MULTIROBOT SYSTEMS

Transforming science labs into automated factories of discovery

Angelos Angelopoulos[1], James F. Cahoon[2], Ron Alterovitz[1]*

Laboratories in chemistry, biochemistry, and materials science are at the leading edge of technology, discovering molecules and materials to unlock capabilities in energy, catalysis, biotechnology, sustainability, electronics, and more. Yet, most modern laboratories resemble factories from generations past, with a large reliance on humans manually performing synthesis and characterization tasks. Robotics and automation can enable scientific experiments to be conducted faster, more safely, more accurately, and with greater reproducibility, allowing scientists to tackle large societal problems in domains such as health and energy on a shorter timescale. We define five levels of laboratory automation, from laboratory assistance to full automation. We also introduce robotics research challenges that arise when increasing levels of automation and when increasing the generality of tasks within the laboratory. Robots are poised to transform science labs into automated factories of discovery that accelerate scientific progress.

INTRODUCTION

Laboratories in chemistry, biochemistry, and materials science are at the leading edge of technology, discovering molecules, materials, and complex chemical systems of these components. These discoveries power our society and enhance our environment, health, and productivity via sustainable energy solutions, pharmaceuticals, electronic devices, and more. The current processes for developing molecules, materials, and chemical systems typically require extensive effort in a laboratory to synthesize them and characterize their properties, followed by analyzing the results, designing revised compounds, and then repeating the process until the desired properties are achieved (*1*, *2*). This process is time consuming and labor intensive. To discover optimal molecules and materials, a vast chemical space often needs to be explored—akin to finding a needle in a haystack. Although intuition, computational modeling, and advances in artificial intelligence (AI) provide valuable insights, physical synthesis and testing remain essential. From the perspective of a roboticist, these laboratories are akin to factories, where the raw materials of the factory are chemical reagents and the output of the factory is a newly synthesized molecule, material, or chemical system of optimal properties. Yet, despite these laboratories being at the cutting edge of science, most science laboratories today resemble factories from generations past, with a large reliance on humans who manually perform tedious tasks.

Expanding the use of robots and automation in science laboratories has the potential to accelerate scientific discovery (*3*, *4*). Automating experiments with robots could enable experiments to be conducted faster by leveraging the high speed of robots and their ability to operate 24 hours a day, 7 days a week. Robots can improve the accuracy, precision, and reproducibility of experiments by eliminating the variability of human movements. For instance, robots can consistently execute exacting experimental procedures, such as dispensing precise amounts of powder (*5*) or depositing liquid at an exact location on a sample, reducing uncertainty in experimental outcomes. Robots can also reduce safety risks to humans given that laboratory research often involves interacting with hazardous materials. Robots can increase productivity by focusing human labor on higher-level tasks and can enable efficient round-the-clock use of expensive specialized equipment. By accelerating experimentation, robots and automation have the potential to help generate unprecedented quantities of experimental data, which AI agents can learn from and analyze. Consequently, AI agents could become more effective at automating or helping in designing molecules, materials, and chemical systems, unlocking frontiers in AI-driven scientific discovery.

Science laboratories can be automated to varying degrees. Lab automation has traditionally relied on systems such as benchtop apparatus assemblies (*6*–*14*), fixed robotic arms (*15*–*17*), Cartesian robots (*18*), and flow chemistry systems (*13*, *19*–*21*). However, these setups are only capable of automating laboratories tailored to narrow experiments and require substantial human effort to set up. More advanced types of robots can be used to develop more sophisticated, flexible, and cost-effective automation that would otherwise require human intervention or expensive bespoke equipment. For instance, dual-arm manipulation robots can automate bimanual tasks and reduce task completion time (*5*, *22*). Mobile robots can transport items between lab stations and even rooms (*23*). In addition, mobile manipulation robots, which include both a mobile robotic base and an attached robotic arm, have been shown to work with laboratory apparatuses to automate larger labs with more diverse instruments (*23*–*27*). The increasing commoditization of robot hardware is also leading to declining costs. The time is ripe to develop robotics techniques tailored to science laboratory automation to enable faster, safer, and more reproducible research.

Here, we define five levels of a laboratory's physical automation, ranging from simple laboratory assistance to full automation. These levels focus on the automation of physical tasks in the laboratory, such as chemical synthesis and characterization of synthesized materials. We discuss the robotics and automation

[1]Department of Computer Science, University of North Carolina at Chapel Hill, Chapel Hill, NC 27599, USA. [2]Department of Chemistry, University of North Carolina at Chapel Hill, Chapel Hill, NC 27599, USA.
*Corresponding author. Email: ron@cs.unc.edu

research challenges that will arise as we increase the automation level. Lower automation levels, which are already commonplace, incorporate automated instruments operated by humans. Intermediate automation levels will require robots to operate in a mixed-use lab populated by humans and robots, where safety and human-robot interactions are paramount challenges. Higher automation levels will require robots to complete most or all tasks without human intervention to independently advance the scientific frontier.

Science laboratories vary substantially in the range of tasks and experiments that they support. Some labs are highly specialized and focus on a single task, and they often require only a benchtop or a single room. Other labs are more general-purpose, support diverse tasks, and may require multiple rooms or buildings to house their diverse apparatuses. We also introduce levels of laboratory generality, which range from single-process labs to general labs encompassing a broad spectrum of scientific endeavors. A lab's generality is independent of the lab's level of physical automation. Full automation for single-process labs may be feasible in the short term, but fully automating more general labs is more complex and may require multipurpose robots such as mobile manipulators. We discuss the robotics research challenges that will arise by increasing lab generality at any automation level. As we increase the levels of both automation and generality, robots can transform science labs into efficient factories of discovery, accelerating scientific progress.

