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SYMPHONY: Efficient Compilation for Hamiltonian Simulation via Global Binary Symplectic Form Simplification

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► **Introduction**

► Preliminary

► Motivation

► Methodology

► Evaluation

► **Conclusion**



- A core workload across chemistry, materials, condensed matter, and optimization.
- One computational paradigm behind various algorithms:
 - **NISQ**: Trotterized time evolution (product formula), VQE, QAOA, etc.
 - **Fault-tolerant**: Qubitization, quantum signal processing, etc.
- The task is to implement/approximate

$$U(t) = e^{-iHt}, \quad H = \sum_{k=1}^m c_k P_k, \quad P_k \in \{I, X, Y, Z\}^{\otimes n}.$$

by quantum circuits (1Q and 2Q gate sequences), with $e^{-iHt} \approx \prod_{k=1}^m e^{-ic_k P_k t}$ when t is small.

- Therefore, the compiler input reduces to a sequence of Pauli rotations $\{e^{-i\theta_k P_k}\}$, which we call the **Pauli-IR**.

Objective: preserve semantics while reducing **two-qubit gate count and circuit depth**, targeting NISQ and early fault-tolerant regimes.

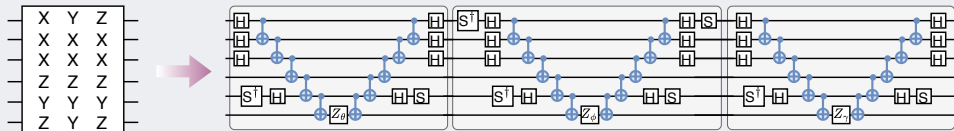
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¹1, 2.

Pauli-IRs as the compiler input:

$$\mathcal{P} = ((P_k, \theta_k))_{k=1}^m, \quad R_{P_k}(\theta_k) = e^{-i\theta_k P_k}.$$

Naïve term-by-term synthesis



Naïve CNOT-tree synthesis

A weight- w Pauli rotation is usually synthesized as $e^{-i\theta P} = C R_Z(2\theta) C^\dagger$, where C is a Clifford frame, typically a parity/CNOT tree with single-qubit Cliffords.

- The naïve term-by-term cost is $2(w - 1)$ CNOTs per rotation.
- In a compute–rotate–uncompute sandwich construction.

Global optimization via simultaneous simplification



Simultaneous simplification through Clifford conjugation

Conjugating multiple Pauli rotations in a shared Clifford frame exposes **simultaneous simplification** — one Clifford transformation can reduce several Pauli strings at once.

- Avoid repeated parity compute–uncompute.
- Lower both two-qubit gate count and circuit depth.

*Built on this mechanism, our work aims at developing a holistic compilation paradigm (**exhaustive global optimization**) that systematically exploits the intrinsic algebraic structures of Pauli-IRs.*

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- A **binary symplectic form (BSF)** represents m Pauli operators on n qubits in a tableau

$$T = [X \mid Z] \in \mathbb{F}_2^{m \times 2n}.$$

- Row i encodes P_i through bit pairs $(X_{i,q}, Z_{i,q})$

$$(X_{i,q}, Z_{i,q}) = (0, 0), (1, 0), (0, 1), (1, 1)$$

- Support and weight reduce to Boolean operations:

$$w_i = \|X_{i,:} \vee Z_{i,:}\|_1.$$

- Commutation relation representation:

$$[P_i, P_j] = 0 \quad \Leftrightarrow \quad x_i z_j^T + z_i x_j^T = 0 \pmod{2}.$$

Why BSF?

- Formally encoding global information and algebraic properties of Pauli-IRs.
- Support, weight, overlap, and commutation become linear/Boolean operations over $\mathbb{F}_2$.
- Row weight directly implies synthesis cost.

- The Clifford group is the normalizer of the Pauli group:

$$CPC^\dagger = sP', \quad s \in \{+1, -1\}.$$

- Clifford conjugation preserves the Pauli-rotation form:

$$Ce^{-i\theta P}C^\dagger = e^{-i(s\theta)P'}.$$

- In BSF, a Clifford acts as an invertible *symplectic transformation* over $\mathbb{F}_2$.

