Revised algorithm description section

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1 ISA framework and implementation

1.1 ISA framework

The ISA framework iterates two steps: select and prepare. In the select step, a sparse quantum state $|x'\rangle$ is selected to approximate the target state $|x\rangle$. In the prepare step, the quantum state preparation method for $|x'\rangle$ is used to approximately prepare $|x\rangle$. The select and prepare steps are iterated until the resultant state is sufficiently close to $|0\rangle$.

$$|\langle 0|x_{final}\rangle|^2 \geq 1 - \epsilon$$

The ISA framework is summarized in Figure [number]. In the following sections, we describe our implementation of the ISA framework, starting with some definitions, then the description of a subroutine, followed by our sparse quantum state preparation method, after which we give a formal description of the select and prepare steps, and finish by describing some optimizations.
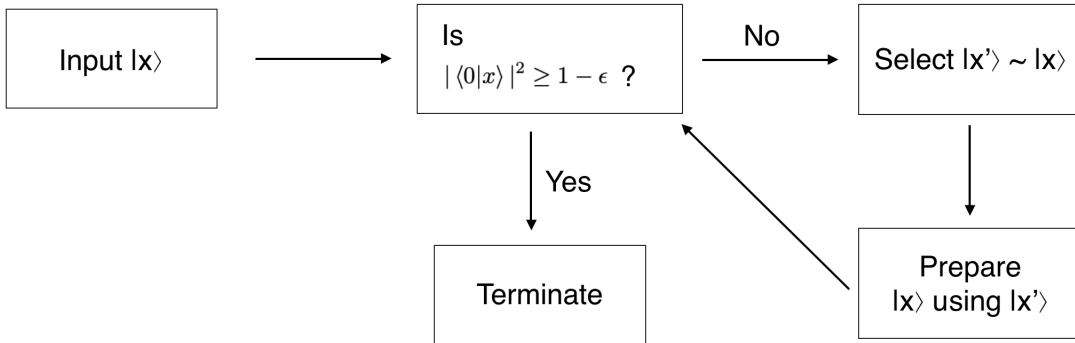

Figure 1: Block diagram summary of the proposed ISA framework

1.2 Pattern and Substate Definition

A k-bit pattern over n-qubits is defined as a length-n string in $\{0, 1, *\}^n$, containing exactly k '$*$' characters. The parameter k may be 0, in which case p would be a length-n bitstring. An n-bit integer i matches a pattern p if each bit in the binary representation of i matches the corresponding character in p ('$*$' matches both 0 and 1). Then, let I_p denote the set of 2^k integers that match the k-bit pattern p.

Next, define the p-substate of a quantum state $|x\rangle$ as:

$$|x\rangle_p = \sum_{i \in I_p} |i\rangle \langle i|x\rangle.$$

When $|x\rangle$ is written in the computational basis, $|x\rangle_p$ contains the subset of basis states $|i\rangle$ where i matches p. In most cases, the norm of $|x\rangle_p$ is less than 1, and therefore does not represent a proper quantum state, but is instead a complex-valued vector. Still, we define the action of quantum gates on these substates as we would for normal quantum states.

An X or CX gate may be applied to a pattern p as long as their relevant qubit indices do not correspond to indices where p has a $*$. If an X gate targeting qubit i is applied to a pattern p, the result is p but with the ith character inverted from 0 to 1 or vice versa. If a CX gate with control qubit i and target qubit j is applied to p and $p[i] = 0$, the result is p; otherwise, the result is p with the jth character inverted. This behavior of X and CX gates on patterns is chosen to match the behavior of those gates on substates, as described in Lemma 1.

Lemma 1: If an X or CX gate g may be applied to a pattern p, then for all quantum states $|x\rangle$, $g(|x\rangle_p) = (g\,|x\rangle)_{gp}$.

