Robotic-arm-based self-driving laboratories powered by NIMO and IvoryOS

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1. Introduction

With the aim of accelerating scientific discovery, self-driving laboratories (SDLs) [1] are actively studied worldwide. Advanced SDLs require sophisticated software to control automation hardware through autonomous decision-making algorithms. To address this need, we developed NIMO (formerly NIMS-OS) [2], a software platform designed to facilitate the creation of closed-loop robotic experiments integrated with artificial intelligence for automated materials exploration. Although NIMO has lowered the barrier to incorporating data-driven algorithms into SDLs, users are still required to write custom programs for their own robotic environments. This requirement can hinder the widespread adoption of SDLs, as their primary users are often non-experts in programming. Furthermore, most existing SDL implementations that incorporate NIMO rely on gantry-based automation systems with limited degrees of freedom, thereby limiting experimental flexibility.

In this work, we demonstrate the integration of NIMO into IvoryOS [3], an open-source orchestration software that provides accessible web interfaces automatically generated from Python code. This integration enables us to leverage IvoryOS's intuitive graphical user interface in combination with the decision-making algorithms provided by NIMO. As a proof of concept, we developed two robotic-arm-based SDLs that utilize the PDC algorithm [4] implemented in NIMO to explore the phase diagrams of the coffee ring effect and the patterns of milk droplet splashing.

2. Integration of NIMO into IvoryOS

The integration of NIMO is through the implementation of the abstract optimizer module in IvoryOS. The abstract optimizer provides a standard input-output between the workflow engine and the NIMO interface. In this integration, the `suggest()` method calls `nimo.selection()` and converts the generated `proposal.csv` to a list of keyword arguments for the workflow engine. The `observe()` method takes the previous data from the workflow engine and calls `nimo.output_update()` to insert the data to the NIMO backend. Additional algorithm-specific parameters and experimental configurations are visualized by providing a schema to the IvoryOS frontend. The integration of two software is illustrated in Fig. 1.

3. Coffee ring effect SDL

The coffee ring effect is a phenomenon in which particles suspended in a liquid form a ring-like structure when a drop of liquid dries on a solid surface. Suppressing this effect is important for various industrial applications, such as inkjet printing. It is known that the addition of surfactants can mitigate the coffee ring effect. In this study, we selected the autonomous exploration of conditions controlling the coffee ring effect as a demonstrative example of the proposed automation setup.

The hardware setup of this SDL is shown in Fig. 2. In this system, a robotic arm transports well plates between instruments. A liquid handler prepares sample solutions by mixing pure water, silica, and two surfactants: polyvinyl alcohol (PVA) and dodecyltrimethylammonium bromide (DTAB). A droplet of the sample is dried on a heat plate at 60 °C. Images of the resulting dried deposits are captured by a camera and automatically analyzed using image analysis software.

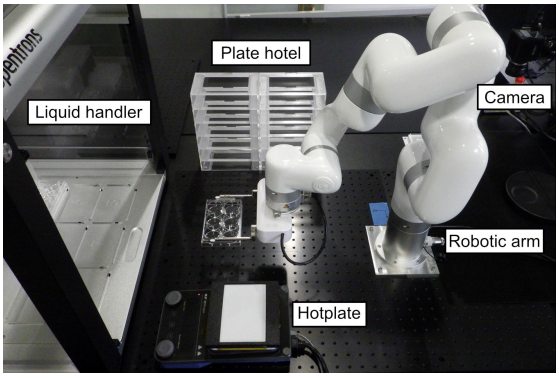

Fig. 2: Hardware setup of the coffee ring effect SDL.

NIMO autonomously determines the concentrations of PVA and DTAB using the PDC algorithm and the overall system is controlled via the IvoryOS web interface. The resulting phase diagrams is shown in Fig. 3.