Example

CNOT on qubits (a, b) updates four columns:

$$[X_a, X_b \mid Z_a, Z_b] \rightarrow [X_a, X_a \oplus X_b \mid Z_a \oplus Z_b, Z_b].$$

	q_0	q_1	q_2	q_3	q_0	q_1	q_2	q_3	
IXYX	0	1	1	1	0	0	1	0	IXYI
ZYXX	0	1	1	1	1	1	0	0	ZYXI
YZIZ	1	0	0	0	1	1	0	1	YIIZ
ZXZI	0	1	0	0	1	0	1	0	ZXZI

$\xrightarrow{\text{CNOT}_{1,3}}$

	q_0	q_1	q_2	q_3	q_0	q_1	q_2	q_3	
IXYI	0	1	1	0	0	0	1	0	IXYI
ZYXI	0	1	1	0	1	1	0	0	ZYXI
YIIZ	1	0	0	0	1	0	0	1	YIIZ
ZXZI	0	1	0	1	1	0	1	0	ZXZI

Takeaways

- Single-qubit Clifford (e.g., S , H) permutes Pauli letters on one qubit, so cannot change weight.
- Only two-qubit Clifford (e.g., CX , CZ , $i\text{SWAP}$) can change the support structure and therefore the row weights of BSF.

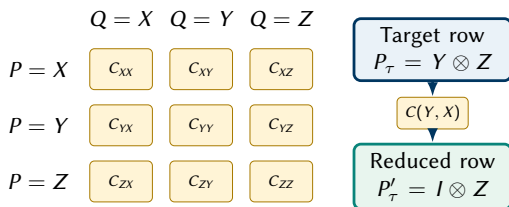
- A convenient two-qubit Clifford family is the **controlled-Pauli Clifford**, known as **universal controlled gate (UCG)** [5]:

$$C(P, Q) = \frac{1}{2}((I + P) \otimes I + (I - P) \otimes Q),$$

$$P, Q \in \{X, Y, Z\}.$$

- Nine choices (at least five) span the entire two-qubit Clifford group.
- Each UCG is Hermitian, self-inverse, and locally equivalent to CNOT/CZ.
- Different Pauli axes induce different symplectic updates while keeping a uniform gate cost.

UCG as BSF simplification primitive



Takeaways

- Each non-trivial weight-2 Pauli can be reduced by **four** UCGs.
- The UCGs provide a uniform way to simplify the BSF with broad optimization space without pre-diagonalization.

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Local / structural methods

- PAULIHEDRAL [6], TETRIS [7], PAULIFOREST [8]: reorder Pauli-IR synthesis variants, cancel gates, and co-optimize routing.
- TKET [9], PCOAST [10], QUCLEAR [11]: diagram- and graph-based rewriting, Clifford extraction.

Global tableau-based methods

- RUSTIQ [3], PMST [12]: first diagonalize the target row, then apply directional CNOTs via path-based search (graph matching, minimum spanning tree).
- PHOENIX [4]: support-grouped BSF simplification plus inter-group ordering.
- PAULIRL [13], MONTEQ [14]: reinforcement learning and Monte Carlo tree search.

Remaining bottlenecks

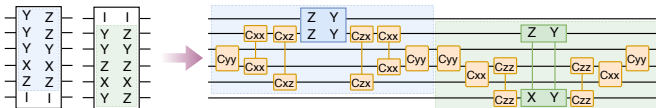
- Rigid first-diagonalization synthesis paradigm; fragmented support or commuting groups.
- Expensive long-horizon heuristics / searches.
- Extra inter-block stitching passes.

Consequence

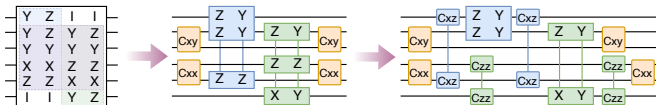
The algebraic structure of Pauli-IRs and Cliffords remains underexploited. A holistic, global, streamlined formulation is needed.

