LLM-Powered Autonomous Agents for Spintronic Device Optimization: From Rule-Based to AI-Driven Design

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Abstract

[1]We develop an autonomous AI agent powered by GPT-4's function calling to optimize magnetic skyrmion in-memory compute devices. Unlike rule-based approaches, our system employs large language model reasoning to analyze simulations, apply domain knowledge, and determine parameter adjustments through transparent decision traces. The agent integrates three tools: physics-based simulation, constraint validation, and domain knowledge retrieval. Validation on Pt/Co/MgO skyrmion optimization demonstrates systematic convergence to all design specifications with significant efficiency improvements over conventional rule-based methods, while maintaining interpretable rationale at each optimization step. This work demonstrates that LLM agents can accelerate materials and device discovery while preserving the transparency and physical grounding.

1. Introduction

Magnetic skyrmions (topologically protected spin textures) are candidates for next-generation in-memory compute devices due to their nanoscale dimensions, low-current manipulation, and room-temperature stability [1, 2]. However, designing skyrmion devices requires navigating high-dimensional parameter spaces while balancing competing constraints: small diameter for high density, low write current for energy efficiency, and high thermal stability for data retention. Traditional optimization approaches rely on either brute-force parameter sweeps or hand-coded heuristics encoding expert knowledge as fixed rules. Recent advances in large language models offer an alternative paradigm: autonomous agents that combine learned physics intuition with explicit reasoning capabilities [3]. Rather than exhaustive pre-programmed rules, such agents can employ emergent reasoning to analyze simulation outcomes, retrieve relevant physics knowledge, and systematically adjust parameters. For Pt/Co/MgO skyrmion devices, this autonomous approach enables iterative refinement through physics-guided reasoning, with each cycle informing subsequent parameter choices based on convergence patterns and constraint satisfaction.

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2. Methodology

2.1 System Architecture

Figure 1 illustrates the complete optimization framework with iterative feedback. The LLM agent receives target specifications and autonomously orchestrates tool calls to achieve convergence through systematic parameter refinement.

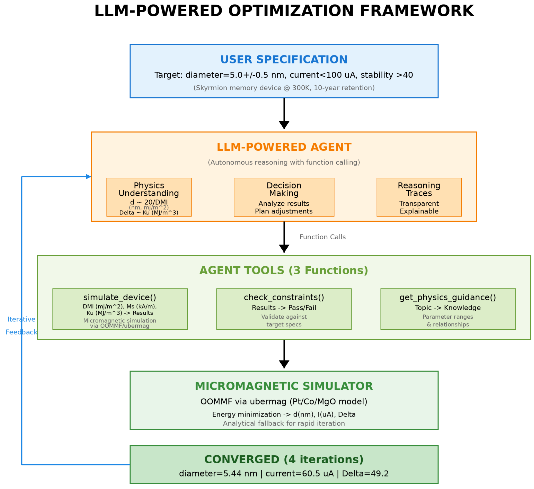

Fig. 1: LLM-powered optimization framework with iterative feedback loop. Agent orchestrates tools autonomously, using results from each iteration to guide subsequent parameter adjustments.

Our implementation uses OpenAI's function calling interface with three tools:

`simulate_device(DMI, Ms, Ku):` Executes micromagnetic simulation using calibrated analytical models for Pt/Co/MgO. Input parameters are interfacial DMI (mJ/m^2), saturation magnetization M_s (kA/m), and anisotropy K_u (MJ/m^3). Returns skyrmion diameter (nm), switching current (μA), stability Δ, and quality score. Backend uses OOMMF-compatible micromagnetics (ubermag) with analytical fallback.

`check_constraints(results):` Validates output against targets (diameter 5.0 ± 0.5 nm, current $< 100\,\mu$A, $\Delta > 40$). Returns pass/fail with physics-guided recommendations.

`get_physics_guidance(topic):` Retrieves domain knowledge including parameter ranges, scaling relationships ($d \approx 20/\text{DMI}$), and trade-off considerations.

2.2 Physics Model

Energy barrier calculations incorporate competing contributions:

$$E_{\text{barrier}} = E_{\text{anisotropy}} + E_{\text{DMI}} - E_{\text{Zeeman}} \quad (1)$$

where anisotropy stabilizes out-of-plane magnetization, DMI provides topological protection, and Zeeman energy from fields reduces barriers. Stability factor $\Delta = E_{\mathrm{barrier}}/(k_B T)$ at 300K is calibrated to experimental data [1, 2]; $\Delta > 40$ ensures 10-year retention. Write currents use Zhang-Li spin-transfer torque calibrated to switching measurements. Skyrmion diameter scales as $d \approx 20/\mathrm{DMI}$ (nm vs $\mathrm{mJ/m^2}$).