Proof: Define $g(i)$ such that $g\,|i\rangle = |g(i)\rangle$. Then, one can verify that $g(i) \in I_{gp}$ for all $i \in I_p$. Since applying g twice, in the context of both patterns and substates, amounts to the identity transformation, $g(j) \in I_p$ for all $j \in I_{gp}$. This implies that g creates a bijection between I_p and I_{gp}. In addition, given that X and CX gates on quantum states represent amplitude permutations in the computational basis, $\langle g(i)|g|x\rangle = \langle i|x\rangle$. Then,

$$g(|x\rangle_p) = g \sum_{i \in I_p} |i\rangle \langle i|x\rangle$$

$$= \sum_{i \in I_p} g\,|i\rangle \langle g(i)|g|x\rangle$$

$$= \sum_{i \in I_p} |g(i)\rangle \langle g(i)|g|x\rangle$$

$$= \sum_{g(i) \in I_{gp}} |g(i)\rangle \langle g(i)|g|x\rangle$$

$$= (g\,|x\rangle)_{gp}$$

as desired.

1.3   Substate merging

Our implementation of the ISA framework makes extensive use of a substate merging subroutine, which we describe here. Given a quantum state $|x\rangle$, a k-bit pattern p, and an X gate g that can be applied to p, the substate merging subroutine applies a single qubit rotation R to $|x\rangle$ to the target qubit of g such that the norm of $(R\,|x\rangle)_p$ is maximized.

Any single qubit rotation can be decomposed into an RZ-RY-RZ sequence. Since RZ gates apply only complex phases to amplitudes in the computational basis, the last RZ gate has no effect on the norm of $(R\,|x\rangle)_p$, and can be left out. Thus, we parameterize $R = RY(\theta)RZ(\phi)$.

To compute the optimal θ and ϕ, we perform casework on $p[i]$. If $p[i] = 0$, then $gp[i] = 1$, and

$$(R\,|x\rangle)_p = (RY(\theta)RZ(\phi)\,|x\rangle)_p$$

$$= cos(\frac{\theta}{2})\,|x\rangle_p - e^{i\phi}sin(\frac{\theta}{2})(g\,|x\rangle)_p \quad \textit{(up to global phase)}$$

The squared norm of this vector is:

$$|(R\,|x\rangle)_p|^2 = \left(cos(\frac{\theta}{2})\langle x|_p - e^{-i\phi}sin(\frac{\theta}{2})(\langle x|\,g)_p\right)\left(cos(\frac{\theta}{2})\,|x\rangle_p - e^{i\phi}sin(\frac{\theta}{2})(g\,|x\rangle)_p\right)$$

$$= cos^2(\frac{\theta}{2})\langle x|_p\,|x\rangle_p - 2cos(\frac{\theta}{2})sin(\frac{\theta}{2})\mathrm{Re}(e^{-i\phi}(\langle x|\,g)_p\,|x\rangle_p) + sin^2(\frac{\theta}{2})(\langle x|\,g)_p(g\,|x\rangle)_p$$

$$= cos^2(\frac{\theta}{2})\langle x|_p\,|x\rangle_p - 2cos(\frac{\theta}{2})sin(\frac{\theta}{2})\mathrm{Re}(e^{-i\phi}\langle x|_{gp}\,g\,|x\rangle_p) + sin^2(\frac{\theta}{2})\langle x|_{gp}\,|x\rangle_{gp},$$

2

Where the last step used Lemma 1 to simplify. The first and third terms of this expression are nonnegative, and do not depend on the sign of θ. Therefore, θ can be chosen such that the coefficient $-2cos(\frac{\theta}{2})sin(\frac{\theta}{2})$ of the second term is positive. Then, the expression is maximized when $e^{-i\phi}(\langle x|_{gp})g\,|x\rangle_p$ is a positive real number with no imaginary part, which is achieved by assigning

$$\phi = \text{phase}(\langle x|_{gp}\, g\, |x\rangle_p)$$

Performing this substitution and simplifying using half-angle laws gives:

$$|(R\,|x\rangle)_p|^2 = cos^2(\frac{\theta}{2})\,\langle x|_p\,|x\rangle_p - 2cos(\frac{\theta}{2})sin(\frac{\theta}{2})|\,\langle x|_{gp}\, g\, |x\rangle_p\,| + sin^2(\frac{\theta}{2})\,\langle x|_{gp}\,|x\rangle_{gp}$$