Key design choices

- **One tableau.** A single BSF over $\mathbb{F}_2$ naturally represents the intrinsic algebraic structures of Pauli-IRs.
- **UCG primitive.** Native $C(P, Q)$ conjugations as simplification primitives.
- **Holistic scope.** No support- or commutation-based pre-grouping; cross-support overlaps stay visible.



Group-wise: cross-support overlap is split.



Holistic: half the two-qubit Clifford conjugations.

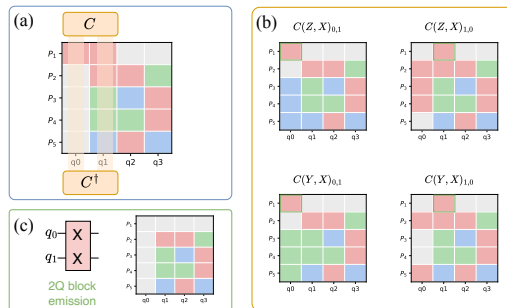
One Clifford conjugation can benefit many Pauli rows at once even among heterogeneous-weight Pauli-IRs.

- Prior tableau methods terminate a target row only once it reaches **weight-1**, emitting a single-qubit rotation.
- Forcing weight-1 can **inflate** unresolved rows: collateral growth outweighs benefit.
- Weight-2 is already cheap: two-qubit Pauli blocks do not always cost 3 CNOTs.
- Early weight-2 emission shortens the Clifford chain and yields coarser, schedulable blocks.
- **Termination boundary should be adaptive**: always emit weight-1; release weight-2 once the tableau is sparse.

Average synthesis cost in CNOT count over all fixed-cardinality

subsets $\mathcal{P} \subseteq \{X, Y, Z\}^{\otimes 2}$.

$ \mathcal{P} $	3	4	5	6	7	8	9
#CNOT	2.07	2.29	2.64	2.93	3	3	3



Pushing P_1 to weight-1 inflates other rows (b); early weight-2 emission avoids the degradation (c).

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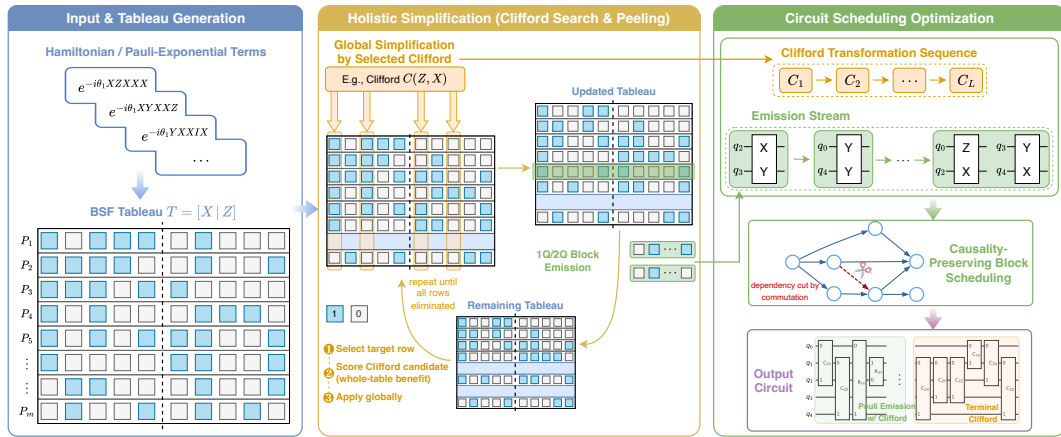
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- UCG conjugations searched via greedy heuristic iteratively simplify the BSF tableau.
- Adaptive emission extracts executable Pauli blocks in a forward frame.
- Causality-preserving ASAP scheduling exposes two-qubit block parallelism finally.

1. Target descent

Choose the active row with the lowest non-trivial weight:

$$\tau = \arg \min_{i \in A} \text{wt}(P_i).$$

Consider only UCGs on $\text{supp}(P_\tau)$ that reduce its weight by one.

2. Global greedy selection

Maximize $\beta = (-\Delta W, N_-, -N_+)$ lexicographically over the full active tableau.