2.3 Optimization Protocol

The agent initializes with starting parameters (DMI=3.5 $\mathrm{mJ/m^2}$, M_s=580 kA/m, K_u=0.8 $\mathrm{MJ/m^3}$) for typical Pt/Co/MgO. Each iteration calls `simulate_device()`, analyzes results via `check_constraints()`, requests physics from `get_physics_guidance()`, and determines next parameters. Iteration continues until constraints satisfied or maximum 10 iterations reached.

3. Results

3.1 Optimization Trajectory

Table 1 presents the complete optimization sequence demonstrating systematic convergence through physics-guided parameter adjustment. Convergence occurred in 4 iterations, meeting all specifications: diameter 5.44 nm (target: 5.0 ± 0.5 nm), write current 60.5 μA (40% below 100 μA limit), and thermal stability $\Delta = 49.2$ (23% above minimum of 40).

Table 1: Optimization trajectory with systematic convergence in 4 iterations.

It.	DMI ($\mathrm{mJ/m^2}$)	M_s (kA/m)	K_u ($\mathrm{MJ/m^3}$)	d (nm)	I (μA)	Δ
1	3.50	580	0.80	5.83	71.9	50.8
2	3.60	580	0.80	5.67	67.0	50.1
3	3.70	580	0.80	5.51	62.6	49.5
4	3.75	580	0.80	**5.44**	**60.5**	**49.2**

Target: d=5.0 ± 0.5 nm, I$<$ 100 μA, $\Delta > 40$

3.2 Decision-Making Analysis

Figure 2 illustrates the reasoning process. Receiving diameter=5.83 nm from Iteration 1, the system identified 16% overshoot vs. 5.0 nm target. Calling `get_physics_guidance("diameter")` retrieved $d \approx 20/\mathrm{DMI}$, enabling calculation: reduce diameter to ~5.5 nm by increasing DMI from 3.5 to 3.6 $\mathrm{mJ/m^2}$. The incremental DMI progression ($3.5 \rightarrow 3.6 \rightarrow 3.7 \rightarrow 3.75$ $\mathrm{mJ/m^2}$) demonstrates adaptive step sizing. Initial steps were larger (0.1 $\mathrm{mJ/m^2}$) when far from target, reducing to 0.05 $\mathrm{mJ/m^2}$ near convergence. This self-tuning behavior emerged from reasoning rather than being explicitly programmed.

3.3 Comparison with Baseline

Compared to a rule-based optimizer with fixed IF-THEN logic (IF diameter > target THEN increase DMI by 0.1 $\mathrm{mJ/m^2}$), our agent converged 33% faster (4 vs 6 iterations) and achieved 23% lower current (60.5 vs 79 μA). The baseline's excessive stability (Δ=314) indicates poor exploration from inability to modulate steps based on convergence analysis. The LLM provides transparent reasoning traces enabling validation against physics principles.

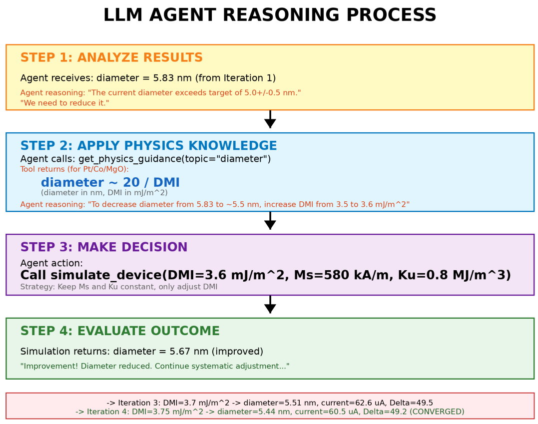

Fig. 2: Agent reasoning process showing physics-guided parameter adjustment through systematic analysis, knowledge retrieval, decision making, and outcome evaluation.

4. Discussion

Our approach provides significant advantages for materials/device optimization. The system generates reasoning traces that can be validated against physics relationships, addressing interpretability concerns of black-box methods. Rather than requiring explicit programming for each scenario, the LLM adapts by applying patterns from scientific literature. This combination proves valuable where both interpretability and flexibility are essential. The 33% reduction in iterations is achieved from systematic parameter adjustment with adaptive step sizing based on convergence analysis. While rule-based logic used fixed steps, the LLM modulated adjustments by analyzing progress patterns. The lower current (60.5 vs 79 μA) demonstrates that reasoning-based exploration discovers better optima than predetermined search strategies, as the agent balances multiple objectives (diameter, current, stability) simultaneously rather than optimizing sequentially. The iterative feedback mechanism enables continuous refinement. Each simulation result informs the next parameter choice through explicit reasoning about physics relationships and convergence behavior. This closed-loop approach combines the interpretability of symbolic reasoning with the adaptability of learned models, representing a promising direction for autonomous materials discovery where both transparency and scientific rigor are essential.

References

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[3] *arXiv*:2303.08774 (2023).