LEVELS OF SCIENCE LABORATORY AUTOMATION

We begin by defining the degree to which a laboratory's physical tasks are automated. These physical tasks correspond to performing the individual steps of synthesis (such as making a molecule or material from reagents or creating a chemical system of these components) and characterization (such as testing the properties and performance of the synthesized components). These steps in a science lab are analogous, respectively, to the fabrication/assembly and the quality control steps of a manufacturing factory. The physical tasks to perform are predefined by humans or an AI agent. Inspired by the Society of Automotive Engineers (SAE) International Standard J3016 for self-driving car levels of automation, we define five levels of automation for physical laboratory automation, labeled A1 through A5, as shown in Fig. 1.

The first automation level, assistive automation (A1), requires automating single steps of a synthesis and characterization process. At this automation level, humans manually complete the bulk of the synthesis and characterization and set up the automated components between experiments. Level A1 is the most prevalent form of laboratory automation today, in which a human operates a laboratory apparatus that automates a single task. Example apparatuses are magnetic mixers, proportional-integral-derivative (PID)–controlled thermal reactors, and autosampling mass spectrometers, which automate single steps that are tedious, difficult, inefficient, or impossible for a human to perform.

The second automation level, partial automation (A2), requires automating multiple sequential steps of a synthesis or characterization process. At this automation level, humans manually perform some synthesis and characterization steps and set up, supervise, and maintain the automated systems. Setting up an automated system may involve tasks such as loading reagents (which can include preparing reagents, fetching reagents from a storage room, and loading reagents into a flow chemistry apparatus), configuring equipment parameters and operating modes, repositioning samples and equipment such that automation can proceed (for example, moving a scale from a closet and placing it next to a robotic arm that will use it), and connecting necessary components (such as connecting tubes for flow chemistry setups). This automation level is increasingly being used in science laboratories, typically in the form of bespoke setups situated on a single table, often composed of apparatuses interconnected with tubes for flow chemistry or with Cartesian robots and fixed robotic arms for batch processing. For example, level A2 can be achieved using an automatic pipetting robot (*28*) for synthesis, which can execute multiple sequential pipetting steps involving

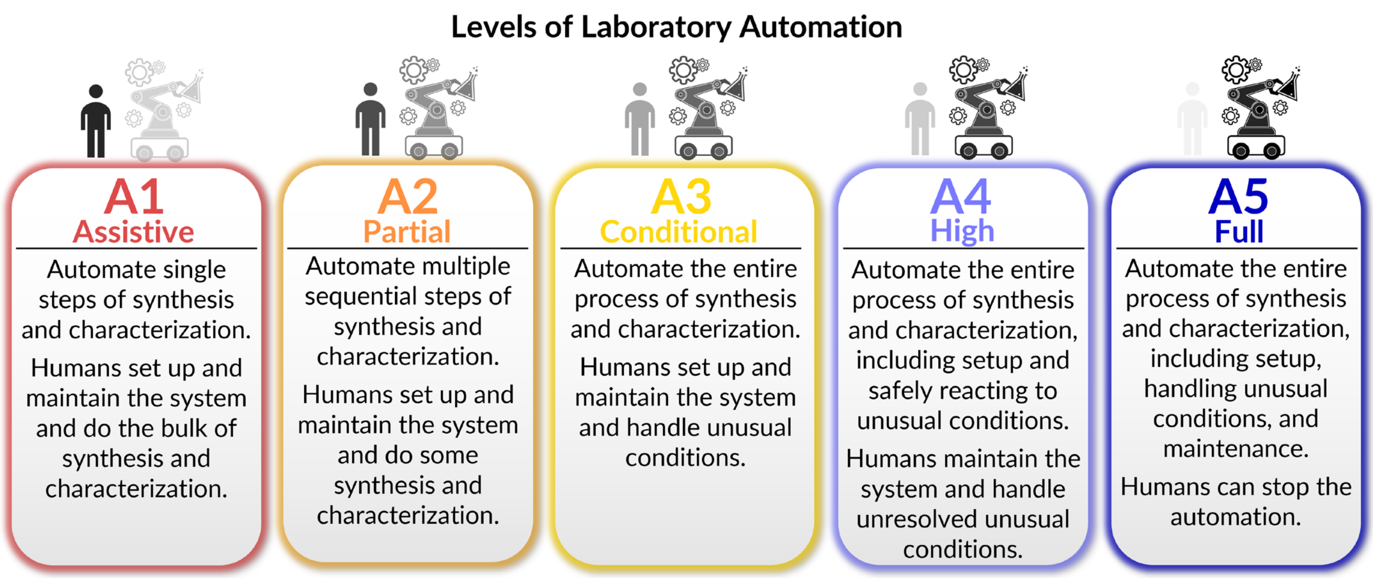

Fig. 1. Levels of physical automation for science laboratories. Laboratory automation ranges from "assistive," whereby the automation helps with single steps, to "full," whereby the laboratory completes entire processes autonomously, manages uncertainty, maintains itself, and requires no human intervention.

multiple reagents across multiple samples (for example, in 96-well plates). Fixed robotic arms can also automatically transport samples between nearby apparatuses, enabling level A2 by stringing together multiple sequential synthesis or characterization tasks (*15*, *29*).

The third automation level, conditional automation (A3), requires automating the entire process of synthesis and characterization. At this automation level, humans are required to set up and maintain the system, and the term "conditional" indicates that humans must intervene in unusual conditions, such as objects not being where expected or a spill occurring on the laboratory floor. As such, level A3 is often dependent on the laboratory environment being fixed or unchanging. An example of level A3 is the A-lab (*29*), which used fixed robotic arms and other apparatuses to entirely automate a workflow. This workflow included tasks such as moving samples between equipment with a fixed robotic arm, opening and closing a furnace door, turning on and off a vacuum pump, and capping samples. Another example is AlphaFlow (*21*), a flow chemistry lab for automated multistep synthesis and characterization. Mobile manipulation robots can also help achieve level A3. A mobile manipulation robot together with apparatuses was shown to automate hundreds of experiments for finding more active photocatalysts (*25*). The robot's role was to transport samples and load/unload them from apparatuses. Mobile manipulation robots can unlock higher automation levels because of their flexibility in using an existing laboratory infrastructure without bespoke automation setups (*23*–*27*).

