NIMO: Universal Middleware for Closed-Loop Materials Exploration

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1. Introduction

To accelerate the discovery of advanced materials, the realization of self-driving laboratories (SDLs) for materials science is essential. Machine learning-based black-box optimization (BBO) has proven to be a powerful "AI" for proposing promising materials candidates[1]. However, a significant technical barrier remains: the seamless integration of these algorithms with diverse, stand-alone robotic hardware to form a unified closed-loop workflow. Most existing laboratory infrastructures are not designed to be easily interfaced with external AI modules, often requiring extensive custom programming and complex system architecture.

To address this challenge, we developed NIMO (NIMS-OS), an open-source middleware library designed for high modularity and interoperability[2]. NIMO treats robotic experimental systems and BBO methods as independent, swappable modules, allowing researchers to bridge the gap between AI and robotic experiments with minimal effort. This architecture significantly lowers the hurdle for transforming traditional laboratory equipment into autonomous, closed-loop systems (Fig. 1).

In this presentation, we first introduce the core algorithms implemented within NIMO. We then demonstrate its versatility through successful implementations in four distinct experimental and functional domains: (1) an automated electrochemical measurement system, (2) a Chemspeed platform for liquid-phase chemical synthesis, (3) a thin-film deposition apparatus, and (4) an automated calibration system for liquid-handling robots. These case studies showcase how NIMO facilitates rapid, human-free materials exploration and system optimization by effectively integrating with heterogeneous laboratory infrastructure, providing a scalable foundation for the future of AI-driven materials science. The GitHub of NIMO is available at https://github.com/NIMS-DA/nimo.

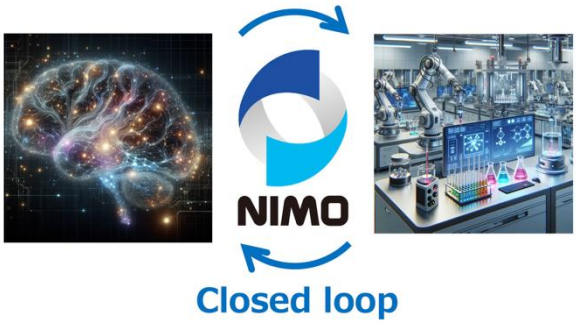

Fig. 1: Conceptual diagram of NIMO-enabled autonomous closed-loop workflow.

2. AI algorithms

To select the next experimental conditions, BBO serves as the "AI engine" for autonomous materials science. Depending on the specific exploration goals, NIMO allows users to switch between different BBO algorithms seamlessly. For instance, when the objective is to optimize a specific material property, Bayesian Optimization (BO) is highly effective. NIMO integrates the PHYSBO library[3], enabling both single- and multi-objective BO with batch proposal capabilities.

Beyond simple optimization, NIMO supports specialized search strategies for various research needs:

- ✓ PTR (Probabilistic Target Region): Useful when the goal is to identify a large number of materials within a specific desired property range[4].
- ✓ BLOX (Bound-Less Objective-free eXploration): Ideal for discovering a diverse variety of materials across the search space[5].
- ✓ COMBI: A specialized BO algorithm designed for combinatorial experiments[6].
- ✓ PDC (Phase Diagram Construction): Tailored for phase diagram mapping, where categorical variables (phase names) require a distinct approach from continuous variables[7].

To facilitate rapid switching between these strategies, each algorithm is implemented as an independent module. These AI modules can be executed through a unified Python interface, as shown below:

```
nimo.selection(method = "PHYSBO",
               input_file = candidates_file,
               output_file = proposals_file,
               num_objectives = 1,
               num_proposals = 10)
```

By simply specifying the algorithm name in the method parameter, researchers can pivot their exploration strategy without restructuring their entire workflow.

3. Self-driving laboratories enabled by NIMO

In this section, we present four distinct SDL implementations that utilize NIMO as their core integration engine (Fig. 2).

3.1 Autonomous electrochemical experiments

This system, originally developed by NIMS in 2017, automates electrolyte preparation and battery performance evaluation, capable of handling up to 96 experiments in parallel[8]. By integrating NIMO, we have achieved a fully closed-loop electrolyte discovery process. The BBO module in NIMO proposes optimal electrolyte compositions, which the robot then prepares and tests without any human intervention[2].

3.2 Automated chemical synthesis workflow

Using the Chemspeed automated synthesis platform coupled with an HPLC (High-Performance Liquid Chromatography) system, an end-to-end workflow for chemical reaction and measurement was realized. NIMO serves as the orchestrator, analyzing HPLC results and suggesting the next synthesis conditions. This integration has successfully realized a closed-loop system for the rapid optimization of chemical reactions[9].

3.3 Composition-spread film synthesis

Combinatorial film deposition is a powerful method for exploring vast compositional spaces simultaneously. By employing the COMBI algorithm implemented in NIMO, we developed a system that automates the cycle of deposition, characterization, and prediction. This allows for the efficient exploration of thin-film materials by evaluating a large number of samples in a single autonomous loop[6].

3.4 Automated liquid-handling calibration

To ensure the precision of robotic experiments, we developed a calibration system for BioDot automated liquid handlers. We integrated a camera to monitor dispensing results, which are then analyzed by NIMO to optimize the dispensing parameters. This closed-loop approach allows for the fully automated calibration of liquid-handling tasks, significantly improving the reliability of subsequent materials experiments[10].

4. Conclusion and future perspective

In this study, we introduced NIMO, an open-source middleware that bridges the gap between diverse robotic hardware and AI-driven optimization algorithms. Through four practical applications, we demonstrated that NIMO's modular architecture effectively lowers the technical barriers to implementing closed-loop systems. By transforming stand-alone instruments into autonomous laboratories, NIMO enables researchers to focus on high-level scientific strategy rather than low-level system integration.

We aim to enhance NIMO's interoperability by establishing seamless interfaces with other lab orchestration software (OS), such as IvoryOS[11]. By combining NIMO's advanced optimization modules with the robust device control and workflow management capabilities of other OSs, we can create more complex and reliable SDL ecosystems. Furthermore, we plan to integrate Large Language Models (LLMs) for intuitive experimental planning and move toward a globally "Connected SDL" network. These efforts will fundamentally accelerate the pace of materials discovery and promote the democratization of autonomous science.

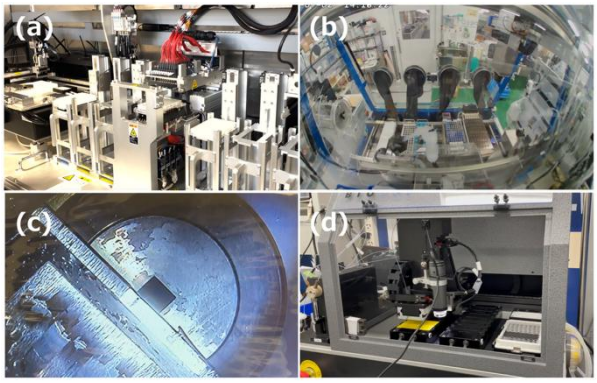

Fig. 2: Examples of NIMO-integrated SDL systems: (a) electrochemical, (b) chemical synthesis, (c) thin-film deposition, and (d) liquid-handling calibration.

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