

Physical Design for Field-coupled Nanocomputing with Discretionary Cost Objectives

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Abstract—*Field-coupled Nanocomputing* (FCN) represents a class of emerging post-CMOS technologies that achieve nanoscale computation without relying on the flow of electrical current. Despite their potential, existing FCN physical design algorithms predominantly focus on minimizing either layout area or execution runtime, neglecting the complexity of real-world design constraints. This work introduces the first physical design method for FCN that accommodates discretionary cost objectives, marking a significant advancement in the field. This approach integrates insights from both simulation and manufacturing, facilitating more comprehensive and optimized design solutions. An open-source implementation is available, and the proposed algorithm has been validated experimentally on a set of common benchmark functions, demonstrating its effectiveness across a range of different scenarios and cost objectives.

I. INTRODUCTION

Field-coupled Nanocomputing (FCN, [1]) represents a class of post-CMOS technologies that operate at the nanoscale without relying on electrical current, aiming to meet the growing demand for computational power while addressing environmental concerns. Recently, FCN has gained momentum due to advances in the manufacturing [2] and simulation [3]–[5] of logic gates using *Silicon Dangling Bonds* (SiDBs, [6]) and the physical design [7]–[14] and optimization [15], [16] of gate-level layouts.

To efficiently design layouts with these logic gates, physical design algorithms are essential. However, due to the numerous technological constraints imposed by FCN, these methods typically focus on either minimizing the layout area, which directly affects both simulation computational costs and manufacturing expenses, or on reducing the execution time of the layout generation process, at the expense of layout area.

While minimizing layout area is a critical target, recent developments emphasize the importance of considering additional factors. For example, physical simulation revealed varying levels of gate robustness to external disturbance in specific FCN technologies [17]. Furthermore, wire segments incur area and delay costs comparable to standard gates [16], [18] while wire crossings impose great hindrances to manufacturability [19]. While logic synthesis and technology mapping can optimize gate selection and the number of crossings in the logic network, the actual number of crossings and wire segments ultimately depends on the specific placement and routing of the gates within the layout.

Moreover, current algorithms are limited in their ability to handle more complex cost objectives, such as those incorporating the distance between gates or weighted combinations of multiple targets.

This work introduces the first physical design algorithm for FCN that accommodates discretionary cost objectives, allowing cost factors to be flexibly adjusted or selected based on specific needs or preferences, and thereby enabling the integration of insights from both simulation and manufacturing processes into the layout design.

An open-source implementation on top of the *fiction* framework [20] is available as part of the *Munich Nanotech Toolkit* (MNT, [21]).¹ Furthermore, the generated layouts have been included in the benchmark suite *MNT Bench* [22].²

The remainder of this paper is structured as follows: Section II reviews technical background on selected FCN technologies. Section III discusses state-of-the-art design automation methods for FCN. The physical design algorithm with discretionary cost objectives is proposed in Section IV, which constitutes the main contribution of this work. It is experimentally evaluated on a set of common benchmark functions in Section V. Finally, Section VI concludes the paper.

II. BACKGROUND

This section introduces the fundamentals of FCN technologies, including *Quantum-dot Cellular Automata* (QCA, [23]) and *Silicon Dangling Bonds* (SiDBs, [6]), along with the technological constraints inherent to most FCN implementations.

A. *Quantum-dot Cellular Automata* (QCA)

In QCA, the fundamental components are called *cells*, each consisting of four *quantum dots* arranged in a square frame, which host two charges. Due to stronger Coulomb interaction along the shorter distance between adjacent dots compared to the diagonal distance, the charges stabilize in one of two configurations, as illustrated in Fig. 1a, representing binary values of 0 and 1. When multiple cells are placed adjacent to each other, the polarization of one cell influences its neighbor through electrical fields, thereby creating a wire capable of propagating information, as shown in Fig. 1b. Additionally, standard logic gates, such as the majority-of-three (MAJ3) function, AND, OR, and inverters, can be constructed by arranging cells in specific configurations, as depicted in Fig. 2 to create gate libraries [24].