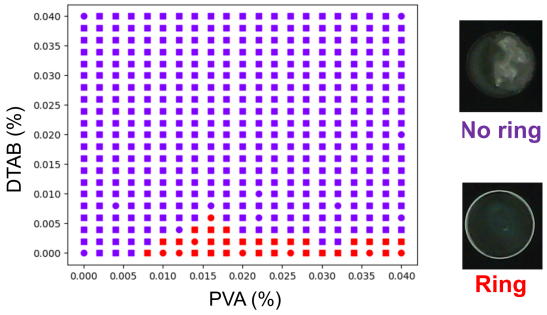

Fig. 3: Phase diagram of the coffee ring effect. Red points indicate conditions under which coffee ring was observed, whereas purple points indicate the coffee ring effect was suppressed.

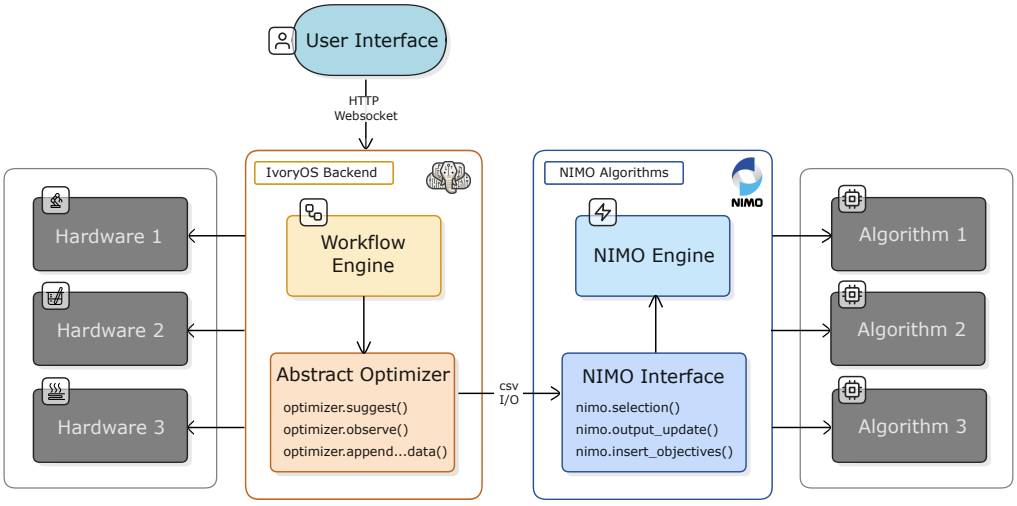

Fig. 1: Integration of NIMO into IvoryOS.

4. Milk crown SDL

When a droplet of milk collides with a thin milk layer, different splash patterns are observed depending on the droplet impact velocity and the depth of the milk layer. The crown-shaped splash observed under certain conditions is referred to as a milk crown. The shape pattern is classified into three phases [5]: axisymmetric (form 1), non-axisymmetric (form 2), and fragmentation (form 3), as shown in Fig. 4.

To investigate this phenomenon, we developed a robotic-arm-based SDL to construct the phase diagram of milk droplet splashing (Fig. 5). In this system, a small robotic arm equipped with an electronic pipette adjusts the volume of milk in the dish, while a large robotic arm releases a milk droplet using a dropper, which is operated by controlling the gripper opening. The droplet collision is recorded by a camera at 240 fps, and the splash pattern is classified into three phases based on human judgment.

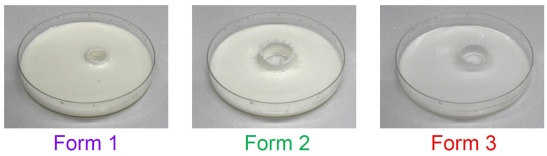

Fig. 4: Three phases of milk droplet splashing.

NIMO determines the droplet release height, which controls the impact velocity, and the milk volume, which controls the layer depth, using the PDC algorithm. The resulting phase diagram of splashing is shown in Fig. 6.

