

# RTL-to-Atoms Synthesis of a Machine Learning Accelerator on Atomic-Scale Computers

Samuel S. H. Ng, Marcel Walter, Simon Hofmann, Jan Drewniok, Robert Wille, and Konrad Walus

**Abstract**—As CMOS scaling slows and AI demand soars, atomic-scale platforms such as quantum-dot logic based on silicon dangling bonds (SiDBs) offer a promising path toward energy-efficient computation, yet practical design flows from register-transfer level (RTL) specifications to manufacturable layouts remain limited. This work presents an RTL-to-atoms synthesis framework for a quantized matrix multiply unit targeting SiDB-based field-coupled nanocomputing (FCN). Building on recent advances in SiDB-aware electronic design automation (EDA), the framework combines a hierarchical, parameterized RTL architecture with platform-optimized arithmetic logic units, reducing the synthesized logic core of processing elements by about 15% compared to prior flows. Key improvements were also made to the synthesis workflow, retargeting tools previously tuned for other FCN technologies toward SiDB logic and incorporating figure-of-merit awareness, which together ensure that the synthesized layouts achieve favorable area scaling and throughput while balancing operational robustness. Evaluations across multiple bit-widths show substantial footprint reductions for configurations within the practical range of latest placement-and-routing algorithms while preserving testbench-validated correctness from RTL to dot-accurate SiDB layouts, thereby establishing a reproducible benchmark for EDA on atomic-scale computing. This represents a significant milestone, bridging manually-intensive workflows with scalable, automated methodologies, thus providing a valuable foundation for future design efforts for SiDB-based accelerators.

## I. INTRODUCTION

GLOBAL computing infrastructure increasingly devotes its resources to AI inference and training, making the associated energy demand a central constraint and spurring efforts to develop hardware platforms that operate far more efficiently than traditional CMOS processors. Among these, field-coupled nanocomputing (FCN) has emerged as an appealing post-CMOS computing paradigm, in which local field interactions encode logic states in the position of charges [1] or in the magnetic polarity of nanomagnets [2], [3], enabling both computation and signal transmission.

Among the various physical implementations of FCN, quantum dots made of silicon dangling bonds (SiDBs) stand out as a promising platform due to their atomically precise fabrication [4], [5] and discretely controllable charge states [6], [7]. Motivated by the experimental demonstration of an SiDB

OR gate measuring just  $5\text{ nm} \times 6\text{ nm}$  [8], specialized CAD tools and electronic design automation (EDA) frameworks have emerged to support SiDB logic exploration. At the physical design level, *SiQAD* [9] and an ecosystem of simulators [10]–[12] have enabled the exploration of logic structures and design rules at the gate and circuit levels [13], [14]. However, the fully manual design of these layouts remained a time-consuming process, motivating the automation of multiple stages of the design flow. At the quantum-dot level, automated SiDB gate designers [15] enabled the creation of standard-tile libraries [16]. With the addition of SiDB support in *fiction* [17], an EDA framework specialized for FCN, new pathways have been opened for large-scale designs by synthesizing gate-level netlists down to dot-accurate SiDB layouts.

Prior to the maturity of SiDB EDA tools, application-scale research targeting SiDBs was scarce and relied on manually verified SiDB building blocks, which were then extrapolated into system-level designs to estimate their behavior and implementation costs [10], [18]. Among them was a quantized matrix multiply unit (MXU) inspired by Google’s tensor processing unit (TPU) [19] and optimized for SiDB’s architectural constraints [18], where simulation-proven SiDB logic components were used to approximate the area cost and performance figures. To facilitate practical exploration, an earlier conference version of this work [20] implemented the MXU as a register-transfer level (RTL) Verilog design, employing clocked registers as an abstract proxy for the underlying FCN clocking behavior. With a workflow spanning multiple EDA frameworks, the study synthesized the RTL implementation into dot-accurate SiDB layouts, realizing an automated, scalable, and verifiable end-to-end SiDB design flow using state-of-the-art EDA tools.

Despite this progress, the conference version of the RTL-to-atoms flow in [20] left several aspects only coarsely explored: the choice of arithmetic logic units (ALUs) was left to logic synthesis frameworks, which do not take FCN’s unique architectural preferences into account. Weights and activations were fixed to a single 8-bit configuration, preventing systematic study of how the synthesized layouts scale with precision. This work therefore provides a substantial extension upon the original methodology at multiple layers: at the RTL design layer, parameterized quantization enabled a systematic study of downstream trade-offs in the synthesis pipeline; for RTL-to-netlist synthesis, the introduction of technology-appropriate ALUs reduced the resulting area; and for netlist-to-atoms synthesis, multiple SiDB-oriented refinements to technology mapping, placement-and-routing, and hexagonalization further had a

S. Ng and K. Walus were with the Department of Electrical and Computer Engineering, University of British Columbia, Canada ({samueln, konradw}@ece.ubc.ca); M. Walter, S. Hofmann, J. Drewniok, and R. Wille were with the Chair for Design Automation, Technical University of Munich, Germany ({marcel.walter, simon.t.hofmann, jan.drewniok, robert.wille}@tum.de). M. Walter, S. Hofmann, and R. Wille were also with the Munich Quantum Software Company GmbH, Germany. R. Wille was also with the Software Competence Center Hagenberg (SCCH) GmbH, Austria.