B. *Silicon Dangling Bonds* (SiDBs)

Unlike QCA cells, which consist of four quantum dots, SiDBs utilize pairs of dots to implement a concept known as *Binary-dot Logic* (BDL, [25]) to develop standard gate libraries [26]. To create SiDBs, which act as atomically-sized, chemically identical quantum dots, a scanning tunneling

¹Code is available at <https://github.com/cda-tum/fiction>.

²<https://www.cda.cit.tum.de/mntbench>

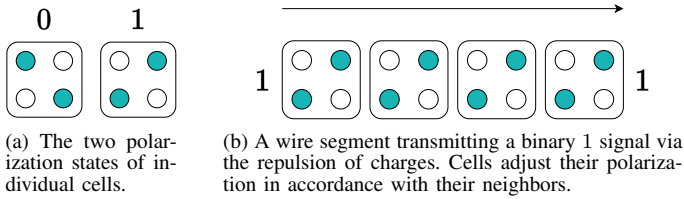


Fig. 1: Elementary QCA cells and a wire segment.

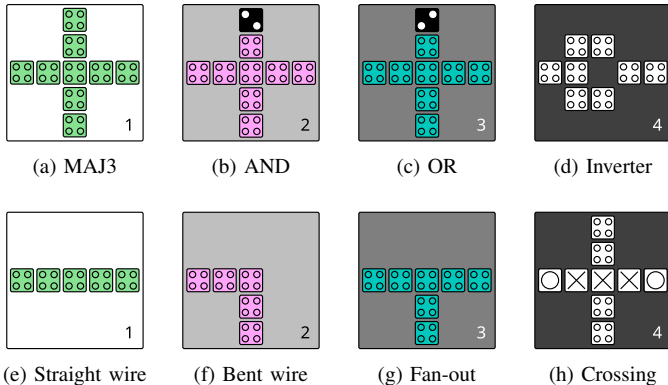


Fig. 2: Standard tiles in the QCA ONE gate library [24].

microscope tip [6] is employed to remove hydrogen atoms from a passivated silicon (H-Si(100)-2×1) surface [27]. Recent advancements that allow for exceptional precision in the placement of these dots [2], [28]–[31] have enabled the successful fabrication of a fully functioning SiDB OR gate with a footprint of less than 30 nm² [25].

C. Technology Constraints

To assemble standard FCN components into layouts computing meaningful functionality, physical design algorithms are commonly applied. However, it has to be ensured that they operate within the realms of technological constraints imposed by FCN. Due to these constraints, especially wire routing is complex, as most implementations are planar with limited crossing capabilities [19], [32] and signal synchronization has to be ensured by managing the length of wire segments throughout the layout [33].

FCN layouts are segmented into uniform *tiles*, visually represented by the black outlines around the standard gates and wire segments in Fig. 2. The total area is then defined by the number of tiles in the layout. To ensure signal stability and manage information flow, a clocking mechanism utilizing four consecutive signals (clock 1 through 4) is implemented. These signals are distributed to the individual tiles via buried electrodes embedded within the circuit substrate [34]. To facilitate the design process, tailored arrangements of regular clock zones, also called clocking schemes, have been proposed, such as *2DDWave* [35], where information flow is restricted from left to right and top to bottom only.

Addressing synchronization constraints, minimizing the number of crossings and wire segments, and optimizing layout area are extremely challenging tasks. In fact, finding an optimal layout with respect to even the single cost objective layout area is \mathcal{NP} -complete [36]. Furthermore, in contrast to traditional

CMOS design, where entire cells are placed and routed, the design process in FCN requires individual gate placement. Each gate is subsequently replaced by its corresponding cell representation from one of the available gate libraries [24], [26]. This underscores the necessity for a physical design algorithm capable of managing all these constraints while accommodating discretionary cost objectives.

III. RELATED WORK: PHYSICAL DESIGN FOR FIELD-COUPLED NANOCOMPUTING

This section reviews existing placement and routing algorithms, which either focus on optimizing the layout area or the execution runtime.

