (up to logarithmic factors), due to the appearance of the subnormalisation s in κ_s in the number of queries to the block encoding, see Equation (6).

Here, we study the method of preamplified quantum multiplication [29]. In the spirit of methods constructing preamplified block encodings [28, 24], separate parts of the quantum circuit are amplified individually to reduce the total figure of merit. Singular value amplification allows to improve the subnormalisation of a block encoding by a factor of γ with approximately

$$\gamma \frac{3}{\delta} \log \frac{\gamma}{\epsilon}$$
 (8)

 $\gamma \frac{3}{\delta} \log \frac{\gamma}{\epsilon} \tag{8}$ queries to the block encoding [24]. The parameters ϵ and δ determine the accuracy and range of singular value amplification.

For preamplified quantum multiplication of block encodings, U_A and U_P are first amplified by amplification factors $\gamma_1 < \alpha, \gamma_2 < \beta$, and then multiplied with the usual method for multiplying block encodings. The resulting block encoding has subnormalisation $\alpha\beta/(\gamma_1\gamma_2)$ and requires $\gamma_{1/2}\frac{3}{\delta}\log\frac{\gamma_{1/2}}{\epsilon}$ queries to U_A and U_P , respectively. The figure of merit is

$$\alpha\beta \left(\frac{1}{\gamma_2} \frac{3}{\delta} \log \frac{\gamma_1}{\epsilon} \cdot \operatorname{gates}(U_A) + \frac{1}{\gamma_1} \frac{3}{\delta} \log \frac{\gamma_2}{\epsilon} \cdot \operatorname{gates}(U_P)\right). \tag{9}$$

Preamplified multiplication is advantageous to regular multiplication (with figure of merit (8)) if

$$\gamma_1 > \frac{3}{\delta} \log \frac{\gamma_2}{\epsilon} \text{ and } \gamma_2 > \frac{3}{\delta} \log \frac{\gamma_1}{\epsilon},$$
(10)

which can be achieved if the original subnormalisations α , β allow for strong amplification. For the example matrices and matrix sizes considered in this work, we find that for preamplification of U_A , $\gamma_1 \simeq 1.25$ is the best that can be achieved. For U_P , $\gamma_2 \simeq 1.25 - 2.0$ can be achieved with more levels of infill allowing higher values of γ_2 . However, these are not sufficient to reduce the figure of merit, and we use regular quantum multiplication [28]. However, if the matrices involved have worse subnormalisations, the preamplified quantum multiplication method will provide an advantage.

3.4 Preconditioning by classical multiplication

The second approach is to perform the product of P and A as a classical preprocessing step and the encode PA. This is only feasible for TPAI and SPAI as PA retains some degree of sparsity. Figure 8 shows the resulting values of s and κ_s for encoding PA.

The subnormalisation factors, Figure 8a and Figure 8b, for TPAI and SPAI have similar values and are relatively insensitive to the size of the mesh and the number of levels of infill. When encoding the preconditioner, P, by itself, the subnormalisation factors for SPAI were significantly larger than TPAI due to the fact that the infill created more diagonals, see Table 1. However, when encoding PA, SPAI creates more diagonals than TPAI, but many of the diagonals contain only zeros to within the precision of the matrix product as discussed in Section 2.6. The presence of the zero-valued diagonals in SPAI does not influence the subnormalisation factor as the PREP operator just loads a zero coefficient. However, removing them from the encoding reduces the number of qubits needed for the PREP register. The net result is that SPAI with 3 levels of infill reduces the QSVT condition number, κ_s , by almost an order of magnitude. This, in turn, leads to a reduction of over 20 in the number of QSVT phase factors.

Although the reduction in κ_s is significant this comes with two costs:

- The product PA must be computed on the classical computer.
- The number of diagonals to be encoded is significantly higher than for the original matrix.

Counter-intuitively, the number of diagonals to encode PA is less than the number to encode P and A separately. For 3 levels of infill, separate encoding requires 41+5 diagonals, encoding PA after removing the zero diagonals requires only 21 diagonals, see Table 1.