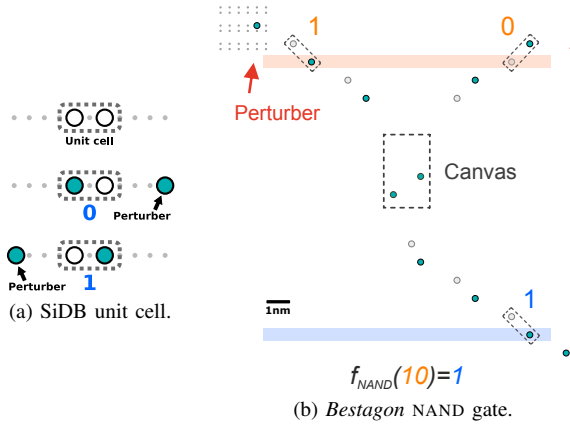


Fig. 1. (a) SiDB logic unit cell: a pair of closely-spaced SiDBs share a charge whose position encodes logic 0 or 1, controlled by the location of a nearby “perturber” SiDB. (b) Example NAND gate from the *Bestagon* library, with inputs applied at the upper pins via perturbers, and the output sensed at the lower pin; the central region hosts SiDBs that implement the gate function. With permission, (a) is reproduced from [18], (b) is adapted from [21].

significant impact on the quality of result. These contributions transform a one-off demonstration into a concrete framework optimized for SiDB logic synthesis, revealing how architectural and layout decisions shape the strengths and limitations of current tools. The remainder of this manuscript is structured as follows: Section II reviews SiDB logic background and EDA infrastructure; Section III summarizes prior SiDB MXU designs; Section IV details the hierarchical RTL architecture and the RTL-to-atoms synthesis flow; Section V presents the synthesis results and discuss their trade-offs; and Section VI concludes with directions for future work.

## II. BACKGROUND

SiDBs can be fabricated on the surface of hydrogen-passivated Si(100)- $2 \times 1$  with the tip of a scanning-tunneling microscope [4], [5]. Each SiDB can hold discrete charge states, including negative, neutral, or positive. In densely packed ensembles, the charge state of each SiDB is determined by their collective interaction, bulk doping levels, and external electrostatic influences [5]. Binary logic states can be encoded by the position of a charge shared among closely positioned SiDBs (Fig. 1a), enabling the experimental demonstration of an OR gate with a footprint of only  $5 \times 6 \text{ nm}^2$  [8]. Further exploration of SiDB logic designs was enabled by *SiQAD* [9], a CAD tool specialized for SiDB logic. Building on these tools, the *Bestagon* standard-tile library [16] was introduced, featuring standardized input/output (I/O) pin locations and a central canvas on which SiDBs are placed to implement logic (Fig. 1b). The *Bestagon* library has allowed *fiction* [17], an EDA framework specialized for FCN, to take gate-level netlists as input and synthesize dot-accurate, fabricable SiDB layouts [16], forming the backbone of this work.

SiDB logic, like other FCN families, uses spatially partitioned clock zones to enforce directed data flow [9], [10]. Hanging or buried electrodes apply phase-shifted sinusoidal potentials that modulate the surface band bending and thereby the local charge density [10]. Adjacent electrodes are offset

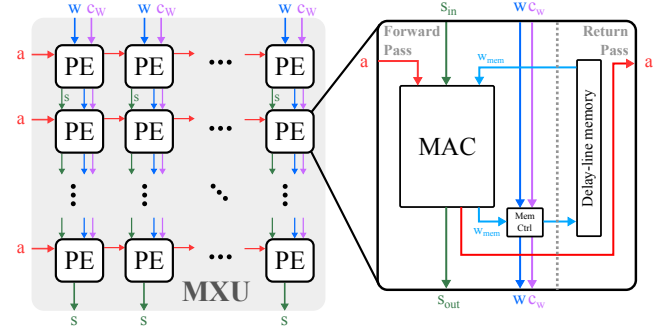


Fig. 2. A 2D systolic array MXU receiving quantized activations  $a$ , weights  $w$ , control signals  $c_w$ , and partial sums  $s$ . Each PE consists of a MAC unit, memory controller, and memory for weight storage. Signals propagate downward on the left (forward pass) and upwards on the right (return pass).

by  $90^\circ$  in phase, producing “active” regions where charges are present, and computation occurs, separated by “inactive” regions that are effectively charge-free buffers. An area-efficient arrangement places these clock zones in rows to support unidirectional, purely combinational logic [10], [22]. Interfacing with CMOS can be achieved by biasing inputs electrostatically via electrodes [10], while outputs can be sensed using charge-sensitive devices such as single-electron transistors [23]–[25].

## III. RELATED WORK

In this section, Section III-A surveys existing FCN EDA frameworks, and Section III-B reviews SiDB MXU designs. Together, they contextualize the proposed RTL-to-atoms flow.