A. Exact Approaches

To generate layouts from specifications that are optimal concerning the layout area, exact physical design algorithms, e.g., [7], [9], have been proposed. By framing the design task of implementing a given function in a symbolic formulation and submitting it to a reasoning engine, the algorithm systematically tests every layout size, beginning with the smallest, to determine whether a realization of the underlying logic function can be achieved. Additionally, if multiple layouts exist with the same area cost, exact approaches enable the consideration of secondary optimization criteria. Due to the \mathcal{NP} -completeness [36] of the underlying physical design problem, this approach only scales to logic functions up to ≈ 40 gates.

B. Heuristic Approaches

To overcome the scalability challenges of exact methods, heuristic approaches provide a practical alternative by employing approximations to generate layouts efficiently. These algorithms either prioritize scalability by disregarding layout area overhead altogether or focus on reducing layout area for logic functions that exact methods cannot manage effectively.

The heuristic algorithms *ortho* [8] and *input-ordering SDN* [10] design large-scale layouts for QCA circuits by restricting the search space drastically. They achieve scalability at the costs of result quality, particularly in terms of layout area.

Another method utilizes reinforcement learning for gate placement [11], [13], where the layout area is incorporated into the reward function for the learning agent.

C. Search-Based Approaches

To find a trade-off between runtime and scalability, a recent addition called *gold* [14] generates compact layouts by representing the physical design problem as path finding in a search space graph. In this graph, each placement event corresponds to a vertex, representing the partial layout at that particular stage. An edge between two vertices, representing partial layouts *a* and *b*, exists if *a* can be transformed into *b* through a single placement event. Similar to finding a path in a maze, the *A**-search algorithm can be used to determine a path from the starting vertex (an empty layout) to a goal (a functionally correct layout with all gates placed).

Example 1: An example of this process is illustrated in Fig. 3 by the means of a 2:1 multiplexer. At the first level, the primary input can be placed on any tile in the first row. As the algorithm progresses to the next level, it prioritizes expanding the partial layout with the smallest area, i.e., the one using the fewest tiles. By traversing to the final level of the search space graph, a functional layout with all gates placed is obtained. In Fig. 3,

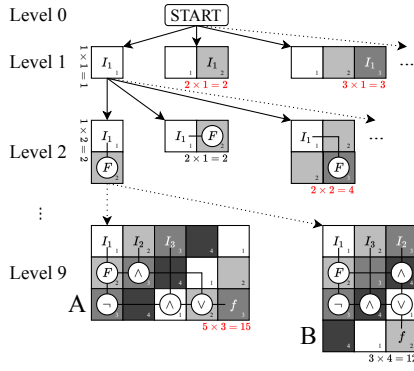


Fig. 3: The search space graph created for the 2:1 multiplexer, with two possible solutions at the bottom.

two possible solutions (A and B) are shown, which are both functionally correct but have different layout areas. The layout in the final level with the smallest area (B) is then returned by *gold*.

This algorithm acts as a basis for the cost-aware physical design approach described in Section IV.

D. Post-Layout Optimization

To address the layout area overhead introduced by heuristic algorithms during the physical design stage, post-layout optimization techniques [15], [16] are employed to eliminate this excess area and refine the design. This is achieved by relocating gates to more advantageous positions and shortening redundant wire segments, thereby refining and minimizing the layout area even after the initial design is complete.

IV. PROPOSED APPROACH: COST-AWARE LAYOUT DESIGN

This section details the key principles of the proposed approach, encompassing the generation of layouts based on discretionary cost objectives introduced in Section IV-A, the formulation of these cost objectives in Section IV-B, and the construction of multiple search space graphs to further accelerate and optimize the layout design process as described in Section IV-C.

A. General Idea: Cost-Aware Expansion

The general idea of the proposed approach is extending the graph-oriented layout design (*gold*) method discussed in Section III-C to enable the creation of layouts guided by discretionary cost objectives. Beginning with an empty layout, gates are placed at positions that minimize that cost. Consequently, the entire search space graph is constructed based on the cost objective, which allows the A*-search algorithm to choose the partial layout with the lowest cost out of the possible vertex expansions.

