Vertical Cloud Labs and Frugal Twins for Accelerated Materials Discovery of Structural Alloys and Energy Materials

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1. Introduction

Many materials have been discovered through brute force, serendipity, and intuition. AI & automation increasingly accelerate materials discovery through "self-driving" (i.e., autonomous) laboratories [1]. We explore three autonomous lab concepts: (1) vertical labs, (2) cloud labs, and (3) frugal twins [2], with applications in solid-state materials science.

Vertical labs maximize *automation-friendly* vertical space utilization—so equipment comes to the operator (e.g., via a vertical lift module) rather than the operator moving between instruments (Figure 1), significantly reducing automation complexity while maximizing space utilization.

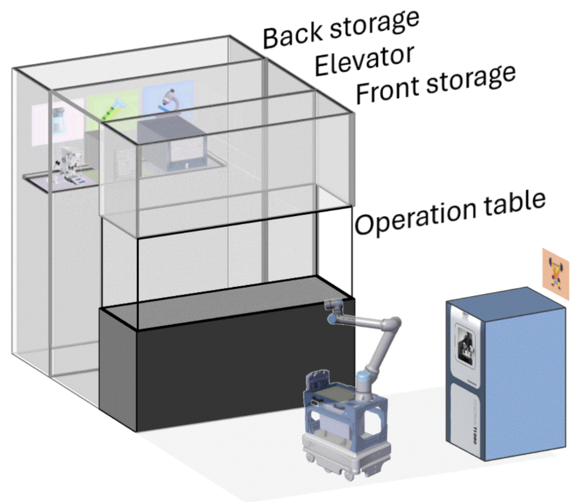

Fig. 1: An "electrified" tray of a vertical lift module carries synthesis and characterization equipment, bringing equipment to the operator for experiments and maintenance.

Cloud labs enable remote, decentralized access to experimental resources—democratizing hardware, computation, and domain expertise (Figure 3).

Frugal twins are low-cost, modular physical twins (like digital twins, but for hardware) that complement high-cost systems, enabling low-risk prototyping, lower barriers to lab automation, and multi-fidelity optimization.

We present an initial workflow for a remotely accessible self-driving lab integrating a vertical lift module, low-cost powder dosing units, a metal alloy ultrasonic atomizer, a small-scale metal 3D printer, and mechanical testing hardware for alloy discovery. We also present early results for autonomous electrochemistry for energy applications, including Ni electrode stress testing for alkaline fuel cells.

2. Scientific Applications

2.1 Autonomous Alloy Discovery

We aim to discover high-performing additively manufactured aerospace alloys through a remotely accessible self-driving lab workflow integrating a vertical lift module, low-cost powder dosing units, an ultrasonic atomizer (Figure 2) [3], a small-scale metal 3D printer, and mechanical testing equipment.

Fig. 2: A metal alloy ultrasonic atomizer creates additive-manufacturing friendly powders by turning inductively heated molten metal into spherical droplets via ultrasonic vibration.

2.2 Autonomous Electrochemistry

We are developing autonomous electrochemistry workflows for energy applications, integrating potentiostats, liquid handling robots, and 3D printed electrochemical cells for accelerated stress testing of Ni electrodes for alkaline electrolysis in fuel cell applications (Figure 4).

3. Conclusion

We envision these examples to help derisk transfer of vertical cloud labs to the community and advance accelerated materials discovery.