### A. Electronic Design Automation for FCN

Aside from *fiction*, other FCN EDA frameworks target nanomagnetic logic (NML), a field-coupled style in which information is stored and propagated via the collective magnetization of interacting nanomagnets rather than mobile charges. Within this setting, *ToPoliNano* [26] provides a top-down flow from structural VHDL descriptions to in-plane NML layouts with clocking-aware placement and routing. Complementing this, *FUNCODE* [27] infers VHDL netlists from custom NML layouts, enabling device-to-system analysis of NML circuits using HDL simulators. These works demonstrate FCN CAD capabilities in the NML domain. In contrast, the present work targets the emerging atomic-scale SiDB logic platform, for which RTL-to-atoms design flows are maturing.

### B. SiDB ML Accelerators

Before dedicated SiDB-aware EDA tooling became available, studies of SiDB applications were limited and largely depended on manual CAD prototyping with extrapolated area and latency estimates. One such example was an SiDB MXU [18] for machine learning (ML) acceleration, which mirrored design choices from Google’s TPUv1 [19]: the matrix-vector multiplications underpinning ML workloads were realized as 8-bit integer multiply-accumulate (MAC) operations to reduce computational cost, and both designs employed a systolic-array architecture relying on regular arrangements of processing elements (PEs)—homogeneous logic modules that operate

on their inputs and pass results to adjacent PEs—to perform computation (Fig. 2). At the PE level, the core operation is a MAC:  $s_{\text{out}} = s_{\text{in}} + (w \cdot a)$ , where  $s_{\text{in}}$  the partial sum from the preceding PE,  $w$  is the stored weight,  $a$  is the activation, and  $s_{\text{out}}$  is the updated partial sum.

In the implementation of [18], each matrix-multiplication job consisted of two primary phases: 1) *preloading*, where weights ( $w$ ) are loaded into the array from the top edge and traverse column-wise until they arrive at the designated PEs for storage; 2) *computing*, where activations ( $a$ ) are streamed from the left side and are multiplied with the stored weights and accumulated with partial sums; activations continue to traverse row-wise while partial sums traverse column-wise for further accumulation until they reach the array’s bottom edge. Additional input signals control the operating phase. At the PE granularity, each PE comprises two signal paths: a *forward pass* containing the MAC and memory controller, and a *return pass* that drives a weight bus upward to close the delay-line memory feedback loop and an activation bus to align activations with neighboring PEs (Fig. 2). Both paths are purely combinational, enabling row-wise clocking on each path. Row-wise clocking incurs deep pipeline stages, which can be taken advantage of by interleaving different inputs by clock cycle to increase the computational throughput.

While that blueprint study reported promising area and power estimates against the TPUv1 [18], [19], its extrapolated nature offered neither a manufacturable layout nor formal verification. The preceding conference version of this work [20] bridged this gap by applying latest SiDB EDA techniques to demonstrate a RTL-to-atoms synthesis flow to a quantized SiDB MXU, which this work substantially refines by introducing technology-specific optimizations and exploring the scaling behavior of different quantization bit-widths, as detailed in the next section.

#### IV. PROPOSED METHODOLOGY

This section presents the proposed end-to-end RTL-to-atoms design and synthesis flow. Section IV-A describes the hierarchical RTL architecture at the core of the flow, which satisfies tooling requirements. Subsequently, Section IV-B covers the RTL-to-netlist conversion, and Section IV-C describes the netlist-to-atoms physical design with optimizations for SiDBs.

##### A. Matrix Multiply Unit in Hierarchical RTL

To achieve this work’s objectives, the RTL implementation must satisfy the following requirements: 1) the RTL must be purely combinational for *fiction* compatibility; and 2) operation of the pipelined PE must be verifiable so that test benches can establish operational correctness, addressing the lack of formal verification in prior work [18]. Because the PE includes forward and return paths that form an internal feedback loop, a direct RTL implementation of the full PE would be incompatible with *fiction*. In reconciliation, this work adopts a hierarchical RTL organization which compartmentalizes the design:

**Combinational core:** The PE’s forward-pass logic is implemented in strictly combinational RTL, as shown in Alg. 1, ensuring compatibility with subsequent synthesis steps.

#### Algorithm 1 Forward Pass Logic in Processing Element

##### Inputs:

$PE_y \leftarrow$  y-index assigned to each PE (constant per PE)  
 $m \leftarrow$  PRELOAD (0) or COMPUTE (1) mode  
 $w_{\text{load}} \leftarrow$  weight to be loaded into memory  
 $PE_{\text{target-}y} \leftarrow$  target Y-index of  $w_{\text{load}}$   
 $s_{\text{in}} \leftarrow$  input partial product  
 $a \leftarrow$  input activation  
 $w_{\text{mem}} \leftarrow$  weight loaded from delay-line memory