Example 2: In Fig. 4, a layout with three input pins and one gate already placed is depicted at the top. Depending on the selected cost objective, different placements for the subsequent gate must be chosen. If minimizing area is the primary objective, placing the AND gate to the right of the existing AND gate results in a layout with an area of $5 \times 3 = 15$ tiles in the bottom left. However, this placement introduces two wire crossings, as the connection to I_1 must cross two other wires. On the other hand, if minimizing the number

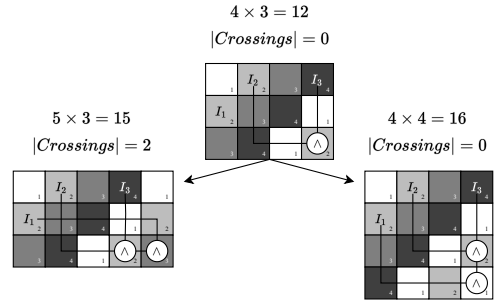


Fig. 4: Depending on the cost objective, different expansions are prioritized.

of crossings is the priority, placing the AND gate below the existing AND gate avoids adding any new crossings in the bottom right layout. This comes at the cost of increasing the layout area to $4 \times 4 = 16$ tiles, which is slightly larger than the other expansion.

B. Cost Objectives

With the proposed method, any discretionary cost objective can be used, as it is calculated based on the current partial placement. On top of the number of tiles, number of crossings, or number of wire segments, also the specific location of gates can be used, e.g., to maximize the distance between gates which are more sensitive to close negative charges [17], and other gates in the layout.

Additionally, this allows for the utilization of composite cost objectives as in traditional physical design for CMOS like the *Power-Delay Product* (PDP), or *Energy-Delay Product* (EDP) [37]. Due to the special technological features and constraints of FCN, a viable composite cost objective could be the *Area-Crossing Product* (ACP):

$$ACP = A \cdot (|C| + 1). \quad (1)$$

C. Multiple Search Space Graphs

To further increase the efficiency of the proposed method, multiple search space graphs are spanned and searched using A* simultaneously. These graphs are created based on different design choices, such as the order in which the gates are placed. Additionally, multiple search space graphs are created for the four cost objectives—layout area, number of crossings, number of wire segments, and area-crossing product—since layouts optimized for these objectives often also achieve a low cost with respect to the defined cost objective.

Overall, incorporating all aspects proposed above yields a physical design method that allows for generating designs optimized for discretionary cost objectives as illustrated by the following example:

Example 3: For the *Parity Check* function and the cost objectives layout area, number of crossings, and number of wire segments, the proposed algorithm generated three distinct layouts, as shown in Fig. 5. The first layout (Fig. 5a) has the smallest area of 50 tiles but requires 4 crossings and 22 wire segments. The second layout (Fig. 5b) achieves the fewest crossings, of only 3, but has a larger area of 60 tiles and 27 wire segments. The third layout (Fig. 5c) minimizes wire segments to 21, but it has a higher area of 54 tiles and the highest number of crossings, totaling 5.

Table I: Experimental evaluation of the proposed algorithm for different cost objectives.