Beyond A3 is the current research frontier. The fourth automation level, high automation (A4), requires robustly automating the entire process of synthesis and characterization, including setup, and safely reacting to unusual conditions. At this automation level, humans only maintain the system and handle any unresolved unusual conditions. Automating setup includes tasks such as preparing input reagents, renewing reagents when they run low, connecting reconfigurable tubes of a flow chemistry apparatus, and setting equipment parameters. Safely reacting to unusual conditions requires adapting a workflow to bypass or resolve the unusual condition; for example, a mobile robot navigates around an unexpected obstacle or searches the vicinity when an object is not in its expected location. For any unusual conditions that cannot be handled, the system would automatically transition into a safe state and seek assistance from a human. Detecting the cause of unusual conditions is a substantial challenge, and level A4 systems must include sensors to do so to react appropriately. For example, a mobile robot could perceive its environment to detect objects at unanticipated locations (because of an error or human interaction) and react appropriately.

The fifth automation level, full automation (A5), takes level A4 a step further by requiring that the system handle all unusual conditions (except catastrophic failures) and be self-maintaining. Unusual conditions that should be automatically handled at this level include resolving safety hazards, such as cleaning up a hazardous spill, and detecting and safely handling unexpected chemical reactions that could pose danger. A level A5 system should be able to detect, contain, and resolve hazards. Self-maintenance requires that the system calibrate, inspect, and clean itself; maximize software uptime; detect hardware failures and request servicing when they occur; and continuously ensure that all items are in their correct locations and satisfy safety requirements. Industries such as manufacturing have made progress toward self-maintenance. An example is predictive maintenance (*30*), where machines inspect their condition using sensors and the data are analyzed to schedule preventative maintenance to minimize system downtime.

LEVELS OF SCIENCE LABORATORY GENERALITY

Science laboratories greatly vary in the breadth of experiments that they support. This breadth is dependent on the laboratory's scale, which can be a benchtop, a room, a building, or even a collection of many buildings (for example, the science buildings of a university campus or a national laboratory like Lawrence Berkeley National Laboratory). Some laboratories, typically at the scale of a benchtop or room, are specialized and designed to perform a single experiment. For instance, they might support optimizing a specific material, such as enhancing the luminescence of an organic light-emitting diode (OLED). A single-process laboratory is akin to a factory that manufactures a single item. Some larger-scale laboratories, typically at the scale of a building or a national laboratory, are more general-purpose and support experiments across multiple science domains, from semiconductor materials to drug design. A general or multidomain laboratory is akin to a factory that manufactures a diversity of products. As science advances and disciplinary boundaries erode, the benefits of more general, multidomain laboratories will likely increase.

Achieving a given physical automation level is more challenging for a science laboratory that supports a broader range of processes and domains. Developing more general automation that can be reused for different problems and workflows is an important dimension of lab automation and a research frontier where robots can be very beneficial. To understand the robotics needs of a particular science laboratory, one must identify both the laboratory's desired physical automation level and its generality. Hence, we now define five levels of generality for science laboratories, labeled G1 through G5, as shown in Fig. 2.

It is important to emphasize that the generality level and the physical automation level are independent of each other. The generality level refers to the scope of science that can be completed in the laboratory independent of the ratio of effort between humans and automated systems, whereas the physical automation level refers specifically to the ratio of effort between human and automated systems in completing the tasks of the laboratory.

The first generality level, a single-process laboratory (G1), supports a specific laboratory process or very related or derivative processes. We define a process as a sequential set of tasks designed to achieve a specific experimental outcome. Processes are specialized for a particular experiment. For instance, a laboratory designed to optimize the photoluminescence of a specific OLED by adjusting key design parameters (such as the organic components) is at level G1. Level G1 is prevalent today, given that many laboratory apparatuses that perform a single process, or some very related processes, are at this level. These labs typically consist of one or several adjacent benchtop systems.

The second generality level, a multiprocess laboratory (G2), supports various distinct laboratory processes. For example, such a laboratory could be capable of several organic or inorganic synthesis processes (for instance, mixing reagents at specific times and temperatures or separating product mixtures) and loading generated samples into a photoluminescence spectrometer. Such a laboratory could be used for multiple processes, such as the optimization of the light emission spectrum from quantum dots and organic components

