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Navigating the landscape of modular reconfigurable laboratory automation in chemistry

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Easily reusable lab automation is the next frontier in automating experiments. Equipment must be repurposed often for experiments, making the current generation of lab automation too costly and too complicated to apply. However, with the rise of platforms in which modules encapsulate operations, connections and equipment can be swapped around quickly and, in some cases, automatically to perform different experiments. This article reviews the current state of the art of reconfigurable modular laboratory automation systems in chemistry. We discuss the key barriers of adoption of these systems and the importance of standardized benchmarks to compare capabilities of different platforms. We provide an outlook on the most promising research paths, including the possibility that AI systems can help guide the layout of processes and operations, leading to improved efficiency and possibly new process layouts. We conclude that the field of laboratory automation should continue to advance, benefiting chemists and the broader scientific community.

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1 Introduction

Automation has secured its place in the modern laboratory. Simple glass apparatuses driven by heat, density and phase changes have evolved into sophisticated systems capable of intricate liquid and gas manipulations.[1] In particular, robotic pipetting systems and robot arms have allowed the customisation of automation in various experimental scenarios.[2–6]

Automated experimental setups have many advantages, including increased precision and the ability to persistently repeat tasks. Furthermore, thanks to the miniaturization and integration of electronic sensors and actuators, automated setups can be monitored in or close to real time.[5] Most automated experimental setups today are built to repeat a single specific set of steps,[5–8] allowing for variations in input materials and process variables like temperature or pressure. The number of different samples that a setup can manage at the same time is often referred to as throughput. High Throughput Screening (HTS) systems that can process hundreds to thousands of samples in a run demonstrate the high level of advancement and utility these setups offer.

Using their ability to repeat tasks, automated experiment setups are often combined with AI techniques to explore vast libraries of compounds and accelerate the discovery of new materials or drugs.[9] These same compound libraries and the results of the experiments can be used as input to the AI system in a closed-loop fashion, which has led to self-driving laboratories (SDL).[6,7,10,11]

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However, as new different experiments need to be performed, considerable work and engineering expertise is needed to redesign and build new setups. Finding hardware parts that allow the material transfer system to connect to different devices, finding parts with materials compatible with the chemicals involved, and making different hardware and software interfaces talk to each other and the main control system are usually the most expensive and time-consuming tasks and are the subject of entire research projects and system lines by vendors. This leads to automated systems that are often used for one project and then discarded as the person in charge moves to another place or the agreement with the vendor expires, since they are really difficult to reuse for other researchers, which consequently have to repeat a lot of work.

Multipurpose modular reconfigurable laboratory automation systems offer the flexibility to set up varied experiments by quickly reconfiguring pre-existing modules. They have existed for decades,[12] and have seen different improvements over the years.[13] In this work, we extend the definition of modularity proposed by Lo *et al.*:[7] modularity refers to the assembly of a cohesive system or device that has discrete, self-contained modules which can be easily [and quickly] interconnected [using standard hardware and software interfaces], replaced [and reconfigured]. Each module performs a specific [chemical operation or process], and they can be combined or modified independently. This definition is closer to the idea of modularity developed in the field of modular robotics, in which robots are formed by units that encapsulate functionality and can attach to each other using standard interfaces to create more complex robotic structures[14,15] in minutes[16] and perform tasks that cannot be done by one module alone. It defines also a class of systems in which modules are designed with the idea of quick and easy interconnection (for hardware, software and material transfer) and reconfiguration from the start, and therefore to be easily and rapidly adapted and extended to different experimental contexts and multiple new experiments that need different processes steps and operations.

Although the software side has seen important developments in modularization that have propelled the laboratory automation area (see Section 3.4), software modularization has been studied extensively for various decades[17,18] and modern software systems take advantage of modularity for performing different tasks[19] or coordinating distributed machine systems.[20,21] We examine modular laboratory automation systems mainly from the hardware side.

Hardware modularity can be implemented in laboratory automation systems at different levels (Fig. 1). A level 4 reconfigurable laboratory automation system is represented by a system in which each module is completely self-contained, that is, it encapsulates a single chemical process or operation, and, at the same time, contains interfaces that allow it to communicate, share power, and transfer materials to any neighboring module (Fig. 2). Modules can perform, for example, a mixing operation, a liquid–liquid extraction operation, or a filtering operation, and then autonomously transfer the result to the next module. Ideal modules should also be able to be connected and quickly reconfigured in a large number of configurations to be able to create any kind of experiment, or even have the ability to self-reconfigure. In contrast, a reconfigurable set of commercial devices loosely connected by means of a robot arm represents a system at the lowest level (level 1).[22] The robot arm acts as a central transfer system that transports material from one device to the next to fit specific protocols.