##### Outputs:

$s_{\text{out}}$ : new partial sum  
 $w_{\text{memOut}}$ : weight to write to delay-line memory  
1: **procedure** PROCESSINGELEMENTLOGIC  
2:  $p \leftarrow \text{signed}(w_{\text{mem}}) \times \text{signed}(a)$   $\triangleright$  Multiply stored  $w$  with  $a$   
3:  $s_{\text{out}} \leftarrow s_{\text{in}} + \text{signExtend}(p, 24)$   $\triangleright$  Sum with partial sum  
4: **if**  $m = \text{PRELOAD}$  **and**  $PE_{\text{target-}y} = PE_y$  **then**  
5:  $w_{\text{memOut}} \leftarrow w_{\text{load}}$   $\triangleright$  Update stored weight  
6: **end if**  
7: **return**  $s_{\text{out}}$ ,  $w_{\text{memOut}}$ , and other pass-through wires  
8: **end procedure**

**Clocked shell:** A higher-level RTL module captures the clocked operation of the full PE, defining the component’s input and output signals, pipelined internal signal steering, and synchronized signal timing for the return pass.

Both are parameterized by the weight and activation bit-widths, allowing the study of their scaling behavior in Section V.

Correctness was validated with test benches across both layers. These tests confirmed correct weight storage in preload mode and accurate MAC results in compute mode for representative inputs. In particular, interleaved inputs for concurrent MAC operation across all pipeline stages was also verified. All simulations were performed using Icarus Verilog [28], establishing logical correctness of the PE prior to synthesis and physical mapping. The codebase is fully open sourced.<sup>1</sup>

##### B. RTL-to-Netlist

With the RTL design verified, the first stage of the synthesis flow is to generate a gate-level netlist. To accomplish this, this work uses *Yosys* [29] to map arithmetic operators such as accumulation (+) and multiplication (\*) into gate-level ALUs. Absent explicit directives, *Yosys* selects CMOS-optimized ALUs, which underperform in FCN due to differences in area and latency trade-offs under the strictly planar fabric [30]. To ensure technology-appropriate choices, this work supplies explicit gate-level descriptions of a ripple-carry adder and an array multiplier to *Yosys*, both of which have been shown to be suitable for FCN thanks to their regular structure, which eases wiring congestion [30]. The mapped netlist is then rewritten as an And-Inverter Graph (AIG) and optimized with ABC’s & *deepsyn* [31] strategy to reduce its node count, and re-validated against test benches to confirm functional correctness.

##### C. Netlist-to-Atoms

The optimized AIG is then passed to *fiction* for the second stage of the synthesis flow: physical design. This stage transforms the netlist into a dot-accurate SiDB layout through a multi-step process, which this work enhances with several optimizations for the SiDB platform.

<sup>1</sup>GitHub repository: <https://github.com/samuelshng/sidb-mxu-verilog>

1) *Synthesis Flow*: This work starts with the SiDB-specific flow in *fiction* proposed by [16]:

**Technology mapping** maps the AIG onto the *Bestagon* gate library [16], exploiting the library’s richer primitives to shrink the logic compared with an AND/INV-only basis.

**Placement and routing** with the *ortho* [32] or graph-oriented layout design (*gold*) [33] algorithm produces a layout on a Cartesian grid.

**Post-layout optimization (PLO)** [34] reduces the footprint of the routed design.

**Hexagonalization** projects the Cartesian layout onto a hexagonal grid [35] to align with *Bestagon* gates.

**SAT-based equivalence checking** [36] confirms that the hexagonalized layout preserves the gate-level behavior.

**Atom mapping** maps each tile in the verified layout to the corresponding *Bestagon* gate’s SiDB arrangement, yielding a dot-accurate, manufacturable SiDB layout.

While this established workflow provides a robust foundation, its application to the SiDB platform revealed opportunities for technology-specific enhancements as detailed below.

2) *FoM-aware Technology Mapping*: Previous SiDB synthesis flows within *fiction* treated all gates in the technology library as equivalent, without physical robustness considerations. Recent SiDB logic robustness studies have culminated in the creation of a unified cost function for figures of merit (FoMs) [37]. The cost function encompasses the dominant cost drivers—operational domain size [9], [38], thermal stability [39], band-bending effects [7], defect sensitivity [40], and related factors—into a single FoM. This work adopts it as the objective for the technology mapper to prioritize gates with higher predicted robustness, accepting a potential trade-off in other layout metrics like area or quantum-dot count.

3) *Placement and Routing Optimizations*: The placement-and-routing framework within *fiction* was first established for quantum-dot cellular automata (QCA) circuits on a Cartesian grid [17]. Subsequent support for SiDB logic was enabled through a coordinate mapping that performs a 45° rotation of the Cartesian layout followed by its projection onto the hexagonal SiDB lattice [35]. This rotation, however, can lead to suboptimal results: a layout that is compact on the Cartesian grid may become significantly taller after hexagonalization when there exists numerous diagonal signal paths in the Cartesian layout that are strongly offset from the northwest corner, which map to long vertical paths in the hexagonal layout. Layouts with a more balanced aspect ratio are therefore preferred. While the older *ortho* algorithm offers no configurable compensation, the more recent *gold* algorithm [33] exposes a customizable cost objective for placement and routing, enabling SiDB-specific optimizations. Whereas the default cost objective for *gold* is the total area, this work introduces new cost objectives that reduce the aspect-ratio distortion introduced by the 45° rotation by encouraging more square footprints, which is further detailed in Section V-B.