The classical product PA can be parallelised and since each row-column multiplication leads to one multi-controlled rotation, the encoding circuit can be written directly without the need to form an intermediate matrix. Since the rotations for each diagonal commute, the parallel circuit generation does not create any loop-order dependencies.

Reducing the depth of the encoding circuit is described in the next section and relies on the fact that, as well as creating zero valued diagonals, SPAI also tends to equalise the values along each of the non-zero diagonals.

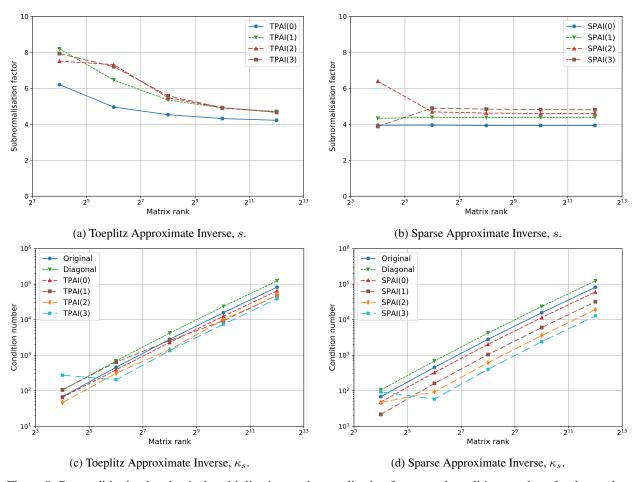


Figure 8: Preconditioning by classical multiplication - subnormalisation factors and condition numbers for the product PA using the TPAI and SPAI preconditioners. The blue and green lines in Figures (c) and (d) are the non-preconditioned reference lines as in Figure 7. Numbers in brackets indicate levels of infill.

4 Query oracle circuit trimming

The circuit trimming approach reduces the circuit size required for block encoding a band diagonal matrix (see Section 2.4. It relies on finding multiplexed rotations where the rotation angles are the same and the multiplexed controls differ by a Hamming distance of 1. The effectiveness of this is enhanced if the matrix is filtered to increase the number of equal-valued entries along each diagonal. We take a digitisation approach where values that are close to each other are placed in *bins* of equal value. However, the filtering needs to take account of the physical characteristics of the matrix and, for example, just because an entry is close to zero does not mean it can be rounded to zero. We use the double-pass filter approach described in Appendix E. The filter involves a free parameter, f that controls the size of the bins. This is a relative factor that sets the bin size to $\left[\left(1-\frac{f}{2}\right)\bar{d}_i, \left(1+\frac{f}{2}\right)\bar{d}_i\right]$ where \bar{d}_i is the average value of the i^{th} bin. The first pass creates a list of overlapping bins that all meet the size criterion. The second pass selects non-overlapping bins giving preference to bins with a large number of entries.

Figure 9 shows the influence of the smoothing factor, f, on the encoding of PA for the 16x16, 32x32 and 64x64 CFD meshes. The preconditioner is SPAI with 3 levels of infill. The overall trends are as expected: increasing f reduces the number of unique angles (i.e. fewer bin with more entries in each bin) and rotation gates, but increases the L_2 error of the solution vector.

There are two other notable features in Figure 9. The first is that the reduction in the number of unique angles is far greater than the reduction in the number of rotation gates. This is because not all multiplexed controls meet the requirement to be coalesced. The second feature is that the percentage reduction in the number of unique values and rotations increases with the size of the mesh. Taking the circuits for which the L_2 error is $\leq 10^{-2}$, the number of

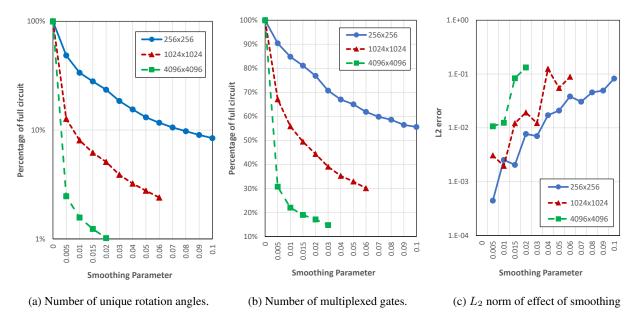


Figure 9: Effect of the smoothing parameter on the encoding circuit for PA where P uses SPAI with 3 levels of infill. The numbers of angles and rotations are shown as percentages of the unsmoothed values. Legends refer to the matrix dimensions not the CFD mesh dimensions.

rotations relative to the unsmoothed case is 70.7%, 49.5%, 30.7% for the 16x16, 32x32 and 64x64 meshes respectively. These features are discussed in Appendix E.3.