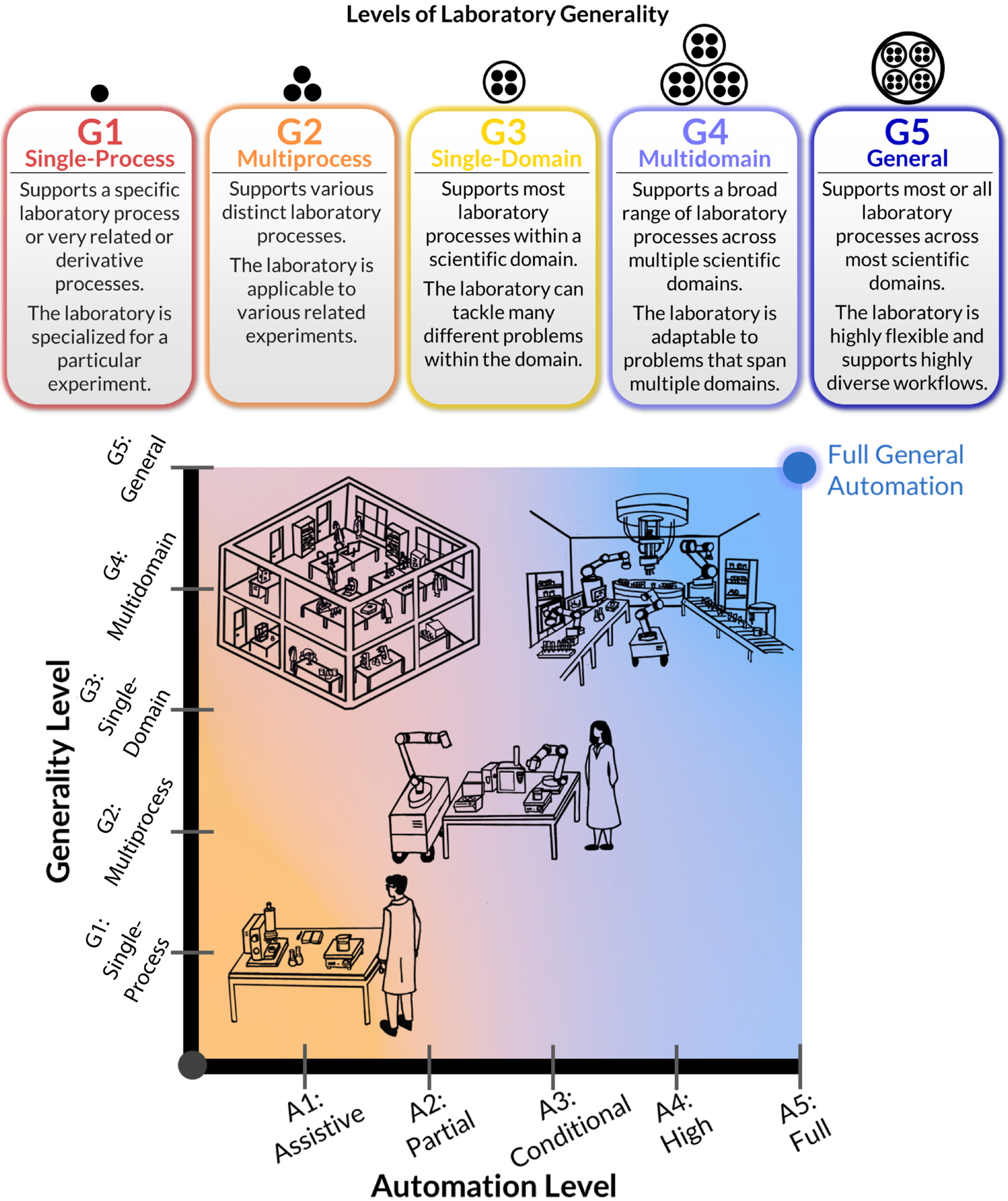

Fig. 2. Levels of generality for science laboratories and their relationship with physical automation levels. Achieving a level of physical automation is more challenging for a science laboratory that supports a broader range of processes and domains. We define levels of generality for science laboratories. We also show the spectrum of physical automation levels versus generality levels, where orange corresponds to the current state of the art and blue indicates the research frontier.

for OLEDs. Some current automation setups achieve level G2 by automating multiple processes and typically consist of one laboratory room.

The third generality level, a single-domain laboratory (G3), supports most laboratory processes within a scientific domain. This level indicates versatility within that domain (for example, metal halide perovskite chemistry for solar cells, lithium-ion chemistry for batteries, or quantum dot chemistry for light emission), supporting a range of processes relevant to that domain. Laboratories with level G3 and higher paired with low physical automation levels are common and typically take the form of groups of laboratory rooms with semiautomated instruments staffed by people. Creating a G3 and higher laboratory becomes more challenging as we aim for higher physical automation levels. To achieve generality level G3 at automation levels A3 and higher, the laboratory must incorporate robots and automation capable of automating most experimental workflows within a specific scientific domain. Reducing dependence on humans is challenging to achieve in a G3 laboratory because of the wide variety of tasks performed by humans, from fetching reagents from a variety of locations to operating diverse specialized instruments. Hence, creating laboratories with generality level G3 at automation level A3 or higher is a research frontier.

The fourth generality level, a multidomain laboratory (G4), supports a broad range of laboratory processes across multiple scientific domains. The laboratory must be usable in a flexible and adaptable manner to support processes and workflows relevant to various forms of experimentation and testing in different domains. For a laboratory to be at level G4, it must first achieve level G3 in each of its target domains and will typically take the form of laboratory buildings or complexes. Science laboratories can be far more general in the variety of tasks that can be performed compared with manufacturing factories. For example, a chemistry building at a university can include a variety of lab rooms and shared resources such as gas chromatographs (GCs), nuclear magnetic resonance (NMR) and mass spectrometers, x-ray diffractometers, and electron microscopes. Such a laboratory building could cover a wide variety of experimental research and span domains from materials science to drug design. This implies that automation solutions to enable higher physical automation levels in these labs will need to be more flexible and modular than traditional automation solutions in current industrial factories.

Last, the fifth generality level, a general laboratory (G5), supports most or all types of laboratory processes. At this generality level, the processes and workflows are highly flexible and applicable to a wide variety of domains. Such a laboratory necessarily consists of multiple buildings and facilities with a large, diverse array of equipment, supplies, and reagents. A G5 laboratory that is also at physical automation level A5 is the pinnacle of laboratory automation.

ROBOTICS CHALLENGES FOR HIGHER LABORATORY AUTOMATION AND GENERALITY LEVELS

Research innovations that push the frontier of laboratory automation closer to full automation (A5) for a general laboratory (G5) would bring us closer to creating automated factories of discovery. We show the spectrum of laboratory automation and generality in the plot in Fig. 2, where orange shading indicates the current state of the art and blue indicates the research frontier.