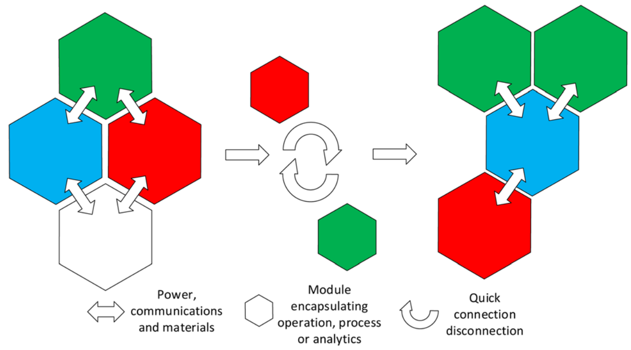

Fig. 2 An ideal modular reconfigurable laboratory automation system is a system in which each module encapsulates a chemical process or operation, and, at the same time, contains interfaces that allow it to communicate, share power and transfer materials to any other neighboring modules. Modules can be quickly rearranged with minimal effort to create a high number of different configurations.

Devices like incubators, analytic machines, and shakers may be able to automatically handle the incoming materials, or may have been heavily modified for this purpose. Modular workcell systems[12] offered by different vendors as packages since the 90s constitute the next level (level 2). They offer a more integrated transfer system between devices or workcells using belts and smaller robot arms in each cell, however they cannot be reconfigured easily by an user (chemist technician), requiring a high level of engineering skill to do so, adding to this the expertise needed to program the robots and belts movements to fit the new modules. Most advances in modular lab automation involving robot arms[13,23,24] live in between these two levels, including mobile robot platforms,[25] although some are closer level 3.

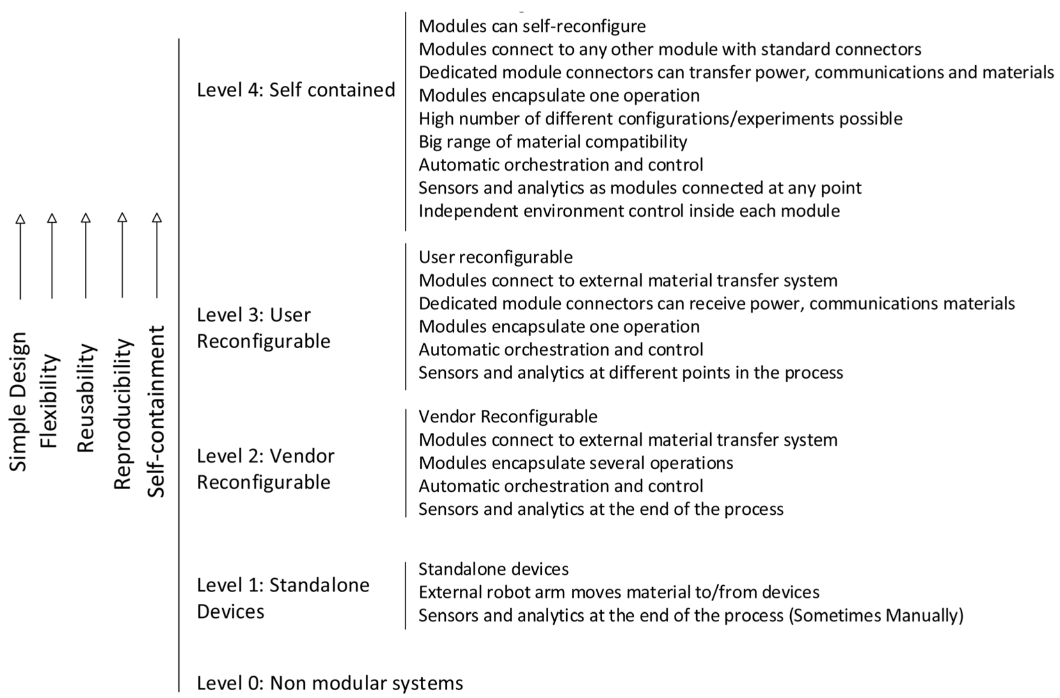

Fig. 1 Different modular systems implement different levels of modularity in hardware. In this review we focus in systems above level 2.