5 CFD Applications using QSVT

In this section we consider two test cases that have not been modelled previously due to the number of emulated qubits required. The QSVT phase factors are calculated with the Remez method [30, 31] using the open-sourced QSPPACK ⁴ software package.

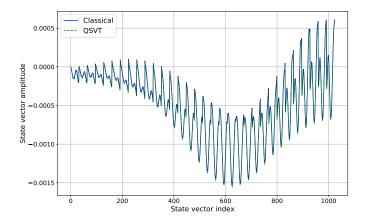


Figure 10: Comparison of QSVT and classical solutions from the pressure correction matrix of a 32x32 CFD mesh.

The solution contains corrections to the pressure field.

The first case is the pressure correction matrix for a 2D cavity with a 32x32 mesh sampled after 100 outer non-linear iterations. Figure 10 compares the QSVT and classical state vector solutions. These are stored at every point in the 2D

⁴https://github.com/qsppack/QSPPACK

mesh and are ordered in sweeps across the horizontal grid lines starting at the lower left corner of the cavity and ending at the top right. The results show good agreement with small differences due to the application of oracle trimming. The details of the QSVT calculation are:

- SPAI with 3 levels of infill.
- Diagonal smoothing factor, f = 0.015
- Number of unique angles reduced from 17374 to 1077.
- Number of nonzero rotations reduced from 18,378 to 8,928.
- Subnormalisation factor from classical multiplication, PA = 4.81
- 14,011 QSVT phase factors based on $\kappa_s=2,500$ and $\epsilon=0.01$
- L_2 norm of difference with the classical solution = 2.22×10^{-2}
- Total number qubits is 17 of which 16 are used for encoding PA, (with reference to Figure 2, there are $10 |j\rangle$ qubits, $5 |s\rangle$ qubits and $1 |d\rangle$ qubit) and 1 for signal processing.

As shown in Figure 9 the large reduction in the number of unique values does not translate into an equivalent reduction in the number of rotation gates. For comparison, previous HHL investigations estimated that this case would require 29 qubits [32]. Without preconditioning, QVST would require of the order 350,000 phase factors, a reduction of a factor of 25. Without preconditioning the number of rotation gates to block encode A is 4,290. Hence, the overall circuit depth is reduced by a factor of 12.5 with preconditioning.

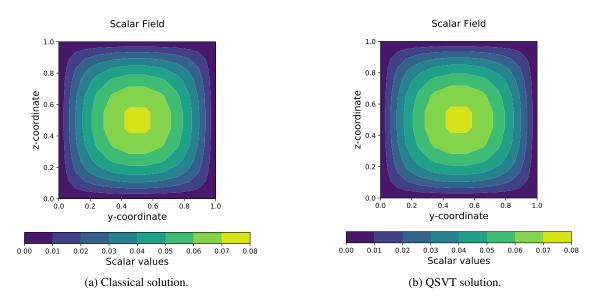


Figure 11: Solution of a 16x16x16 Laplacian matrix system for a scalar field representative of fully developed flow in a square sided channel. Contours are taken at a slice mid-way along the channel.

The second testcase is a 3D 16x16x16 Laplacian matrix system, set up using the open source L-QLES ⁵ framework [33]. The boundary conditions are set up to model fully developed Stokes flow in a square cross-section channel. The subnormalised condition number for encoding A is $\kappa_s=123.6$. Using SPAI preconditioning with no infill reduces this to $\kappa_s=65.2$. SPAI with one level of infill, which is used for this calculation, further reduces the condition number to $\kappa_s=36.7$.