4) *Hexagonalization Improvements*: The hexagonalization algorithm was also revised in this work to align generated layouts with SiDB clocking expectations. Under the Cartesian layout’s 2DDWave clocking scheme [41], primary inputs are placed along the north and west borders, and data advances

TABLE I  
SYNTHESIS COMPARISON ACROSS MXU AND EDA CONFIGURATIONS

ALUS	PE	ALG	UNIFORM TM		$A_{\text{FoM}}$
			$w \times h$	$= A_{\text{uni}}$	
Default [20]	W8A8	<i>ortho</i> +PLO	$515 \times 1043$	$= 537\,145$	541\,284
Optimized (This work)	W8A8	<i>ortho</i> +PLO	$474 \times 967$	$= 458\,358$	470\,830
	W4A4	<i>ortho</i> +PLO	$143 \times 333$	$= 47\,619$	56\,744
		<i>gold</i> +PLO	$116 \times 241$	$= 27\,956$	70\,070
	W2A2	<i>ortho</i> +PLO	$67 \times 151$	$= 10\,117$	10\,833
		<i>gold</i> +PLO	$48 \times 98$	$= 4\,704$	5\,457

“Default” and “optimized” ALUs indicate *Yosys*’s ALU selection mode;  $w$  and  $h$  denote the tile counts along the width and height;  $A = w \times h$ ;  $A_{\text{uni}}$  and  $A_{\text{FoM}}$  denote the *Bestagon* variant used for technology mapping.

diagonally toward the southeast. The 45° rotation left many I/O pins recessed from the north and south edges, which reduces the attainable throughput because some signals must be held across multiple cycles for synchronization. The updated flow stretches all I/O pins to the north and south boundaries after projection, producing layouts whose ports are time-aligned as they enter and exit the hexagonal fabric. An optional constraint can be toggled to perform the pin extensions without wire crossings as they are typically less robust against environmental defects.

## V. EXPERIMENTS

This section evaluates the RTL-to-atoms flow using the synthesized PE-core layouts. Section V-A outlines the experimental protocol and configurations. Section V-B presents the resulting synthesis metrics across technology-mapping and placement-and-routing variants. Section V-C discusses these findings and compares them with prior manual estimations.

### A. Experimental Protocol

This comparative study characterizes how activation and weight bit-widths scale and reports synthesis results across various synthesis configurations. To this end, the combinational PE-core (Section IV-A) is synthesized for 2-, 4-, and 8-bit weights and activations, henceforth denoted W2A2, W4A4, and W8A8, respectively. These selections correspond to widely studied quantized regimes for ML workloads where the dominant operations reduce to dense matrix multiplications [19], [42], [43]. The RTL-to-netlist flow from this work instructs *Yosys* to use technology-appropriate ALUs to produce an AIG (Section IV-B), which is then optimized using ABC’s *&deepsyn* strategy [31]. In the netlist-to-atoms flow, two *Bestagon* library [16] variants are compared during technology mapping: a uniform cost baseline, and an FoM-aware counterpart. *ortho* and *gold* are used for placement and routing.

### B. Results

The best achieved synthesis results of the PE-core under the tested configurations are presented in TABLE I. Compared to prior results from [20], which left ALU selection to *Yosys*’s CMOS-aligned defaults, the explicit selection of SiDB-aligned ALUs yields a 15 % area reduction, underscoring the importance of steering EDA tools towards technology-specific

TABLE II  
COST OBJECTIVE COMPARISON FOR *gold* ALGORITHM

PE	COST OBJ	$A_{\min}$	$\bar{A}$
W4A4	Area (baseline)	27 956	37 483.61
	$x + y$	27 956 (+0.00 %)	37 303.28 (−0.48 %)
	$x^2 + y^2$	28 175 (+0.78 %)	36 716.71 (−2.05 %)
W2A2	Area (baseline)	5145	10 156.22
	$x + y$	5145 (+0.00 %)	8107.02 (−20.18 %)
	$x^2 + y^2$	4704 (−8.57 %)	8121.47 (−20.03 %)

$A_{\min}$  and  $\bar{A}$  represent the minimum and mean areas under uniform technology mapping. All trials ran *gold* in single-core mode (400 s timeout on AMD Ryzen 9 9950X3D, maximum effort mode, input pin tile skipping swept 1–6 with randomization). 630 trials were performed per configuration with unsuccessful results discarded. *PLO* had maximum gate relocations set to 1.

component choices. Turning to the FoM-informed technology mapping results, the corresponding layouts are consistently larger than those obtained by treating all gates with equal preference, indicating that the technology mapper has chosen costlier solutions that make use of more robust gates. This area trade-off comes with the benefit that SiDB gates with higher reliability metrics are more often employed in the layout, which can ultimately yield a more robust SiDB logic implementation.