In this study, we examine systems on the next level (level 3) beyond the workcell/TLA model, which can be reconfigured by a user more easily, and in which modules encapsulate more basic operations and connectors contain more functionality. We concentrate on laboratory-scale systems, specifically those ranging from microlitres to litres in scale. While microfluidic platforms posses similar characteristics and offer intriguing possibilities for reconfigurable modular lab automation, they face unique challenges and have been extensively covered elsewhere; for a comprehensive review, we refer the reader to.[26] Similarly, mobile manipulation platforms present an alternative approach. However, due to their substantial challenges in automatic navigation, object recognition, and glassware manipulation,[27,28] that require extensive adaptations to laboratory equipment,[29] we will not include them in this analysis. However, we make an exception with the ARChemist system due to the strategies used in this system to tackle manipulation problems, which make it easier to reconfigure and use. Additionally, while the majority of the systems reviewed have been built as part of self-driving labs (SDL), our focus is not on the self-driving aspect but on their hardware modularity, and we refer the reader to[6] for a comprehensive review from the point of view of SDLs.

Just as glassware has become a standard, quick, and easy to use tool in chemistry for various operations, multipurpose reconfigurable modular automation systems hold the potential to revolutionise experiment automation. They offer a ready-to-use, quickly reconfigurable framework, eliminating the need for the chemist technician to design automation from scratch for each new experiment. This advancement could greatly simplify the automation of experiments. In the age of AI and self-driven experimentation, these systems could also empower AI to modify not only material quantities but also the structure of the experiment itself.

2 Modular design

In theory, the reconfigurable modular design defined in last section has different advantages for improving the implementation of automated laboratory experiments, making it potentially easier to design, use, and reuse, and helping increase system encapsulation, sensorization, and ease environment control. We describe some of these advantages here as well as possible limitations. We will return to these in Section 4.

• Simple to design systems: encapsulating the mechanisms, vessels, electronics, *etc.* of an experiment operation leads to focused and simplified designs as a module only has to be designed to perform one operation inside a standard physical frame.

• Extendability: new modules can be created by making modifications to the base modules, which in turn makes the system easily extendable. Moreover, a module only has to be designed once and can be replicated multiple times.

• Flexibility: different experiments can be put together by swapping modules and connecting them in different ways. Having modules that can be swapped allows an operation to be used at different places in an experiment and even in multiple places.

• Reusability: modules can be reused for multiple types of experiments instead of designing and building them from scratch, saving time and resources.

• Experiment reproducibility: different sensors for measuring process variables, environment conditions and analytics can be implemented in a single module as part of its electronics, obtaining valuable data that can be used to better replicate the experiment afterwards.

• Parallelization: modules can be replicated multiple times to parallelize the same operation.

• Easy debugging: modules implementing analytics equipment can be interleaved at multiple positions in the process and swapped to different positions as the experiment is built, increasing the amount of tests to be performed to catch problems early and increasing the amount of data that can be obtained from a experiment.

• Better environment control: encapsulation allows operation steps to be performed inside their own isolated space, which could be monitored or modified at will (*e.g.* for oxygen-free environments, low humidity environments, *etc*…).

• Reconfigurability: interfaces between modules with mating connectors for material transfer, power and communication make it quicker and easier to connect and disconnect modules to create new configurations for different experiments. Although designing a standard connector can be a hard task at the beginning,[16] once designed it can be easily replicated.

The ability to quickly make and break connections between modules, both in hardware and in software, to reconfigure an experiment, also introduces some disadvantages.

• Leaks: using detachable interfaces between modules increases the risk of faulty connections that could end in failed material transfers as opposed to using monolithic transfer systems. However, quick-connect and re-attachable fittings already exist in the market and can be adapted for this purpose.

• Complex orchestration: orchestration is more complex with modular systems than with monolithic approaches, as the amount of degrees of freedom increases, and modules can be quickly relocated to different positions in a new experiment. Fortunately, software has become modular itself in recent years and different orchestration architectures stemming from similar scenarios (*e.g.* the internet) can be deployed.

• Big overhead: if the tasks are too simple, a modular system can have too big of an overhead to solve the problem (*i.e.* a single pump may be all that is needed for an experiment).

• Cleaning: cleaning is already a difficult task in automated platforms; it can become more difficult as, for example, more flow control components and connectors are added to each module.