Figure 11 compares the classical and QSVT solutions at a cross-section midway along the channel. There is very good agreement between the classical and QSVT solutions. The details of the QSVT calculation are:

- SPAI with one level of infill. The resulting product matrix, PA contains 63 diagonals of which 43 have non-zero entries
- Diagonal smoothing factor, f = 0.1

⁵https://github.com/rolls-royce/qc-cfd/tree/main/L-QLES

- Number of unique angles reduced from 21,262 to 1,852.
- Number of non-zero rotations reduced from 103,872 to 41,181.
- Subnormalisation factor from classical multiplication, PA = 5.48
- 249 QSVT phase factors based on $\kappa_s = 40$ and $\epsilon = 0.01$
- L_2 norm of difference with the classical solution = 8.2×10^{-3}
- Total number qubits is 20 of which 19 are used for encoding PA, (with reference to Figure 2, there are $12 |j\rangle$ qubits, $6 |s\rangle$ qubits and $1 |d\rangle$ qubit) and 1 for signal processing.

For comparison, 879 QSVT phase factors are needed to solve the system without preconditioning. However, the encoding of A requires only 8,348 rotation gates. Hence, in this case, the factor of 3.5 increase in phase factors is more than offset by the 4.9x saving in the number of rotation gates. The larger saving in rotation gates is due to the fact that the Laplacian matrix has a regular structure with many repeated entries, even before smoothing. This is not representative of 3D CFD testcases and savings similar to the 2D testcase are expected.

6 Conclusions

A thorough analysis of preconditioning has been performed using emulated circuits. Banded diagonal encoding using PREP-SELECT to load the diagonals of the matrix produces a low subnormalisation factor and a low qubit overhead. Block encoding P and A separately as a quantum multiplication circuit and encoding the classically multiplied product PA have been evaluated. Disappointingly, the subnormalisation factors for the quantum multiplication of P and A mean there is no reduction in the effective condition number κ_s for QSVT. Preamplified quantum multiplication has been considered but did not offer an advantage for the matrices considered here. This may be different for larger cases or non-banded matrices. The circulant preconditioner was beset by the need to encode a diagonal matrix of inverse eigenvalues with a maximum value over 500 on the largest test case. This has implications for other encodings based on singular value decomposition.

For classical multiplication, encoding PA with either TPAI or SPAI results in low subnormalisation factors that are largely independent of the matrix size and the number of levels of infill. SPAI with infill gives the best reduction in κ_s . An unexpected feature of SPAI with infill is that while the matrix PA has an increasing number of diagonals, over half of them contain only zeros. This has the beneficial effect that PA can be encoded with fewer diagonals than separately encoding P and A.

A diagonal filtering technique has been developed with allows circuit operations to be coalesced if certain criteria are met. The percentage reductions in circuit increase with mesh size giving some indication that sub-linear circuit depths may be achievable.

Given the initial concerns over subnormalisation factors, it was not obvious that encoding a classical matrix product would lead to a reduction in condition number. Indeed, encoding PA using SPAI with no infill gives only a marginal improvement over the classical condition number. Although SPAI with 3 levels of infill gives an order of magnitude reduction, it comes with large classical pre-processing cost. Fortunately, when forming PA in parallel, since the encoding operations commute, each parallel process can directly store its chunk of the circuit. This avoids the need to perform expensive sparse matrix-matrix products during the classical preconditioning step.

Two new emulation results have been achieved that were not previously possible. A 32x32 CFD matrix was emulated using only 17 qubits instead of 29 for HHL. A first 3D case using a Laplacian to approximate fully developed Stokes flow has been run on a 16x16x16 mesh.

Although this work has exploited the diagonal matrix structure of lattice-based meshes, for unstructured meshes the benefits of SPAI with infill are expected to be repeated.

7 Acknowledgements

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A Diagonal preconditioning

Diagonal preconditioning is based on scaling the rows and columns of a matrix by the inverse of the diagonal. If D is the matrix formed by the diagonal entries in A, then preconditioning is applied by:

$$(D^{-1}A)|x\rangle = D^{-1}|b\rangle \tag{11}$$

An alternative is to take D_s as the diagonal matrix of the square root of the diagonal entries which gives:

$$(D_s^{-1}AD_s^{-1}) D_s |x\rangle = D_s^{-1} |b\rangle$$
(12)

The difference between the two formulations is that Equation (11) scales the rows of A and Equation (12) scales both the rows and columns. The former is preferred as the solution vector, $|x\rangle$, is left unchanged. Classically, this is also referred to as Jacobi preconditioning but is rarely used as there are better performing preconditioners which yield a much greater reduction in the condition number. However, for QLES, the benefit is that as well as setting all the diagonal entries to unity, diagonal scaling tends to equalise other entries in the matrix. This is a necessary step prior to the Toeplitz and circulant approximate inverses discussed in Appendix C and Appendix D.