Comparing placement and routing algorithms, while the W8A8 AIG exceeds *gold*'s tractable problem size, W4A4 and W2A2 remain sufficiently small for *gold* to successfully place and route, achieving a  $\approx 40\%$  to  $50\%$  area reduction relative to *ortho*-based counterparts. However, the FoM-aware synthesis of W4A4 using *gold* exhibits a pronounced area increase. This work interprets the outlier as evidence that, under FoM-aware technology mapping, the AIG is already near the upper bounds of *gold*'s ability to provide consistent solutions: only 1 trial succeeded among 630 trials for this configuration. Nevertheless, configurations that remain within *gold*'s effective scaling regime yield area reductions that directly benefit manufacturability and reduce power consumption in practice.

Part of the improvement achieved with *gold* arises from refining the cost objectives in the SiDB-specific synthesis workflow (Section IV-C3). Two additional *gold* cost objectives were implemented—Manhattan distance ( $x + y$ ) and squared Euclidean distance ( $x^2 + y^2$ )—and compared against the default area-based objective in TABLE II. For the W2A2 configuration, both the best and average layout areas improve, with the gains being more pronounced in the average case and the squared Euclidean objective yielding the smallest minimum area. For W4A4, modest improvements persist in the average case, but no benefit is observed in the minimum area. This behavior is consistent with W4A4 already operating near the upper end of *gold*'s practical scaling range, where a reduced number of successful runs can skew the distribution of best-case results.

### C. Discussion

The presented synthesis results implement the PE-core, which represents all the logic operations in the PE; the omitted parts are purely for signal propagation (Section IV-A). A full PE-level estimation would additionally require routing the I/O pins of the PE-core to the outer I/O of the PE module and

accounting for the wiring cost of the return pass. Automating these steps calls for further streamlining of SiDB EDA tools and is therefore left as future work. Despite this estimation gap, the PE-core captures the computational portion of the PE, making it a meaningful comparison against the manual SiDB MXU estimates from [18]. Using the tile dimensions in TABLE I, the physical dimensions can be computed by  $w \times 23.06$  nm and  $h \times 13.06$  nm.<sup>2</sup> Relative to the manually estimated dimensions of  $5000$  nm  $\times$   $8150$  nm [18], the synthesized layout using optimized ALUs represent a  $3.4\times$  area increase; the gap would further widen if the entire PE was synthesized.

Several factors contribute to this discrepancy. Whereas the manual estimation used hand-designed components with relatively high logic gate density [18], the *Bestagon* gate library used in synthesis deliberately chooses a larger footprint to ensure sufficient separation between logic canvases of neighboring tiles to minimize inter-gate interference [16]. In addition, while the manual estimation directly used optimal ALU layouts, this work can only influence ALU selection at the RTL-to-netlist stage. The resulting AIG blurs the boundaries of arithmetic elements, limiting subsequent possibilities of exploiting those structures. Finally, the large W8A8 AIG is computationally intractable for *gold* to place and route, preventing the  $\approx 40\%$  to  $50\%$  area reductions observed for smaller configurations from being realized at this bit-width. Nevertheless, the successful end-to-end design flow achieved in this work demonstrates what state-of-the-art FCN EDA tools can realize on the SiDB platform, combining manufacturable layouts with full testbench-based verification and highlighting opportunities for further optimization.

## VI. CONCLUSION AND FUTURE WORK

This work has demonstrated an end-to-end RTL-to-atoms synthesis flow for a quantized SiDB-based MXU PE with fully verifiable behavior across abstraction levels, enabled by a hierarchical RTL organization that separates a combinational PE-core from its clocked shell. By explicitly selecting SiDB-appropriate ALUs in *Yosys* and tailoring technology mapping, placement-and-routing, and hexagonalization to SiDB logic, the presented framework achieves  $\approx 15\%$  reduction in synthesized PE-core area over prior flows and realizes additional footprint savings of  $\approx 40\%$  to  $50\%$  for configurations within the scaling range of newer placement-and-routing algorithms, while making explicit the trade-off between footprint and device-level robustness under FoM-aware mapping. Together, these components establish a reproducible benchmark for atomic-scale EDA that links RTL design decisions, EDA tooling, and manufacturable SiDB layouts.

The findings also reveal several avenues for future work to bridge remaining gaps with manual expert designs. Preservation of frequently used arithmetic structures across the synthesis stages will allow optimized ALU layouts to be directly applied in the physical layout stage. On physical design, improving the scalability and robustness of *gold* and *PLO* to handle larger scale netlists could allow the demonstrated footprint advantages to carry over to W8A8-scale layouts and larger

<sup>2</sup>These scaling factors differ from [20] due to corrected calculation factors.

accelerators. Finally, automating full PE- and MXU-level synthesis—including routing of the return path and of the PE-core’s pins to the outer PE module—will enable application-scale studies that jointly consider device reliability, clocking constraints, and workload characteristics. Taken together, the successful demonstration of an end-to-end RTL-to-atoms flow for a quantized SiDB-based MXU PE provides a concrete methodological foundation for these avenues and serves as the blueprint for future scalable accelerator studies on SiDBs.