3. Adaptive emission

Emit all weight-1 rows. Emit weight-2 rows only when the active-tableau density satisfies $\rho_A \leq \rho$.

```
while active rows remain:
```

```
   $\tau \leftarrow \arg \min_i \text{wt}(P_i)$ 
```

```
  for  $C(P, Q)$  on  $\text{supp}(P_\tau)$ :
```

```
    if  $\Delta \text{wt}(P_\tau) = -1$ :
```

```
       $\beta \leftarrow (-\Delta W, N_-, -N_+)$ 
```

```
    apply best UCG; Emit()
```

```
Emit() :
```

```
  collect rows with  $\text{wt} \leq 1$ 
```

```
  if any  $\text{wt} = 2$  and  $\rho_A \leq \rho$ :
```

```
    collect them too
```

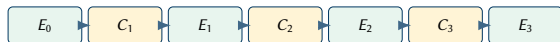
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  remove emitted rows from the active set
```

Guarantee: every chosen UCG reduces the target row, thus terminating in $O(m^2 n^3)$ time.

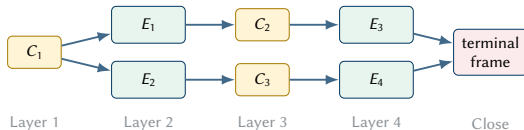
Output:

$$(C_1 \cdots C_L) \cdot E_L C_L \cdots E_1 C_1 E_0 \approx e^{-i \sum_k \theta_k P_k}.$$

Forward-frame stream



Dependency DAG and ASAP layers



Exact commutation rules

- UCG–UCG commute iff their Pauli letters agree on every shared qubit
- UCG–Pauli commute iff the Pauli letters match the UCG axes on overlaps
- Disjoint operations always commute

Closing the frame

The terminal Clifford is resynthesized or absorbed into observables when the application permits it.

Outcome

Preserve causal correctness while executing dependency-ready, resource-disjoint blocks in parallel.

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HamLib: 100 representative Hams [15]

Category	Qubits	Pauli terms	Weight
Binary (15)	4–90	12–2958	2–3
Discrete (15)	8–480	48–5334	2–8
Chemistry (35)	2–64	6–6508	2–24
Condensed (35)	12–930	32–8241	2–361

UCCSD: 6 synthetic, scaled Hams [7]

UCCSD-derived (10–35 qubits, 800–9800 Pauli terms)

Baselines

- Topology-agnostic: QISKIT-RUSTIQ [3], TKET-PCOAST [16], QUCLEAR [11], PHOENIX [4]
- Topology-aware: PAULIHEDRAL [6], TETRIS [7]

Implementation & Platform

- SYMPHONY impl. in Python + Qiskit/NumPy
- Dual-socket server with two 96-core AMD EPYC processors; 1.5 TiB memory

Fairness

- QISKIT O3 is applied after high-level synthesis (Clifford resynthesis, 2Q unitary resynthesis, etc.).
- In limited-connectivity compilation, all outputs go through QISKIT's topology-aware O3 ultimately.

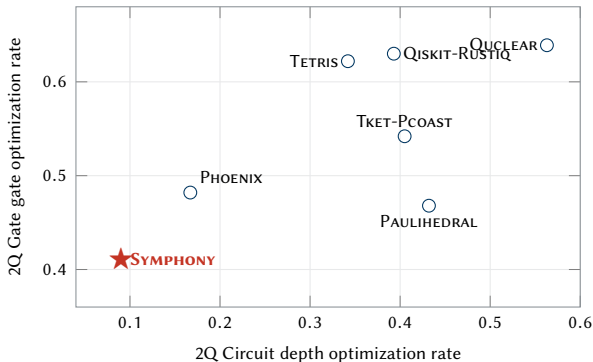
−59%

two-qubit gates vs. naïve synthesis

−91%

two-qubit depth vs. naïve synthesis

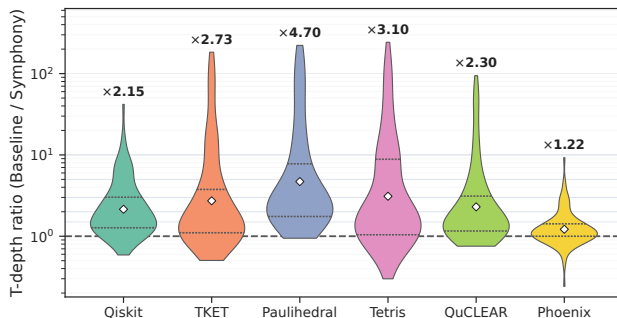
- Versus six baselines:
 - 1.14–1.58× fewer 2Q gates
 - 1.87–5.67× shallower 2Q depth
- Best depth optimization in every HamLib category



Versus grouping-based PHOENIX (Our prior work)

- Opt. rate (gate count) improves 0.482 → 0.411
- Opt. rate (circuit depth) improves 0.167 → 0.09

T -count remains nearly compiler-invariant ($\pm 2\%$) as expected, so **T -depth** becomes the differentiating metric in the early fault-tolerant benchmarking.