Mobile robots for automation in larger laboratories

A key challenge to achieving higher physical automation levels for laboratories with greater generality is the need for flexibility. The laboratory must support a variety of experiments, with each experiment using a different subset of apparatuses and in a different order. This required flexibility is one of the key differentiators between the automation requirements in factories versus science laboratories. Mass-production factories often use workcells specialized for specific steps or components. The workcells are connected by conveyor belts, tracks, or other mechanisms to achieve full automation. Such an automation setup may not be cost effective or scalable for a laboratory at higher generality levels because the connection mechanisms between workcells would constantly need reconfiguration, such as when new experiments require new workflows or when equipment is added or removed from the laboratory, which may be frequently. What if we could provide alternate connection mechanisms that are easily reconfigurable? Mobile manipulation robots could be a potential solution.

Using mobile manipulation robots could enable flexible and scalable automation. Advances in robotics and AI have begun to enable the application of mobile robots in laboratories (*23*–*25*). Recent research has demonstrated that mobile manipulation robots can work with laboratory apparatuses to autonomously conduct experiments (*25*) and to perform accurate manipulations with chemistry instruments (*24*). Mobile manipulation robots can work with equipment originally designed for humans, without major changes to a lab's layout. This could facilitate the creation of mixed-use labs where humans and robots work together, as discussed below. In addition, mobile robots can navigate across multiple rooms, enabling greater automation for laboratories with generality level G3 and above.

Using mobile manipulation robots in laboratory automation setups can offer many benefits, but there are implementation challenges. A primary challenge is manipulation accuracy: A mobile manipulation robot will need to travel multiple meters between stations and then at a station may need to manipulate objects with submillimeter accuracy. One potential solution could be repeated calibration by touching a calibration fixture (*25*), but this demands a rigid environment. A related challenge is perception, given that objects in a laboratory may be small, reflective, or transparent (for example, glassware). Furthermore, navigation in laboratories requires avoiding obstacles in tight spaces. Consideration of safety complicates robot planning and control because of risks associated with hazardous materials and the need to avoid humans if present. One promising approach for more general laboratory automation, similar to approaches used in manufacturing and warehouse automation, is to create workcells that may include robotic arms for specific tasks (*31*), like preparing input solutions and characterizing samples, and the use of mobile robots to transport items between the workcells to achieve higher levels of automation. Optimizing the design and integration of mobile robots and mobile manipulation robots for science labs is an open problem—especially for mixed-use labs shared by humans and robots.

Mixed-use laboratories for higher generality

Laboratories shared by humans and robots, which we refer to as mixed-use laboratories, are arranged such that the apparatuses and supplies are usable by both humans and automation setups. This means that apparatuses have human-accessible interfaces, are not fenced off in an automation setup, and can be moved without breaking automated workflows. Mixed-use labs could allow humans and robots to complete separate tasks in the same space or to collaborate on tasks.

Mixed-use laboratories at intermediate levels of physical automation, however, are challenging to implement. Laboratory robots must be capable of safely working alongside humans. The safety requirements will need to be formally specified, and they will influence both robot hardware and software design, including joint compliance, sensors for situational awareness, and constraints on motion planning (such as avoiding contact with humans and handling hazardous substances and dangerous objects on the basis of safety protocols). Mixed-use laboratories will also require sharing limited lab resources, such as apparatuses and labware, between robots and humans, so appropriate planning, scheduling, and resource management approaches may be needed.

Orchestrating the various resources of an automated laboratory

Achieving higher levels of laboratory physical automation requires a system capable of coordinating and controlling the lab's automation hardware to execute experiments. Some work in this area includes the A-Lab OS (*29*), Chemputer (*14*), and ARChemist (*32*). An experiment orchestration system should include middleware to communicate with the automation hardware, including sending instructions and receiving and processing data and status messages. For higher levels of automation, the orchestration system will also need to schedule tasks on the automation hardware to maximize the lab's performance while considering resource, timing, and task ordering constraints. The middleware will need to handle automation hardware from a variety of vendors and with a variety of experimental capabilities. Developing a standard lab automation "operating system" is an important challenge to facilitate the growth of automated labs.

Cloud laboratories

Laboratories can be made remotely accessible via the internet, enabling scientists anywhere in the world to use them to run experiments. These "cloud laboratories" can be offered as a service by providing software and application programming interfaces (APIs) that can be used to define workflows, submit workflows for execution, monitor their status, and view generated results. Such labs can theoretically operate at any level of physical automation or generality. A few cloud laboratories have already been commercially deployed [see, for example, (*33*)] and currently rely on humans physically in the remote lab to perform tasks. Increasing the level of physical automation could help cloud laboratories lower costs, improve reproducibility of results, and enable greater scalability, opening them up to a broader range of scientists. We believe that cloud laboratories will have an important place in the future of lab automation, offering accessible and cost-effective automation without capital investment for laboratory equipment and custom automation setups.

Intuitive user interfaces for automated laboratories

Evolving the way scientists interact with laboratories is critical to fully leverage the capabilities of laboratories with increasing automation. User interfaces should be developed for experiment orchestration systems that are specifically designed for scientists, allowing them to specify tasks, workflows, and objectives to optimize. This interface can be a graphical user interface, a simple API, or even a voice-based interface. Generative AI may make programming laboratories faster and easier by allowing scientists to communicate with the lab via natural language (*34*) to specify experiments and monitor experiment progress in real time. Cloud laboratories raise an added challenge because the scientists cannot physically see and control a lab's apparatuses. Virtual reality can offer an immersive interface for programming and understanding a cloud laboratory. Seeing up close the layout of the lab, the apparatuses, and how apparatuses are connected could make operating a cloud lab more intuitive. Also, integrating the user interface with a simulated digital twin of the lab could allow viewing of in-progress experiments, providing an even higher understanding of the cloud lab's operation.