$$= \frac{1}{2}(1 + cos(\theta))\,\langle x|_p\,|x\rangle_p - sin(\theta)|\,\langle x|_{gp}\, g\, |x\rangle_p\,| + \frac{1}{2}(1 - cos(\theta))\,\langle x|_{gp}\,|x\rangle_{gp}$$

$$= \frac{1}{2}(\langle x|_p\,|x\rangle_p + \langle x|_{gp}\,|x\rangle_{gp}) + \frac{1}{2}cos(\theta)(\langle x|_p\,|x\rangle_p - \langle x|_{gp}\,|x\rangle_{gp}) + sin(\theta)|\,\langle x|_{gp}\, g\, |x\rangle_p\,|$$

This quantity is maximized when

$$\theta = -arccos(\frac{A}{\sqrt{A^2 + B^2}})$$

$$A = \frac{1}{2}(\langle x|_p\,|x\rangle_p - \langle x|_{gp}\,|x\rangle_{gp})$$

$$B = |\,\langle x|_{gp}\, g\, |x\rangle_p\,|$$

Once θ and ϕ are determined, R can be constructed.

In the other case, $p[i] = 1$, $gp[i] = 0$. Then,

$$(R\,|x\rangle)_p = sin(\frac{\theta}{2})(g\,|x\rangle)_p + e^{i\phi}cos(\frac{\theta}{2})\,|x\rangle_p .$$

The squared norm of this vector is

$$|(R\,|x\rangle)_p|^2 = \left(sin(\frac{\theta}{2})(\langle x|\, g)_p + e^{-i\phi}cos(\frac{\theta}{2})\,\langle x|_p\right)\left(sin(\frac{\theta}{2})(g\,|x\rangle)_p + e^{i\phi}cos(\frac{\theta}{2})\,|x\rangle_p\right)$$

Performing the same calculations as before, this quantity is maximized when

$$\theta = arccos(\frac{A}{\sqrt{(A^2 + B^2)}})$$

$$\phi = \text{phase}(\langle x|_p\, g\, |x\rangle_{gp})$$

where A and B are defined the same as before. This procedure is called substate merging because equations [REF] and [REF] show that the final substate, $(R\,|x\rangle)_p$, is a linear combination of $|x\rangle_p$ and $|x\rangle_{gp}$; it's as if $|x\rangle_{gp}$ is merged with $|x\rangle_p$ to form a new, larger-magnitude substate $(R\,|x\rangle)_p$, while some residue is left behind at $(R\,|x\rangle)_{gp}$. For this reason, the substate merging procedure will be described as "merging $|x\rangle_{gp}$ into $|x\rangle_p$."

In most cases, the substate merging procedure needs to be modified such that it doesn't disturb the amplitude at $|0\rangle$. We call this modified procedure "controlled substate merging" and define it as follows. Given a quantum state $|x\rangle$, a pattern p, and a CX gate g that can be applied to p (and $gp \neq p$), the controlled substate merging procedure applies a transformation R consisting of the CX gate g and single-qubit rotations applied to the target qubit of g, such that the norm of $(R\,|x\rangle)_p$ is maximized and $\langle 0|Rx\rangle = \langle 0|x\rangle$, up to global phase.

The substate merging procedure can be adapted for controlled substate merging as follows. First, the RZ-RY sequence R' is constructed for merging $|x\rangle_p$ into $|x\rangle_{gp}$:

$$R' = RY(\theta)RZ(\phi).$$

In this pair of gates, only the RY gate disturbs the amplitude at $|0\rangle$, thus, the RY gate is replaced with a controlled-RY gate, then decomposed into CX and RY:

$$R' = CRY(\theta)RZ(\phi)$$

$$= gRY(-\frac{\theta}{2})gRY(\frac{\theta}{2})RZ(\phi)$$

where g is the CX gate given in the problem statement. The transformation R' minimizes $(R'|x\rangle)_p$ and maximizes $(R'|x\rangle)_{gp}$, whereas the opposite effect is desired. This problem is amended by removing the trailing g in the gate sequence R' to get the desired gate sequence R:

$$R = RY(\frac{\theta}{2})gRY(\frac{\theta}{2})RZ(\phi).$$

One interesting property of this specific construction is that, for all integers i where $g|i\rangle = |i\rangle$, $\langle i|R|x\rangle = \langle i|x\rangle$ up to a complex phase, and the restriction $\langle 0|Rx\rangle = \langle 0|x\rangle$ is a special case of this more general property of the construction for controlled substate merging. This property will prove useful for our ISA implementation.