Note that diagonal preconditioning is not the same as diagonal encoding.

B Sparse Approximate Inverse (SPAI)

The objective of SPAI [34, 35, 2] is to find a preconditioning matrix M that minimises a function F(M) such that:

$$F(M) = ||I - AM||_F^2 \tag{13}$$

Where the subscript F the Frobenius norm of a matrix A defined by:

$$||A||_F = \sqrt{\sum_{i,j} |a_{i,j}|^2} = \sqrt{\text{Tr}(AA^{\dagger})}$$
 (14)

F(M) is minimised when M is close to A^{-1} . There are two approaches to this described below.

B.1 Sparse-Sparse Iteration Method

The first method uses the global minimal residual descent method [35]. After an appropriate M_0 has been selected, the following iterations are performed.

$$G_k = I - AM_k$$

$$\alpha_k = \operatorname{tr}(G_k^{\dagger} A G_K) / ||AG_k||_F^2$$

$$M_{k+1} = M_k + \alpha_k G_k$$
(15)

Each iteration of the algorithm adds new non-zero entries and reduces the sparsity of M_k as shown in Figure 12. This is called *infill* and the degree of infill is controlled via *numerical dropping*, i.e. ignoring any entries that fall outside the infill sparsity pattern. This can be applied to either M_k or G_k [35]. A common choice is to retain the same sparsity pattern for M_k as A_k .

The recommended starting approximation [35] is $M_0 = \alpha_0 A^T$, where

$$\alpha_0 = \frac{||A||_F}{||AA^{\dagger}||_F} \tag{16}$$

B.2 Column Minimisation Method

The second approach separates the minimisation into a set of independent column based operations that can be easily parallelised on a classical computer [36].

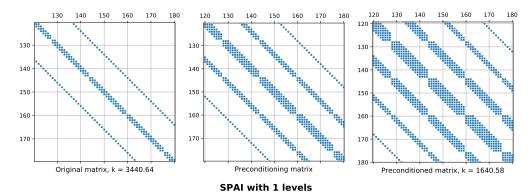


Figure 12: Zoomed in sparsity patterns for SPAI applied to 16x16 pressure correction matrix with 1 level of infill. Left: original matrix (A), centre: preconditioning matrix (P), right: result of preconditioning (PA)

Solving $AA^{-1} = I$ for A^{-1} can be expressed in terms of the column vectors \mathbf{y}_i of A^{-1} as:

$$A\mathbf{y}_{j} = \mathbf{e}_{j} \qquad (j = 0, N - 1) \tag{17}$$

where e_j is the j^{th} column of the identity matrix. If M is an approximation to A^{-1} then:

$$A\mathbf{m}_{j} \simeq \mathbf{e}_{j} \qquad (j = 0, N - 1) \tag{18}$$

For a given sparsity pattern, the entries in \mathbf{m}_i can be reordered to place all s non-zero entries, $\hat{\mathbf{m}}_i$ first:

$$\mathbf{m}_j = \begin{pmatrix} \hat{\mathbf{m}}_j \\ 0 \end{pmatrix} \tag{19}$$

Equation (19) can be achieved by a permutation operator, P_i that can be applied to A to give:

$$P_j A P_j^{-1} = \begin{pmatrix} \hat{A}_j & * \\ * & * \end{pmatrix} \tag{20}$$

And to e_i to give:

$$P_j \mathbf{e}_j = \begin{pmatrix} \hat{\mathbf{e}}_j \\ 0 \end{pmatrix} \tag{21}$$

From which we have N small $s \times s$ systems to solve:

$$\hat{A}_j \hat{\mathbf{m}}_j = \hat{\mathbf{e}}_j \qquad (j = 0, N - 1) \tag{22}$$

The size of s depends on the level of infill. For small values of s, Equation (22) can be directly inverted. For larger values, it can be solved via a least squares minimisation [12] or by finding the minimum of an energy functional [37]. The key to performance is that the N equations are independent and can be solved in parallel. Here, we use a direct Lower-Upper decomposition to solve Equation (22) exactly to within machine precision.