TOWARD FULLY AUTONOMOUS FACTORIES OF SCIENTIFIC DISCOVERY

A common paradigm for laboratory workflows is the design-make-test-analyze (DMTA) loop (*1*, *2*). The design phase consists of specifying the molecule, material, or chemical system to synthesize and the desired workflow for accomplishing this. The make phase involves synthesizing the designed item. The test phase involves characterizing the synthesized item, which may be done using equipment such as GCs and NMR spectrometers to measure properties. Last, in the analysis phase, the results from the test phase are analyzed. This cycle is repeated; on the basis of the analysis, better future experiments can be designed in the design phase, repeating the cycle until the objectives are achieved. Currently, the design and analyze phases are largely performed by scientists on the basis of intuition, knowledge, and data analysis. The make and test phases can be run in a laboratory of any physical automation level and generality. Increasing the physical automation level has the potential to directly accelerate and improve the reproducibility of the make and test phases, which is the primary focus of this Viewpoint article. If the design and analyze phases of DMTA could also be automated, then the entire DMTA loop would be automated. This would create a laboratory that goes beyond the mere physical automation of tasks by providing the lab with the autonomy to decide what experiments to conduct, resulting in a fully autonomous factory of discovery.

Integrating AI in the laboratory

AI can help automate the design and analyze phases of DMTA, thus creating fully autonomous labs (*35*). AI methods have already been shown to succeed in some circumstances for the design and analyze phases, particularly for science problems suitable for a G2 or lower laboratory. For example, AI successfully guided experimental design by predicting new candidate compounds using historical and online data to accelerate the search (*25*). In another example, an AI system was able to rapidly explore a chemical reaction space to discover new reactions (*8*). AI was also successfully used to discover and optimize synthesis routes (*21*). Whereas the make and test phases can benefit from physical automation using robots, the analyze and design phases can benefit from cognitive automation based on AI.

Creating an AI agent for cognitive automation in laboratories with generality levels above G2 could be very beneficial but also raises many technological hurdles. For example, the space of decision variables when designing chemistry experiments is vast, leading to the curse of dimensionality (*21*) when trying to navigate the space of experiments in search of an optimal molecule or material. Also, AI methods typically work best when expressing knowledge in domains that they have already learned, and they may perform poorly when asked to extrapolate beyond their knowledge base, for example, making "hallucinations," which can be uninformative or even dangerous when integrated into a physically automated laboratory. Furthermore, the AI should be provided with a variety of characterization data to reduce the effect of errors in any one characterization method and increase confidence in results. These hurdles could potentially be mitigated by leveraging high physical automation to generate the massive quantities of data desired by data-hungry AI agents.

Software and hardware standardization

Hardware and software components used in laboratories today are either custom built or purchased from a wide variety of vendors. Unfortunately, there currently are no widely accepted standards or protocols for interoperability and communication between laboratory components that would facilitate the easy integration of robotic and AI systems with existing laboratory equipment. Consequently, automated labs today rely on highly bespoke systems that require substantial engineering effort to set up.

The growth of automated labs will greatly benefit from standard communication protocols and a common experimental orchestration system. Examples include standards for communication and interoperability between different hardware and software components, defining tasks, scheduling tasks, aggregating status metrics, implementing AI-optimized experimental campaigns, and communicating with an AI for the design and analyze phases. Such standards, as well as a common experimental orchestration system, would streamline and lower the cost of setting up an automated lab, facilitate the swapping of components such as equipment or AI agents on the basis of experimental needs, increase automation reuse across research groups, help build an ecosystem of reusable components, and enhance reproducibility of experiments. We urge instrument and equipment manufacturers to consider automation needs such as standards-based communication protocols and APIs in their product design and development efforts, which could provide a competitive advantage when working with researchers to increase the level of lab automation.

Prioritizing safety is essential

Building confidence in lab automation and the molecules, materials, and chemical systems found through automated experimentation presents challenges, particularly at higher levels of automation and generality with low human involvement. Lab automation may have unforeseen implementation flaws. For example, an AI-driven automated lab might synthesize hazardous materials without realizing it, which is especially dangerous in a mixed-use lab. Constraints on AI systems driving experiments are critical to control these occurrences. Less human supervision at higher physical automation levels paired with fewer constraints on an AI agent's search through a chemical space will require thorough safety and failure mitigation protocols.

The need for education

Training scientists to operate and cooperate with advanced lab automation systems is critical to harnessing their full potential. The intricacies and nuances of these systems require not only understanding their function but also adapting to their evolution. Therefore, it is important to focus on educating the next generation of scientists to have not only expertise in their science domain but also sufficient familiarity with robotics, automation, data science, and AI to leverage advances in these areas for their specific scientific domains and to be able to configure automated systems to achieve targeted scientific outcomes. Robotics and automation shift the effort of scientists away from tedious tasks, providing more time to focus on designing important basic science questions and to consider ways to advance their research projects by leveraging AI agents, potentially resolving scientific questions that could not be efficiently answered without AI, robotics, and automation. Scientists will need to be adept at evaluating, selecting, and using the most effective lab automation options available, as well as helping drive the automation solutions that should be developed in the future.

CONCLUSIONS

Robotics and automation are poised to help usher in an era of faster, safer, more accurate, and more reproducible experimentation in science labs. We introduced five levels of physical laboratory automation, from laboratory assistance to full automation. Today's chemistry, biochemistry, and materials science labs resemble factories from generations past, with a large reliance on humans performing tasks manually, creating many opportunities to boost the level of automation. We highlighted how labs can also differ in the level of generality of the experiments they can support, ranging from single-process labs to general labs. These automation and generality levels are useful for classifying the current state of the art in laboratory automation as well as setting goalposts for future advancements.