1.4 Sparse quantum state preparation

In this work, we consider sparse quantum states of the form:

$$|x'\rangle = \sum_{i \in I_{p^0}} c_i |i\rangle + \sum_{j \in I_p} c_j |j\rangle$$

where p is a k-bit pattern, $k \leq 2$, p^0 is p but with its '1' characters set to 0, and $p \neq p^0$. We also require the '$*$' characters in p to be adjacent to each other, if there are two of them, and for all pairs k and l where $p[k] = p[l] = 1$, there exists no m such that $k < m < l$ and $p[m] = $ '$*$'. Patterns meeting these latter two criteria regarding the positioning of '1' and '$*$' characters are called "compatible", since these criteria are necessary for our sparse quantum state preparation method to work on linear nearest neighbor architectures specifically.

As a base case, if p contains at most one '1' character, and that '1' character is adjacent to a '$*$' character, then $|x'\rangle$ is a $k+1$-qubit quantum state on neighboring qubits; $k+1 \leq 3$, so existing exact state preparation methods can be used in this case. Otherwise, we can construct a sequence of CX gates $g_1, g_2, ..., g_m$ and a sequence of patterns $p_0, p_1, ..., p_m$ such that $p_k = g_k p_{k-1}$ for all $1 \leq k \leq m$, $p_0 = p$, and p_m is a base case pattern. For this construction to be possible on linear nearest neighbor architectures, the pattern p must satisfy the compatibility criteria described above. From here, we construct the sequence $|x'_0\rangle, |x'_1\rangle, ..., |x'_m\rangle$ such that $|x'_k\rangle = g_k |x'_k\rangle$. Repeatedly applying Lemma 1 shows that

$$|x'_m\rangle = \sum_{i \in I_{p^0}} c'_i |i\rangle + \sum_{j \in I_{p_m}} c'_j |i\rangle,$$

for some complex amplitudes c'_i and c'_j. This is $k+1$-qubit quantum state on adjacent qubits, which can be prepared by existing methods. In summary, our sparse quantum preparation method uses a sequence of CX gates to move the p-substate to qubits adjacent to the p^0-substate, then applies exact quantum state preparation.

The number of CX gates our method needs to prepare sparse quantum states is the minimum possible length m of the CX sequence used to move the p-substate plus the number of CX gates needed for the base case. Let cost(p) denote this quantity. Breadth first search can be used to compute cost(p); despite the inefficiency of this approach, the computation for cost(p) needs to be performed only once and can therefore be precomputed and cached.

1.5 ISA framework implementation

In the previous sections, we described the building blocks for ISA implementation; in this section, we assemble the pieces.

For the select step, we enumerate all compatible k-bit patterns p, with $k \leq 2$. For each pattern, we construct the corresponding (non-normalized) sparse approximation

$$|x'(p)\rangle = |x\rangle_{p^0} + |x\rangle_p .$$

When the sparse quantum state preparation method is applied to $|x'(p)\rangle$, the result is $|\,|x'(p)\rangle\,|\,|0\rangle$; when the same gate sequence is applied to $|x\rangle$ to get $|x_1\rangle$, we expect $\langle 0|x\rangle = |\,|x'(p)\rangle\,|$. This corresponds to a fidelity increase of $\langle x'(p)|x'(p)\rangle - |\langle 0|x\rangle|^2$ using $\text{cost}(p)$ CX gates, or a fidelity increase ratio of

$$ratio(p) = \frac{\langle x'(p)|x'(p)\rangle - |\langle 0|x\rangle|^2}{1 + \text{cost}(p)}.$$

Adding 1 to the denominator is necessary to prevent division by zero errors when $\text{cost}(p)$ is zero. In the select step, we greedily choose p to maximize $ratio(p)$ and select the corresponding sparse approximation $|x'(p)\rangle$.