The infill pattern for the column minimisation method is the same as the sparse-sparse method and is computed by taking successive products with itself. This is an expensive task but can be performed as a one-off calculation. Since only the sparisty pattern is needed, it is sufficient to know whether each row-column multiplication has a common entry.

Finding a preconditioner of the form MA follows the same procedure except that \mathbf{m}_j and \mathbf{e}_j are row vectors and we solve:

$$\hat{\mathbf{m}}_j \hat{A}_j = \hat{\mathbf{e}}_j \qquad (j = 0, N - 1) \tag{23}$$

C Toeplitz Approximate Inverse (TPAI)

A Toeplitz matrix has the form:

$$\begin{pmatrix} t_{0} & t_{-1} & \dots & t_{2-n} & t_{1-n} \\ t_{1} & t_{0} & t_{-1} & \ddots & t_{2-n} \\ \vdots & t_{1} & t_{0} & \ddots & \vdots \\ t_{n-2} & \ddots & \ddots & \ddots & t_{-1} \\ t_{n-1} & t_{n-2} & \dots & t_{1} & t_{0} \end{pmatrix}$$

$$(24)$$

The Toeplitz Approximate Inverse (TPAI) is inspired by the SPAI column minimisation method from Appendix B.2. However, it makes the further approximation that the inverse is itself a Toeplitz matrix. This means that only one $s \times s$ system needs to be inverted instead of N. More importantly from a quantum perspective, the TPAI can be encoded with circuit depth of $\mathcal{O}(d)$ where d is the number of diagonals, rather than $\mathcal{O}(dN)$ for SPAI.

The TPAI method begins by approximating A with a Toeplitz matrix:

$$\hat{A} = S_{diag}(D^{-1}A) \tag{25}$$

Where D is the diagonal scaling matrix described in Appendix A. For the CFD matrices considered here, this creates ones along the main diagonal and tends to equalise the entries along the off-diagonals. S_{diag} is a function that takes the average value along each diagonal and uses the result for the value along the corresponding Toeplitz diagonal. This approach is only appropriate to matrices that have a predominantly diagonal sparsity pattern.

It is further assumed that \hat{A} and its TPAI have infinite dimension. To illustrate consider the case when \hat{A} is tridiagonal with entries a, b, c and the approximate inverse is also tridiagonal with entries a_i, b_i, c_i . Multiplying a row of the inverse with a 3x3 block of \hat{A} gives a row of the identity matrix:

$$\begin{pmatrix} a_i & b_i & c_i \end{pmatrix} \begin{pmatrix} b & c & 0 \\ a & b & c \\ 0 & a & b \end{pmatrix} = \begin{pmatrix} 0 & 1 & 0 \end{pmatrix}$$
 (26)

The inverse of the 3x3 block matrix is:

$$\frac{1}{b^3 - 2abc} \begin{pmatrix} b^2 - ac & -bc & c^2 \\ -ab & b^2 & -bc \\ a^2 & -ab & b^2 - ac \end{pmatrix}$$
 (27)

Solving for the approximate inverse gives:

$$b_i = b/(b^2 - 2ac)$$

$$a_i = -ab_i/b$$

$$c_i = -cb_i/b$$
(28)

Infill is treated the same as SPAI and is illustrated with a pentadiagonal preconditioner for a tridiagonal \hat{A} where a 5×5 system is solved:

$$\begin{pmatrix}
a_i & b_i & c_i & d_i & e_i
\end{pmatrix}
\begin{pmatrix}
b & c & 0 & 0 & 0 \\
a & b & c & 0 & 0 \\
0 & a & b & c & 0 \\
0 & 0 & a & b & c \\
0 & 0 & 0 & a & b
\end{pmatrix} = \begin{pmatrix}
0 & 0 & 1 & 0 & 0
\end{pmatrix}$$
(29)