The automation and generality levels, particularly the levels not yet reached, are helpful for identifying robotics research and automation challenges that must be solved to attain the benefits of greater automation. We highlighted the importance of developing mobile robots for automation in larger labs and addressing human-robot interaction challenges in labs that are not fully automated. We also discussed the importance of developing systems for orchestrating the various resources of an automated lab, creating cloud labs, creating hardware and software standards for interoperability and communication between automation components, prioritizing safety, and educating scientists on effectively leveraging automation. Last, we elucidated the potential of AI to create labs that go beyond the mere physical automation of tasks by providing the laboratory with the autonomy to decide what experiments to conduct, resulting in a fully autonomous laboratory.

Successful laboratory automation at higher physical automation and generality levels will require more engagement of physical/life scientists with computer scientists, engineers, and roboticists. Scientists need the help of the robotics community to unlock the next generation of labs. Robotics and automation are poised to transform science labs into automated factories of discovery that accelerate scientific progress.

REFERENCES AND NOTES

1. A. T. Plowright, C. Johnstone, J. Kihlberg, J. Pettersson, G. Robb, R. A. Thompson, Hypothesis driven drug design: Improving quality and effectiveness of the design-make-test-analyse cycle. *Drug Discov. Today* **17**, 56–62 (2012).
2. B. A. Koscher, R. B. Canty, M. A. McDonald, K. P. Greenman, C. J. McGill, C. L. Bilodeau, W. Jin, H. Wu, F. H. Vermeire, B. Jin, T. Hart, T. Kulesza, S.-C. Li, T. S. Jaakkola, R. Barzilay, R. Gómez-Bombarelli, W. H. Green, K. F. Jensen, Autonomous, multiproperty-driven molecular discovery: From predictions to measurements and back. *Science* **382**, eadi1407 (2023).
3. K. Sanderson, Automation: Chemistry shoots for the Moon. *Nature* **568**, 577–579 (2019).
4. I. Holland, J. A. Davies, Automation in the life science research laboratory. *Front. Bioeng. Biotechnol.* **8**, 571777 (2020).
5. Y. Jiang, H. Fakhruldeen, G. Pizzuto, L. Longley, A. He, T. Dai, R. Clowes, N. Rankin, A. I. Cooper, Autonomous biomimetic solid dispensing using a dual-arm robotic manipulator. *Digit. Discov.* **2**, 1733–1744 (2023).
6. S. Asche, G. J. T. Cooper, G. Keenan, C. Mathis, L. Cronin, A robotic prebiotic chemist probes long term reactions of complexifying mixtures. *Nat. Commun.* **12**, 3547 (2021).
7. V. Dragone, V. Sans, A. B. Henson, J. M. Granda, L. Cronin, An autonomous organic reaction search engine for chemical reactivity. *Nat. Commun.* **8**, 15733 (2017).
8. J. M. Granda, L. Donina, V. Dragone, D.-L. Long, L. Cronin, Controlling an organic synthesis robot with machine learning to search for new reactivity. *Nature* **559**, 377–381 (2018).
9. M. Christensen, L. P. E. Yunker, F. Adedeji, F. Häse, L. M. Roch, T. Gensch, G. dos Passos Gomes, T. Zepel, M. S. Sigman, A. Aspuru-Guzik, J. E. Hein, Data-science driven autonomous process optimization. *Commun. Chem.* **4**, 112 (2021).
10. A. Milo, Democratizing synthesis by automation. *Science* **363**, 122–123 (2019).
11. A.-C. Bédard, A. Adamo, K. C. Aroh, M. G. Russell, A. A. Bedermann, J. Torosian, B. Yue, K. F. Jensen, T. F. Jamison, Reconfigurable system for automated optimization of diverse chemical reactions. *Science* **361**, 1220–1225 (2018).