#### CONTENT GENERATED BY AI

OpenAI LLMs were used for limited writing (wording & clarity) and coding aid. All outputs were reviewed and verified by the authors, who assume full responsibility for the content.

#### REFERENCES

- [1] C. S. Lent, B. Isaksen, and M. Lieberman, “Molecular quantum-dot cellular automata,” *Journal of the American Chemical Society*, vol. 125, no. 4, pp. 1056–1063, 2003.
- [2] G. Bernstein *et al.*, “Magnetic QCA systems,” *Microelectronics Journal*, vol. 36, no. 7, pp. 619–624, 2005.
- [3] D. Giri *et al.*, “Modeling, Design, and Analysis of MagnetoElastic NML Circuits,” *IEEE Transactions on Nanotechnology*, vol. 15, no. 6, pp. 977–985, Nov. 2016.
- [4] R. Achal *et al.*, “Lithography for robust and editable atomic-scale silicon devices and memories,” *Nature Communications*, vol. 9, no. 1, p. 2778, Jul. 2018.
- [5] J. Pitters *et al.*, “Atomically Precise Manufacturing of Silicon Electronics,” *ACS Nano*, p. acsnano.3c10412, Feb. 2024.
- [6] M. B. Haider *et al.*, “Controlled coupling and occupation of silicon atomic quantum dots at room temperature,” *Physical Review Letters*, vol. 102, no. 4, p. 046805, Jan. 2009.
- [7] J. L. Pitters, I. A. Dogel, and R. A. Wolkow, “Charge control of surface dangling bonds using nanoscale Schottky contacts,” *ACS Nano*, vol. 5, no. 3, pp. 1984–1989, Mar. 2011.
- [8] T. Huff *et al.*, “Binary atomic silicon logic,” *Nature Electronics*, vol. 1, no. 12, pp. 636–643, Dec. 2018.
- [9] S. S. H. Ng *et al.*, “SiQAD: A design and simulation tool for atomic silicon quantum dot circuits,” *IEEE Transactions on Nanotechnology*, vol. 19, pp. 137–146, 2020.
- [10] H. N. Chiu *et al.*, “PoisSolver: A tool for modelling silicon dangling bond clocking networks,” in *2020 IEEE 20th International Conference on Nanotechnology (IEEE-NANO)*. Montreal, QC, Canada: IEEE, Jul. 2020, pp. 134–139.
- [11] J. Drewniok, M. Walter, and R. Wille, “The Need for Speed: Efficient Exact Simulation of Silicon Dangling Bond Logic,” in *Asia and South Pacific Design Automation Conference (ASP-DAC)*, 2024.
- [12] W. Lambooy *et al.*, “Mastering the Exponential Complexity of Exact Physical Simulation of Silicon Dangling Bonds,” in *Asia and South Pacific Design Automation Conference (ASP-DAC)*, 2026.
- [13] M. D. Vieira *et al.*, “Three-Input NPN Class Gate Library for Atomic Silicon Quantum Dots,” *IEEE Design & Test*, pp. 1–1, 2022.
- [14] E. V. Ruella *et al.*, “A Comprehensive Analysis of Wire Performance in Silicon Dangling Bonds,” in *2025 38th SBC/SBMicro/IEEE Symposium on Integrated Circuits and Systems Design (SBCCI)*, 2025, pp. 1–5.
- [15] J. Drewniok *et al.*, “QuickCell: Fast Automatic Design of Standard Cells for Silicon Dangling Bond Logic,” *IEEE Transactions on Computer-Aided Design of Integrated Circuits and Systems*, pp. 1–1, 2025.
- [16] M. Walter *et al.*, “Hexagons are the Bestagons: Design automation for silicon dangling bond logic,” in *Proceedings of the 59th ACM/IEEE Design Automation Conference*, ser. DAC ’22. San Francisco, CA: Association for Computing Machinery, 2022, p. 6.
- [17] —, “Fiction: An open source framework for the design of field-coupled nanocomputing circuits,” *ArXiv*, vol. abs/1905.02477, 2019.
- [18] S. S. H. Ng *et al.*, “A Blueprint for Machine Learning Accelerators Using Silicon Dangling Bonds,” in *2023 IEEE 23rd International Conference on Nanotechnology (NANO)*. Jeju City, Korea, Republic of: IEEE, Jul. 2023, pp. 1–6.
- [19] N. P. Jouppi *et al.*, “In-datacenter performance analysis of a tensor processing unit,” 2017.
- [20] S. S. H. Ng *et al.*, “Building a Machine Learning Accelerator with Silicon Dangling Bonds: From Verilog to Quantum Dot Layout,” in *2025 IEEE 25th International Conference on Nanotechnology (NANO)*, 2025, pp. 483–488.
- [21] J. Drewniok, M. Walter, and R. Wille, “QuickTrace: An efficient contour tracing algorithm for defect robustness simulation of silicon dangling bond logic,” in *Proceedings of the 2025 IEEE International Symposium on Circuits and Systems (ISCAS)*. London, United Kingdom: IEEE, May 2025.