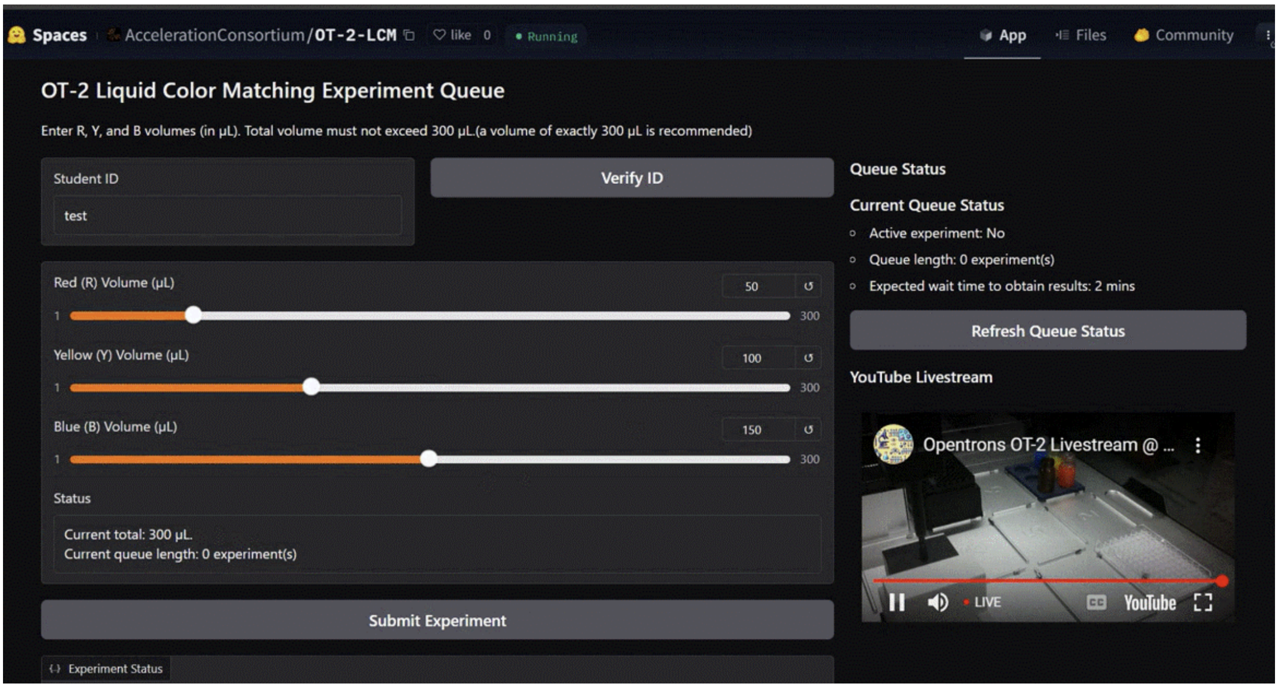

Fig. 3: A remotely accessible cloud lab using a quota-based system, enabling asynchronous and remote experiment requests with shared programmatic and manual control. Over 1000 experiments have been conducted by numerous users in various countries, including Canada, the United States, and Mexico. A 24/7 livestream enables users to view the experiment remotely.

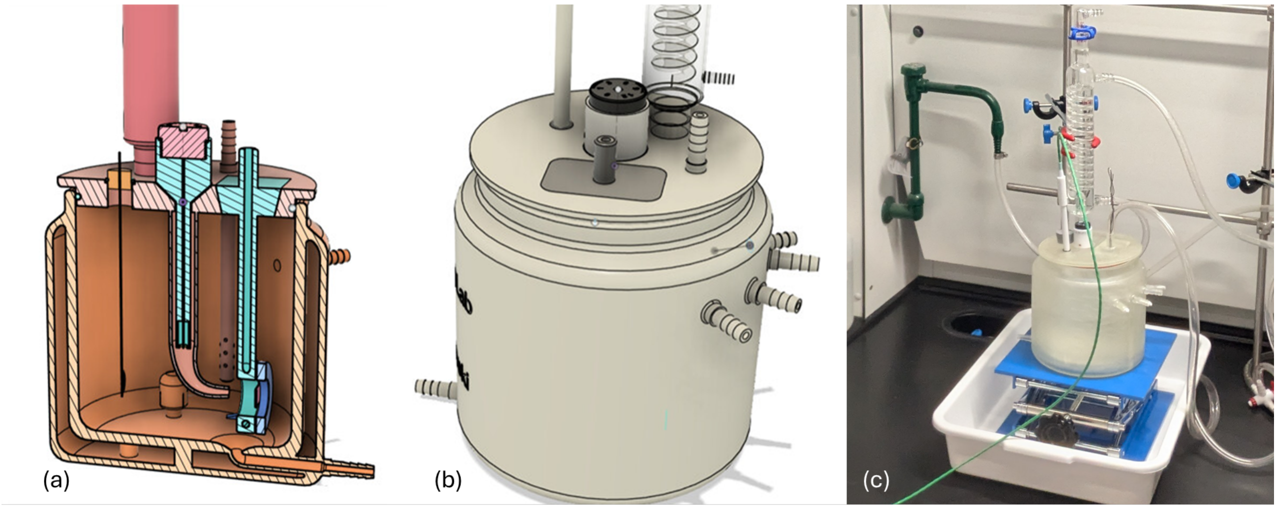

Fig. 4: A resin-based 3D printed electrochemical cell used for accelerated stress testing of nickel electrodes for alkaline fuel cell experiments.

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, Naruki Yoshikawa, Samantha Corapi, Gun Deniz Akkoc, Felix Strieth-Kalthoff, Martin Seifrid, and Alán Aspuru-Guzik. Self-driving laboratories for chemistry and materials science. *Chemical Reviews*, 124(16):9633–9732, 2024.

[2] Stanley Lo, Sterling G. Baird, Joshua Schrier, Ben Blaiszik, Nessa Carson, Ian Foster, Andrés Aguilar-Granda, Sergei V. Kalinin, Benji Maruyama, Maria Politi, Helen Tran, Taylor D. Sparks, and Alán Aspuru-Guzik. Review of low-cost self-driving laboratories in chemistry and materials science: the "frugal twin" concept. *Digital Discovery*, 3(5):842–868, 2024.

[3] S. Mohadeseh Taheri-Mousavi, Michael Xu, Florian Hengsbach, Clay Houser, Zhaoxuan Ge, Benjamin Glaser, Shaolou Wei, Mirko Schaper, James M. LeBeau, Greg B. Olson, and A. John Hart. Additively manufacturable high-strength aluminum alloys with coarsening-resistant microstructures achieved via rapid solidification. *Advanced Materials*, page e09507, 2025.