12. J. Li, S. G. Ballmer, E. P. Gillis, S. Fujii, M. J. Schmidt, A. M. E. Palazzolo, J. W. Lehmann, G. F. Morehouse, M. D. Burke, Synthesis of many different types of organic small molecules using one automated process. *Science* **347**, 1221–1226 (2015).
13. N. Hartrampf, A. Saebi, M. Poskus, Z. P. Gates, A. J. Callahan, A. E. Cowfer, S. Hanna, S. Antilla, C. K. Schissel, A. J. Quartararo, X. Ye, A. J. Mijalis, M. D. Simon, A. Loas, S. Liu, C. Jessen, T. E. Nielsen, B. L. Pentelute, Synthesis of proteins by automated flow chemistry. *Science* **368**, 980–987 (2020).
14. S. Steiner, J. Wolf, S. Glatzel, A. Andreou, J. M. Granda, G. Keenan, T. Hinkley, G. Aragon-Camarasa, P. J. Kitson, D. Angelone, L. Cronin, Organic synthesis in a modular robotic system driven by a chemical programming language. *Science* **363**, eaav2211 (2019).
15. C. W. Coley, D. A. Thomas, J. A. M. Lummiss, J. N. Jaworski, C. P. Breen, V. Schultz, T. Hart, J. S. Fishman, L. Rogers, H. Gao, R. W. Hicklin, P. P. Plehiers, J. Byington, J. S. Piotti, W. H. Green, A. J. Hart, T. F. Jamison, K. F. Jensen, A robotic platform for flow synthesis of organic compounds informed by AI planning. *Science* **365**, eaax1566 (2019).
16. A. Sparkes, W. Aubrey, E. Byrne, A. Clare, M. N. Khan, M. Liakata, M. Markham, J. Rowland, L. N. Soldatova, K. E. Whelan, M. Young, R. D. King, Towards robot scientists for autonomous scientific discovery. *Autom. Exp.* **2**, 1 (2010).
17. H. J. Yoo, N. Kim, H. Lee, D. Kim, L. T. C. Ow, H. Nam, C. Kim, S. Y. Lee, K.-Y. Lee, D. Kim, S. S. Han, Bespoke metal nanoparticle synthesis at room temperature and discovery of chemical knowledge on nanoparticle growth via autonomous experimentations. *Adv. Funct. Mater.* **34**, 2312561 (2024).
18. F. Kong, L. Yuan, Y. F. Zheng, W. Chen, Automatic liquid handling for life science: A critical review of the current state of the art. *J. Lab. Autom.* **17**, 169–185 (2012).
19. M. H. Reis, F. A. Leibfarth, L. M. Pitet, Polymerizations in continuous flow: Recent advances in the synthesis of diverse polymeric materials. *ACS Macro Lett.* **9**, 123–133 (2020).
20. A. Slattery, Z. Wen, P. Tenblad, J. Sanjosé-Orduna, D. Pintossi, T. den Hartog, T. Noël, Automated self-optimization, intensification, and scale-up of photocatalysis in flow. *Science* **383**, eadj1817 (2024).
21. A. A. Volk, R. W. Epps, D. T. Yonemoto, B. S. Masters, F. N. Castellano, K. G. Reyes, M. Abolhasani, AlphaFlow: Autonomous discovery and optimization of multi-step chemistry using a self-driven fluidic lab guided by reinforcement learning. *Nat. Commun.* **14**, 1403 (2023).
22. M. Walker, G. Pizzuto, H. Fakhruldeen, A. I. Cooper, Go with the flow: Deep learning methods for autonomous viscosity estimations. *Digit. Discov.* **2**, 1540–1547 (2023).
23. S. Kleine-Wechelmann, K. Bastiaanse, M. Freundel, C. Becker-Asano, Designing the mobile robot Kevin for a life science laboratory, in *2022 31st IEEE International Conference on Robot and Human Interactive Communication (RO-MAN)* (IEEE, 2022), pp. 870–875.
24. A. Angelopoulos, M. Verber, C. McKinney, J. Cahoon, R. Alterovitz, High-accuracy injection using a mobile manipulation robot for chemistry lab automation, in *2023 IEEE/RSJ International Conference on Intelligent Robots and Systems (IROS)* (IEEE, 2023), pp. 10102–10109.
25. B. Burger, P. M. Maffettone, V. V. Gusev, C. M. Aitchison, Y. Bai, X. Wang, X. Li, B. M. Alston, B. Li, R. Clowes, N. Rankin, B. Harris, R. S. Sprick, A. I. Cooper, A mobile robotic chemist. *Nature* **583**, 237–241 (2020).
26. Q. Zhu, F. Zhang, Y. Huang, H. Xiao, L. Zhao, X. Zhang, T. Song, X. Tang, X. Li, G. He, B. Chong, J. Zhou, Y. Zhang, B. Zhang, J. Cao, M. Luo, S. Wang, G. Ye, W. Zhang, X. Chen, S. Cong, D. Zhou, H. Li, J. Li, G. Zou, W. Shang, J. Jiang, Y. Luo, An all-round AI-Chemist with scientific mind. *Natl. Sci. Rev.* **9**, nwac190 (2022).
27. H. Liu, N. Stoll, S. Junginger, K. Thurow, Mobile robotic transportation in laboratory automation: Multi-robot control, robot-door integration and robot-human interaction, in *2014 IEEE International Conference on Robotics and Biomimetics (ROBIO 2014)* (IEEE, 2014), pp. 1033–1038.
28. P. Dettinger, T. Kull, G. Arekatla, N. Ahmed, Y. Zhang, F. Schneiter, A. Wehling, D. Schirmacher, S. Kawamura, D. Loeffler, T. Schroeder, Open-source personal pipetting robots with live-cell incubation and microscopy compatibility. *Nat. Commun.* **13**, 2999 (2022).
29. N. J. Szymanski, B. Rendy, Y. Fei, R. E. Kumar, T. He, D. Milsted, M. J. McDermott, M. Gallant, E. D. Cubuk, A. Merchant, H. Kim, A. Jain, C. J. Bartel, K. Persson, Y. Zeng, G. Ceder, An autonomous laboratory for the accelerated synthesis of novel materials. *Nature* **624**, 86–91 (2023).
30. T. Zonta, C. A. da Costa, R. da Rosa Righi, M. J. de Lima, E. S. da Trindade, G. P. Li, Predictive maintenance in the Industry 4.0: A systematic literature review. *Comput. Ind. Eng.* **150**, 106889 (2020).
31. A. M. Lunt, H. Fakhruldeen, G. Pizzuto, L. Longley, A. White, N. Rankin, R. Clowes, B. Alston, L. Gigli, G. M. Day, A. I. Cooper, S. Y. Chong, Modular, multi-robot integration of laboratories: An autonomous workflow for solid-state chemistry. *Chem. Sci.* **15**, 2456–2463 (2024).
32. H. Fakhruldeen, G. Pizzuto, J. Glowacki, A. I. Cooper, ARChemist: Autonomous robotic chemistry system architecture, in *2022 International Conference on Robotics and Automation (ICRA)* (IEEE, 2022), pp. 6013–6019.
33. Emerald Cloud Lab: Remote Controlled Life Sciences Lab; www.emeraldcloudlab.com/.
34. N. Yoshikawa, M. Skreta, K. Darvish, S. Arellano-Rubach, Z. Ji, L. Bjørn Kristensen, A. Z. Li, Y. Zhao, H. Xu, A. Kuramshin, A. Aspuru-Guzik, F. Shkurti, A. Garg, Large language models for chemistry robotics. *Auton. Robots* **47**, 1057–1086 (2023).
35. J. H. Montoya, M. Aykol, A. Anapolsky, C. B. Gopal, P. K. Herring, J. S. Hummelshøj, L. Hung, H.-K. Kwon, D. Schweigert, S. Sun, S. K. Suram, S. B. Torrisi, A. Trewartha, B. D. Storey, Toward autonomous materials research: Recent progress and future challenges. *Appl. Phys. Rev.* **9**, 011405 (2022).

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