In the prepare step, the sparse quantum state preparation method is adapted for general quantum state preparation. In our implementation, we replace the iterated application of CX gates to move the p-substate with the iterated application of controlled substate merging. This change allows the p-substate of $|x\rangle$ to increase in length as it moves towards a base-case pattern, instead of keeping the same norm throughout. Also, using controlled substate merging in place of CX gates will not affect the p^0 substate, as argued at the end of [SUBSTATE MERGE SECTION REF]. In addition, we implement a greedy selection procedure to construct the pattern sequence $p_0, p_1, ..., p_m$. Specifically, we implement prepare using the following procedure:

1. If p is a base case pattern, apply exact quantum state preparation and terminate the prepare step.

2. Otherwise, construct P, the set of patterns p' that can be reached from p using one CX gate.

3. For each $p' \in P$, compute the magnitude of the substate that would result from merging $|x\rangle_p$ with $|x\rangle'_p$, call this quantity $mag(p')$.

4. For each p', compute the projected fidelity increase ratio as

$$ratio(p') = \frac{mag(p') + \langle x|_{p^0} |x\rangle_{p^0} - |\langle 0|x\rangle|^2}{1 + min(\text{cost}(p), \text{cost}(p'))}$$

   The numerator is the projected fidelity increase after substate merging, while the denominator is the projected number of CX gates - one for substate merging, and $min(\text{cost}(p), \text{cost}(p'))$ to prepare the resulting sparse approximation.

5. Select p' such that it maximizes $ratio(p')$. If $\text{cost}(p) < \text{cost}(p')$, then apply controlled substate merge to merge $|x\rangle_{p'}$ into $|x\rangle_p$. Otherwise, controlled substate merge $|x\rangle_p$ into $|x\rangle_{p'}$, set $p = p'$, and return to the first step.

It may seem possible that this procedure will always select p' with $\text{cost}(p') > \text{cost}(p)$ in step 5 and get stuck in an infinite loop. However, this will never happen because each time another substate is merged into $|x\rangle_p$, an extra CX gate is used. This extra CX gate can only ever be justified by a corresponding increase in projected fidelity increase, and the projected fidelity increase cannot increase indefinitely.

This concludes the description of our implementation of the select and prepare steps of the ISA framework.

1.6 Optimizations

We describe two optimizations to our implementation of the ISA framework: refinement by RZ-RY, and retroactive base case reduction.

1.6.1 Refinement by RZ-RY

Refinement by RZ-RY seeks to apply approximate quantum state preparation to the target state $|x\rangle$ without using any CX gates, before applying the ISA framework. This is done by selecting a zero-bit pattern p such that $|\,|x\rangle_p\,|$ is maximized (ties are broken randomly), then applying substate merging several times to eventually merge $|x\rangle_p$ into $|x\rangle_p$. The selection procedure resembles the implementation of prepare, but using substate merging instead of controlled substate merging:

1. If p is the string of all zeroes, then terminate this procedure. Otherwise, continue.

2. Construct the set P, containing zero-bit patterns p' that differ from p.

3. Select p' such that $|x\rangle_{p'}$ is maximized, with ties broken randomly.

4. Let i be the index where p and p' differ. If $p[i] = 0$ then merge $|x\rangle_{p'}$ into $|x\rangle_p$, otherwise, merge $|x\rangle_p$ into $|x\rangle'_p$ and update $p = p'$. Return to step 1.

1.6.2 Retroactive base case reduction

When a two-bit pattern p is chosen in the select step, the corresponding quantum circuit takes on the structure shown in Figure [number].
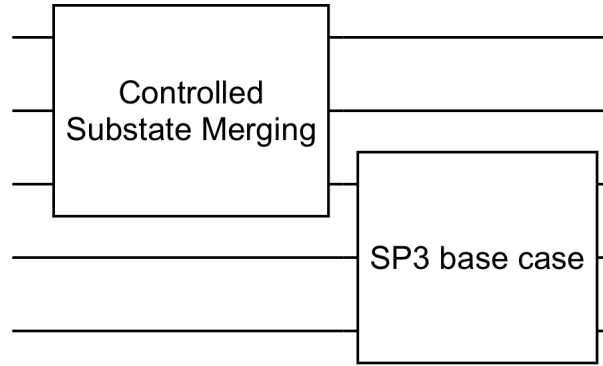