The inverse of the 5x5 block matrix is:

$$\frac{1}{D} \begin{pmatrix} b^4 - 3ab^2c + a^2c^2 & -b^3c + 2abc^2 & b^2c^2 - ac^3 & -bc^3 & c^4 \\ -ab^3 + 2a^2bc & b^4 - 2ab^2c & -b^3c + abc^2 & b^2c^2 & -bc^3 \\ a^2b^2 - a^3c & -ab^3 + a^2bc & b^4 - 2ab^2c + a^2c^2 & -b^3c + abc^2 & b^2c^2 - ac^3 \\ -a^3b & a^2b^2 & -ab^3 + a^2bc & b^4 - 2ab^2c & -b^3c + 2abc^2 \\ a^4 & -a^3b & a^2b^2 - a^3c & -ab^3 + 2a^2bc & b^4 - 3ab^2c + a^2c^2 \end{pmatrix}$$
(30)

where, the determinant D is:

$$D = b^5 - 4ab^3c + 3a^2bc^2 (31)$$

Solving for the approximate inverse gives:

$$a_{i} = (a^{2}b^{2} - a^{3}c)/D$$

$$b_{i} = (-ab^{3} + a^{2}bc)/D$$

$$c_{i} = (b^{4} - 2ab^{2}c + a^{2}c^{2})/D$$

$$d_{i} = (-b^{3}c + abc^{2})/D$$

$$e_{i} = (b^{2}c^{2} - ac^{3})/D$$
(32)

For greater levels of infill, the $s \times s$ system is solved using a Lower-Upper decomposition [1]. Note that the preconditioner is applied to $D^{-1}A$ and not \hat{A} .

The infill for TPAI simply adds new diagonals adjacent to the existing diagonals. This results in lower levels of infill as SPAI. As reported in the main text, this leads to trade-off between the level of reduction in the condition number and the subnormalisation factor for encoding the preconditioning matrix.

D Circulant Approximate Inverse

A circulant matrix is a special case of a Toeplitz matrix and has the form:

$$\begin{pmatrix} c_{0} & c_{n-1} & \dots & c_{2} & c_{1} \\ c_{1} & c_{0} & c_{n-1} & \ddots & c_{2} \\ \vdots & c_{1} & c_{0} & \ddots & \vdots \\ c_{n-2} & \ddots & \ddots & \ddots & c_{n-1} \\ c_{n-1} & c_{n-2} & \dots & c_{1} & c_{0} \end{pmatrix}$$

$$(33)$$

For an arbitrary matrix A, the circulant preconditioner has the form [38, 39]:

$$C(A) = F^{\dagger} \operatorname{diag}(FAF^{\dagger})F \tag{34}$$

where $F_{jk} = \frac{\omega jk}{\sqrt{N}}$ and $\omega = e^{-2\pi i/N}$. F is effectively the Quantum Fourier Transform (QFT) operator. The diagonal term can be computed from:

$$\Lambda_k = \operatorname{diag}(FAF^{\dagger})_k = \frac{1}{n} \sum_{p,q} \omega^{(p-q)k} A_{p,q}$$
(35)

The preconditioned system is $C^{-1}Ax = C^{-1}b$. Hence, an efficient way to compute C^{-1} is needed. From Equation (34) and Equation (35):

$$C^{-1} = F\Lambda^{-1}F^{\dagger} \tag{36}$$

The benefit of the circulant preconditioner is that C^{-1} can be efficiently implemented on a quantum computer.

E Double pass filtering to create equal values

When filtering or smoothing entries in the matrix, it is important to respect the underlying discretisation on which the matrix is based. Non-uniform meshes can create mesh volumes that vary by several orders of magnitude. Variations in flow properties, e.g. between the free-stream and near the walls can also be significant. Hence, matrix entries that are close to zero cannot be arbitrarily rounded to zero.

E.1 Digitising the matrix entries

To avoid rounding non-zero values to zero, the digitisation algorithm creates *bins* based on percentages of the mean value within each bin. The principle is illustrated in Figure 13.