HamLib T -depth ratio: baseline / SYMPHONY. Shaded regions indicate multiplicative-ratio bounds (1–1.5 $\times$, 1.5–2 $\times$, 2–3 $\times$, 3–5 $\times$, and 5–10 $\times$).

Superiority in early-FT

- GridSyth [17] is used for synthesizing R_Z by $\{H, S, T\}$, requiring a median of 102.5 T gates per rotation with precision 10^{-10} .
- SYMPHONY's T -depth strictly shallower in 86% / 85% / 98% / 86% / 78% / 62% vs. baselines.

Limited-connectivity benchmarking on UCCSD UC SANTA BARBARA

2Q gate-count optimization rate

Topology	QISKIT	TKET	PAULIHEDRAL	TETRIS	QUCLEAR	PHOENIX	SYMPHONY
All-to-all	0.256	0.175	0.299	0.311	0.228	0.133	0.131
Square	1.117	0.691	0.427	0.61	0.95	0.395	0.452
Heavy-hex	1.976	1.168	0.914	0.764	1.625	0.571	0.76

2Q depth optimization rate

Topology	QISKIT	TKET	PAULIHEDRAL	TETRIS	QUCLEAR	PHOENIX	SYMPHONY
All-to-all	0.153	0.059	0.307	0.309	0.102	0.112	0.051
Square	0.575	0.309	0.325	0.438	0.455	0.276	0.21
Heavy-hex	0.917	0.47	0.724	0.54	0.702	0.362	0.32

Architectural tradeoff

- SYMPHONY wins 2Q depth on all topologies; on restricted topologies its 2Q gate count trails PHOENIX by 14–33%: holistic simplification dissolves hardware-friendly locality.
- “Logical synthesis + external routing” outperforms “topology-aware co-optimization” here, yet SYMPHONY degrades more steeply: co-optimization bounds search space, but still matters.

Adaptive emission threshold

- Default $\rho = 0.35$ is better than both fixed endpoints.
- Strict weight-1 emission ($\rho = 0$):
 - Depth degrades by +112.5%.
 - Gate count degrades by +6.8%.
- Unconditional weight-2 emission ($\rho = 1$):
 - Largely recovers depth.
 - But loses 8.8% aggregate gate count.

Scheduling pass

- Trivially ordered emission is needlessly serial.
- ASAP without commutation: -60.3% two-qubit depth on average.
- ASAP with canonical commutation: -63.5% depth.
- Gains appear in every benchmark family, and up to 99.1% on individual condensed-matter instances.

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1. SYMPHONY reframes Hamiltonian simulation compilation as **holistic BSF simplification**.
2. Controlled-Pauli Cliffords over a global tableau expose simultaneous simplification across heterogeneous-weight Pauli operators.
3. **Adaptive two-qubit emission** avoids single-qubit-only degradation and exposes more parallelism.
4. **Causality-preserving block rescheduling** unlocks two-qubit depth reductions.

Key result on HamLib

Average reductions of **59% in two-qubit gate count** and **91% in two-qubit depth** relative to naïve synthesis; strict Pareto dominance over evaluated prior compilers.

Open question

- How can holistic BSF simplification remain topology-aware so as to not incur severe degradation from restricted connectivity?
- How can this approach be more effectively extended to early fault-tolerant compilation?
- Can these technical insights be applied to other representations, such as phase polynomials?



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Thank you for your attention!



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