Circuit [38], [39]	COST: AREA (A)			COST: CROSSINGS (C)				COST: WIRES (W)				COST: ACP							
	Name	I	O	$ N $	A	$ C $	$ W $	ACP	A	$ C $	$ W $	ACP	A	$ C $	$ W $	ACP	A	$ C $	$ W $
2:1 MUX	3	1	4	12	1	3	24	15	0	5	15	12	1	3	24	15	0	5	15
XOR	2	1	4	18	1	9	36	21	1	11	42	18	1	7	36	18	1	9	36
Full Adder	3	2	5	32	2	19	96	32	2	19	96	32	2	19	96	32	2	19	96
XNOR	2	1	6	18	1	6	36	18	1	6	36	18	1	4	36	18	1	6	36
Half Adder	2	2	6	24	4	14	120	40	2	23	120	24	4	14	120	28	2	16	84
c17	5	2	8	32	1	13	64	36	1	17	64	32	1	13	64	32	1	13	64
Parity Gen.	3	1	10	40	4	21	200	48	2	25	144	40	3	20	160	45	2	25	135
clpl	11	5	10	90	10	50	990	90	10	50	990	90	10	50	990	90	10	50	990
t	5	2	11	48	6	27	336	48	6	27	336	48	6	27	336	48	6	27	336
t_5	5	2	11	30	1	11	60	30	1	11	60	30	1	11	60	30	1	11	60
b1_r2	3	4	12	56	5	30	336	64	4	30	320	64	4	29	320	64	4	30	320
Parity Check	4	1	15	50	4	22	250	60	3	27	240	54	5	21	324	60	3	27	240
1bitAdderAOIG	3	2	15	72	7	42	576	90	5	48	540	72	7	42	576	78	5	44	468
majority	5	1	17	126	9	81	1260	143	8	75	1287	128	10	75	1408	126	9	81	1260
majority_5_r1	5	1	17	60	3	31	240	60	3	31	240	60	3	30	240	60	3	31	240
newtag	8	1	17	70	7	38	560	102	1	48	204	70	7	37	560	102	1	48	204
XOR5_R1	5	1	26	90	9	46	900	144	7	80	1152	90	9	46	900	90	9	46	900
1bitAdderMaj	3	1	29	200	20	115	4200	238	15	117	3808	200	20	115	4200	238	15	117	3808
cm82a_5	5	3	42	234	44	176	10530	324	40	197	13284	234	44	176	10530	234	44	176	10530
2bitAdderMaj	5	2	54	399	39	195	15960	432	34	190	15120	432	34	190	15120	432	34	190	15120
xor5Maj	5	1	70	759	70	373	53889	759	70	373	53889	759	70	373	53889	759	70	373	53889
parity	16	1	103	549	33	260	18666	630	27	322	17640	549	33	260	18666	549	30	260	17019

I , O , and $|N|$ represent the number of primary inputs, primary outputs, and nodes in the logic network, respectively; A , $|C|$, $|W|$, and ACP denote the resulting layout area, number of crossings, number of wire segments, and area-crossing product, respectively. The timeout for each layout generation was set to 1 min.

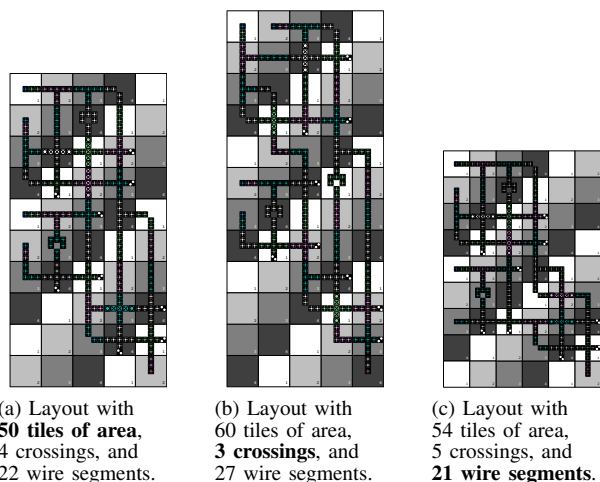


Fig. 5: Three layouts for the *Parity Check* function based on different cost objectives.

V. EXPERIMENTS

This section presents the results of an experimental evaluation of the proposed physical design algorithm, conducted on logic networks from a set of benchmark circuits commonly used in the field [38], [39]. To show that the proposed method is able to generate layouts based on any specified cost objective, the evaluation considers four different ones: layout area, number of crossings, number of wire segments, and the area-crossing product. Furthermore, the correctness of the generated layouts has been validated using formal verification [40]. The comparative analysis was conducted on a macOS 13.0 machine with an Apple Silicon M1 Pro SoC with 32 GB of integrated main memory and set a timeout of 1 min for each layout generation.

VI. CONCLUSION

With the rise of *Field-coupled Nanocomputing* (FCN) as a class of promising post-CMOS technologies, it has become essential to incorporate insights from recent advances in simulation and manufacturing into the automatic physical design process. This work presented an approach capable of generating layouts based on discretionary cost objectives. Its effectiveness was demonstrated experimentally on a set of benchmark functions, focusing on four exemplary cost objectives: layout area, number of crossings, number of wire segments, and area-crossing product. These results are crucial because they demonstrate the potential of our approach to address the complex and varied design requirements of FCN technologies, paving the way for more efficient and adaptable designs as this emerging technology continues to evolve.

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