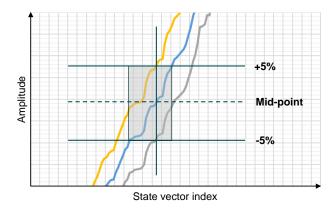


Figure 13: Bin selection for digitising the matrix entries: blue = entries in ascending order, yellow = +5%, grey = -5%. Box indicates the extent of the bin. - all blue values in the bin are reset to the mid-point value.

The algorithm initially applies a convolution operator to the ordered state amplitudes. This creates a number of potential bins, all of which meet the criteria that the values in each bin differ by no more than a given percentage, e.g. 10% as shown in Figure 13. At this stage, there are a number of overlapping bins. A marching algorithm then eliminates any overlaps by retaining bins with the largest number of entries. As with most marching algorithms, it is a *greedy* algorithm and is not guaranteed to produce the minimum number of bins and/or the maximum number of repeats.

E.2 Collapsing equal angled rotation gates

Having created a circuit with a large number of equal angle rotations, the final step is to collapse as many pairs of controlled rotations as possible [27]. The requirements to coalesce two controlled rotations:

- Both rotations must belong to the same matrix diagonal.
- Both rotations must have the same angle. In practice, this is relaxed by a small amount to allow for rounding error
- The bit patterns of the controls on each rotation must have a Hamming distance of 1.

The collapsing of equal-valued rotations is shown in Figure 14.

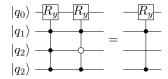


Figure 14: Coalescing multi-qubit controlled gates with a Hamming distance of 1 where the R_y gates have the same rotation angle.

Within each bin, the coalescing process is as follows:

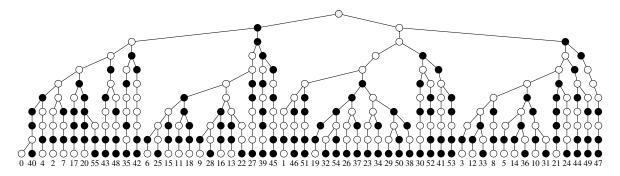
- Collect all operations that are a Hamming distance of 1 away from any other operation.
- Create a binary tree based on the multiplexed controls.
- Sweep through the levels of the tree, coalescing branches that have a Hamming distance of 1.

E.3 Performance

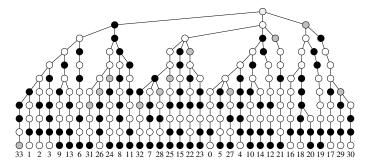
The performance of filtering and collapsing algorithm is illustrated in Figure 15. In this example, the bin contains 56 equal-valued multiplexed rotations, all of which are a Hamming distance of 1 away from at least one other rotation. The

collapsing algorithm reduces this to 34 rotations. Examination of Figure 15a shows that there are 16 rotations that have not been modified and none are within a Hamming distance of 1 of the other. Note that while the matrix entries have been reordered to be monotonic, this does not mean that controls correspond to a contiguous set of integers.

For larger bins, the relative performance is seen to improve. For a bin of 145 equal-valued rotations, the collapsing algorithm reduces this to 45. As the size of the matrix increases, so does the size of the bins resulting in the greater percentage reductions shown in Figure 9.



(a) Binary tree for untrimmed circuit. All paths in the tree are a Hamming distance of 1 away from at least one other path.



(b) Binary tree for trimmed circuit. Grey nodes correspond to controls that have been removed.

Figure 15: Performance of the circuit trimming algorithm, displayed as a binary tree. Each path from the lowest leaves to the root represents a controlled rotation.

Figure 16 shows the circuit with the multiplexed rotations trimmed according to the tree in Figure 15b. The labels on the circuit gates correspond to paths through the tree.

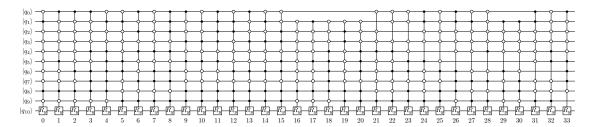


Figure 16: Section of matrix loading circuit after trimming. All R_y gates have the same rotation angle. The gate indices correspond to the path labels in Figure 15b