5. Conclusion and future perspective

We developed a software framework that facilitates the development of SDLs by integrating NIMO and IvoryOS, and demonstrated its effectiveness through two robotic-arm-based SDLs. In future work, we aim to develop additional SDLs using this framework to further enhance its versatility and utility.

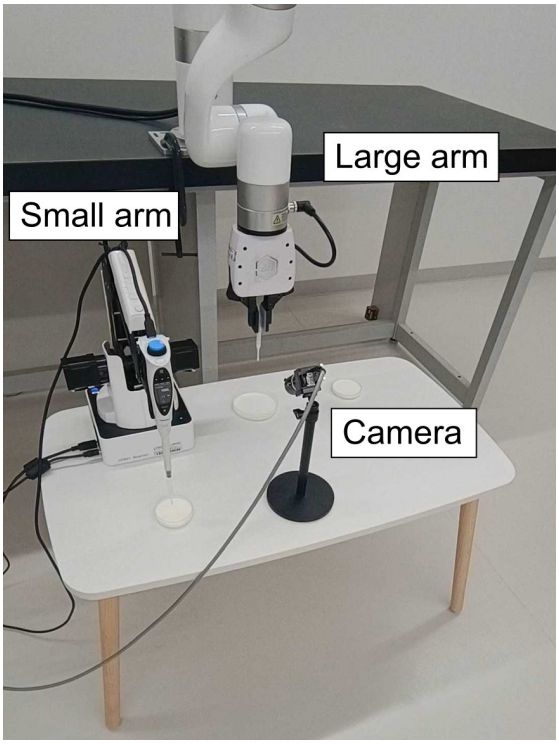

Fig. 5: Hardware setup of the milk crown SDL

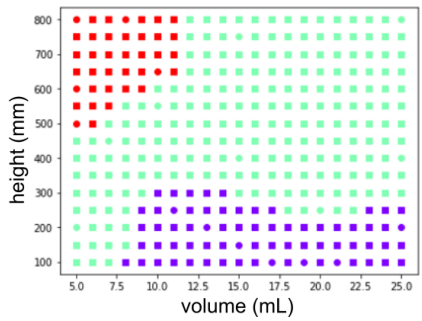

Fig. 6: Phase diagram of milk droplet splashing. Points of different colors indicate the conditions under which each splash phase was observed.

Acknowledgments

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References

[1] Gary Tom, Stefan P Schmid, Sterling G Baird, Yang Cao, Kourosh Darvish, Han Hao, Stanley Lo, Sergio Pablo-García, Ella M Rajaonson, Marta Skreta, et al. Self-driving laboratories for chemistry and materials science. *Chemical Reviews*, 124(16):9633–9732, 2024.

[2] Ryo Tamura, Koji Tsuda, and Shoichi Matsuda. NIMS-OS: an automation software to implement a closed loop between artificial intelligence and robotic experiments in materials science. *Science and Technology of Advanced Materials: Methods*, 3(1):2232297, 2023.

[3] Wenyu Zhang, Lucy Hao, Veronica Lai, Ryan Corkery, Jacob Jessiman, Jiayu Zhang, Junliang Liu, Yusuke Sato, Maria Politi, Matthew E Reish, et al. Ivoryos: an interoperable web interface for orchestrating python-based self-driving laboratories. *Nature Communications*, 16(1):5182, 2025.

[4] Kei Terayama, Ryo Tamura, Yoshitaro Nose, Hidenori Hiramatsu, Hideo Hosono, Yasushi Okuno, and Koji Tsuda. Efficient construction method for phase diagrams using uncertainty sampling. *Physical Review Materials*, 3(3):033802, 2019.

[5] Kensuke Watari, Takaaki Hayashi, Suguru Shiratori, and Taketoshi Hibiya. Effects of gravitational acceleration on formation of coronets. *Journal of The Japan Society of Microgravity Application*, 23(1):46, 2006.