- [22] C. S. Lent and P. D. Tougaw, “A device architecture for computing with quantum dots,” *Proceedings of the IEEE*, vol. 85, no. 4, pp. 541–557, Apr. 1997.
- [23] M. Fuechle *et al.*, “A single-atom transistor,” *Nature Nanotechnology*, vol. 7, no. 4, pp. 242–246, Apr. 2012.
- [24] A. A. Prager, A. O. Orlov, and G. L. Snider, “Integration of CMOS, single electron transistors, and quantumdot cellular automata,” in *2009 IEEE Nanotechnology Materials and Devices Conference, NMDC 2009*, 2009.
- [25] S. Bohloul *et al.*, “Quantum transport in gated dangling-bond atomic wires,” *Nano Letters*, vol. 17, no. 1, pp. 322–327, Jan. 2017.
- [26] F. Riente *et al.*, “ToPoliNano: A CAD Tool for Nano Magnetic Logic,” *IEEE Transactions on Computer-Aided Design of Integrated Circuits and Systems*, vol. 36, no. 7, pp. 1061–1074, 2017.
- [27] U. Garlando, F. Riente, and M. Graziano, “FUNCODE: Effective Device-to-System Analysis of Field-Coupled Nanocomputing Circuit Designs,” *IEEE Transactions on Computer-Aided Design of Integrated Circuits and Systems*, vol. 40, no. 3, pp. 467–478, 2021.
- [28] Icarus Verilog GitHub repository. [Online]. Available: <https://github.com/steveicarus/iverilog>
- [29] C. Wolf, J. Glaser, and J. Kepler, “Yosys-a free verilog synthesis suite,” 2013.
- [30] S. W. Kim and E. E. Swartzlander, “Multipliers with coplanar crossings for quantum-dot cellular automata,” in *10th IEEE International Conference on Nanotechnology*, Aug. 2010, pp. 953–957.
- [31] R. Brayton and A. Mishchenko, “ABC: an academic industrial-strength verification tool,” in *Proceedings of the 22nd International Conference on Computer Aided Verification*, ser. CAV’10. Berlin, Heidelberg: Springer-Verlag, 2010, p. 24–40.
- [32] M. Walter *et al.*, “Scalable design for field-coupled nanocomputing circuits,” in *Proceedings of the 24th Asia and South Pacific Design Automation Conference*, ser. ASPDAC ’19. New York, NY, USA: Association for Computing Machinery, 2019, pp. 197–202.
- [33] S. Hofmann, M. Walter, and R. Wille, “Graph-Oriented Layout Design for Field-Coupled Nanocomputing via Parallel Multi-Objective Search Space Exploration,” *IEEE Transactions on Circuits and Systems I: Regular Papers*, pp. 1–14, 2025.
- [34] —, “Efficient and Scalable Post-Layout Optimization for Field-Coupled Nanotechnologies,” *IEEE Transactions on Computer-Aided Design of Integrated Circuits and Systems*, vol. 44, no. 10, pp. 3790–3803, 2025.
- [35] —, “Scalable Physical Design for Silicon Dangling Bond Logic: How a 45° Turn Prevents the Reinvention of the Wheel,” in *2023 IEEE 23rd International Conference on Nanotechnology (NANO)*. Jeju City, Korea, Republic of: IEEE, Jul. 2023, pp. 872–877.
- [36] M. Walter *et al.*, “Verification for field-coupled nanocomputing circuits,” in *2020 57th ACM/IEEE Design Automation Conference (DAC)*, 2020, pp. 1–6.
- [37] J. Drewniok *et al.*, “Unifying Figures of Merit: A Versatile Cost Function for Silicon Dangling Bond Logic,” in *2024 IEEE 24th International Conference on Nanotechnology (NANO)*. Gijón, Spain: IEEE, Jul. 2024, pp. 91–96.
- [38] M. Walter *et al.*, “Reducing the Complexity of Operational Domain Computation in Silicon Dangling Bond Logic,” in *International Symposium on Nanoscale Architectures (NANOARCH)*, 2023.
- [39] J. Drewniok, M. Walter, and R. Wille, “Temperature Behavior of Silicon Dangling Bond Logic,” in *IEEE International Conference on Nanotechnology (IEEE NANO)*, 2023, pp. 925–930.
- [40] S. S. H. Ng *et al.*, “Simulating Charged Defects in Silicon Dangling Bond Logic Systems to Evaluate Logic Robustness,” *IEEE Transactions on Nanotechnology*, vol. 23, pp. 231–237, 2024.
- [41] V. Vankamamidi, M. Ottavi, and F. Lombardi, “Two-dimensional schemes for Clocking/Timing of QCA circuits,” *IEEE Transactions on Computer-Aided Design of Integrated Circuits and Systems*, vol. 27, no. 1, pp. 34–44, 2008.
- [42] S. K. Esser *et al.*, “Learned Step Size Quantization,” 2020.
- [43] R. Banner, Y. Nahshan, and D. Soudry, “Post training 4-bit quantization of convolutional networks for rapid-deployment,” in *Advances in Neural Information Processing Systems*, vol. 32. Curran Associates, Inc., 2019.