Figure 2: *The quantum circuit structure for the prepare step for a 2-bit pattern*

The three-qubit quantum state preparation step can be broken into two steps: disentangling the third qubit, and two-qubit state preparation on the remaining two qubits.
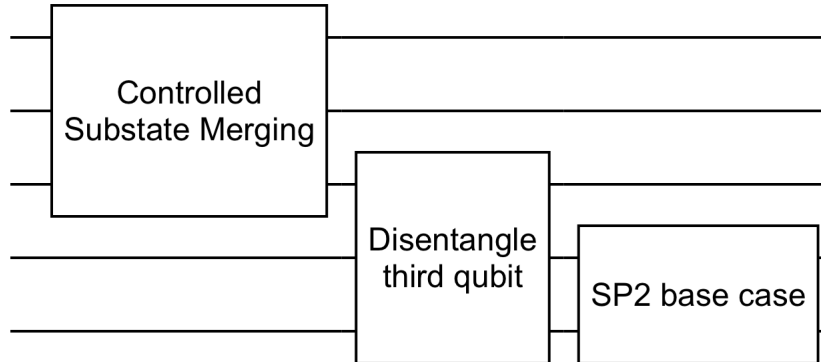

Figure 3: *The quantum circuit structure for the prepare step for a 2-bit pattern, with the base case decomposed*

If two consecutive iterations of ISA both selected a two-bit pattern, and those two patterns had their '∗' characters on the same two qubits, the resulting quantum circuit would have the structure shown in Figure [number].
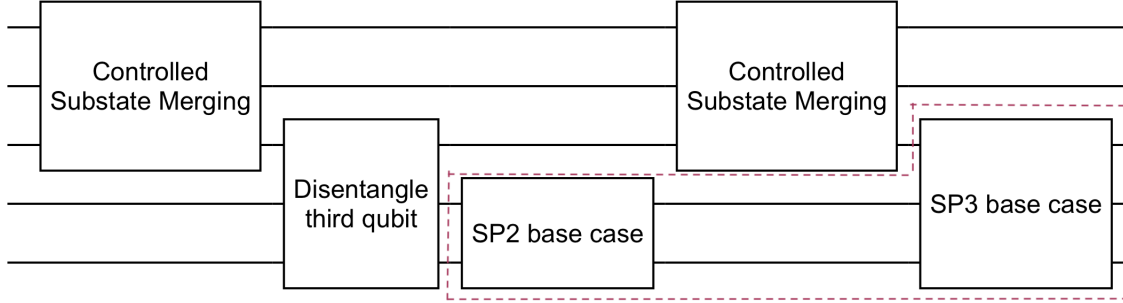

Figure 4: *The quantum circuit structure for two consecutive prepare steps with the same '∗' pattern*

The part of the quantum circuit enclosed in dotted lines first performs two-qubit state preparation on the lower two qubits, then performs three-qubit state preparation on all three relevant qubits. These two transformations have the net effect of transforming the three-qubit substate to $|0\rangle$, and can instead be replaced by a single three-qubit state preparation routine. This procedure saves the one CX gate used by the two-qubit state preparation base case.
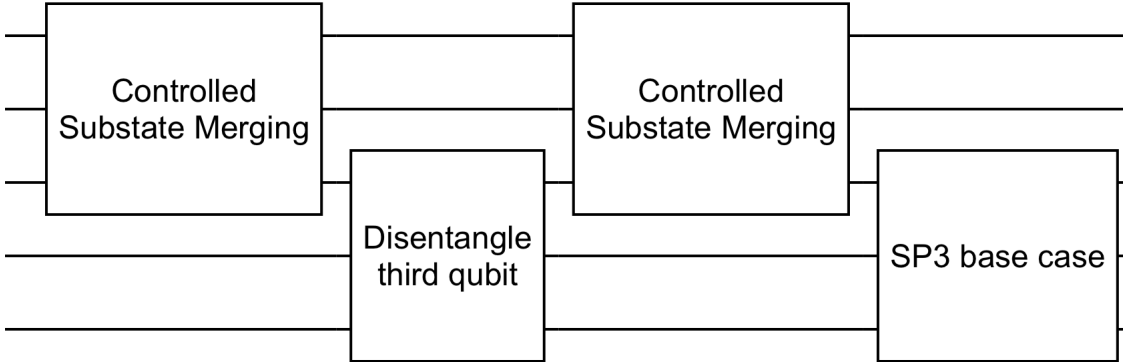

Figure 5: *The quantum circuit structure for two consecutive prepare steps with the same '∗' pattern, simplified*

We use this insight to formally describe the retroactive base case reduction procedure. After each iteration of ISA, starting from the second iteration, the gate sequence for the current iteration and the gate sequence for the previous iteration are examined. If the current iteration has a three-qubit state preparation base case, the preceding gate sequence ends with a two-qubit state preparation, that two-qubit state preparation can be commuted with the controlled substate merging section of the current iteration, and the two-qubit state preparation applies to two of the three qubits for the base case of the current iteration, the two-qubit state preparation part from the preceding iteration is deleted, and the three-qubit base case of the current iteration is recomputed before going on to the next ISA iteration.

Every step of our implementation of the ISA algorithm has been fully described; we summarize our implementation in Figure [number].
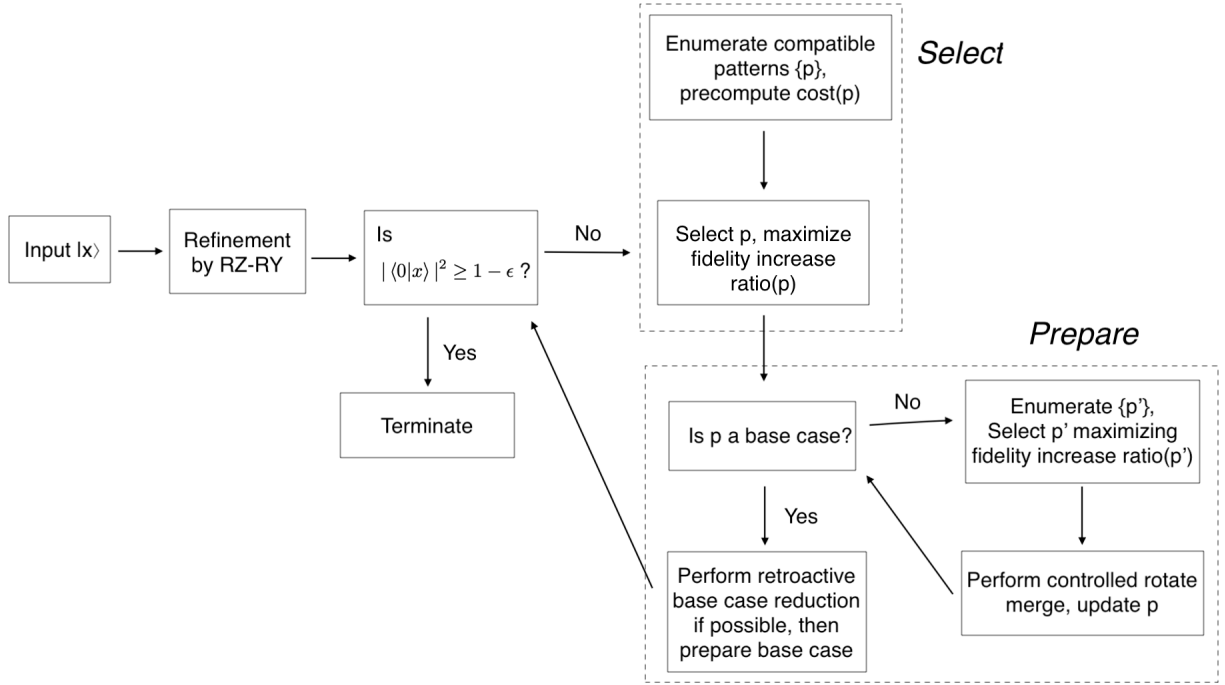
Figure 6: Block Diagram summary of our implementation of the ISA framework