3 State of the art in reconfigurable modular systems

In the simplest automated lab experiment, different pieces of automatic hardware perform an individual process or operation in which steps are arranged in a predetermined order or workflow. The outputs of certain processes are connected to the inputs of others and the whole experiment can be completed from the beginning to the end without manual intervention.[30] Robots Adam and Eve[11] are examples of level 1 modular systems, they introduce some flexibility for changing experiments by way of reorganizing steps in the workflow, however their hardware is static and not designed with a quick reorganization in mind. Similar systems exist across multiple application areas.[31–34]

Syncar and Automated Synthesis Lab (ASL) are two examples of systems that fit into the workcell/TLA description, which are level 2 modular systems. In Syncar[35] modules are connected to a central rail system that moves materials around (Fig. 3). Shuttles carrying glass and plastic vessels can automatically move around in the rail system and bring materials and reagents to different workstation modules on the side of the rail. Similarly, in ASL,[24] racks containing vessels are routed through conveyor belts to different modular workstations (Fig. 4). Some of these modules have pipetting and Scara robots that can move materials to adjacent modules. Although they have the advantage of being able to handle vessels both systems occupy the space of a room, with Syncar using more than one floor. In theory, modules in both systems can be rearranged physically around the central transfer system, nevertheless this task would require a small team of engineers and several days of work (see Section 4).

We present a taxonomy of the level 3 systems included in this review as part of the general category of laboratory automation (Fig. 5) from the point of view of hardware. Level 3 systems are designed with hardware reconfiguration by the user in mind. Modules encapsulate only one operation and can act independently of other modules and can connect to transfer systems or other modules through dedicated connectors to transfer materials, communicate, and transmit power.

Depending on the mechanisms used for the system to be reconfigured three categories can be distinguished:

Fig. 3 The Syncar system, glass or plastic vessels travel to different modular stations using a shuttle rail system. Experiment reconfiguration is achieved by changing the order in which the shuttles visit the different modules in software. Reprinted (adapted) with permission from ref. 35 Copyright 2005 American Chemical Society.

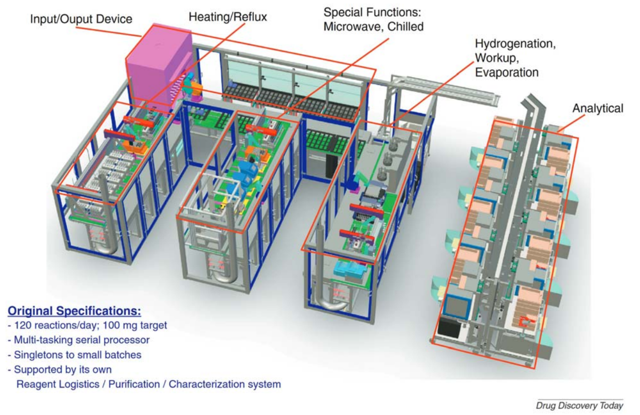

Fig. 4 Automated synthesis lab, vessels travel in racks that are moved by a central belt system. Stations composed by different standard laboratory equipment represent the system modules. Reconfiguration is achieved by changing the order in which the racks visit modules. Reprinted (adapted) with permission from ref. 24 Copyright 2013 Elsevier.

1. Manual systems or systems in which a human is needed to move modules and reconnect the system when changing experiments.

2. Workflow reconfiguration or systems in which manually reconfigurable modules can remain static and only the workflow needs to be altered, with connection routes between modules changing automatically, to run a completely different experiment. Still, these systems can be not completely autonomous, and a technician may be needed to perform analytics in some steps of the majority of these systems or to move modules manually.

3. Hardware reconfiguration includes systems in which hardware modules can be automatically moved around, not only automatically reconnected, adding a new dimension on top of rearranging the workflow to run a different experiment.

Tables 1 and 2 show a collection and comparison of operation or process modules that have been demonstrated in the different platforms described in this work. Using these operation or process modules, different types of experiments have been performed. The experiments demonstrated are concentrated in the area of drug production. This is mainly a consequence of extensive compound libraries already existing for drug applications,[36] the need to produce drugs on site in a reliable way, and the fact that drug companies are pioneers in developing laboratory automation platforms. Nevertheless, some platforms have been developed for other types of chemistries[37] for example solid material synthesis. To the date of this review we have no knowledge of level 3 modular reconfigurable laboratory automation platforms outside of these areas.

3.1 Manual reconfiguration

Manual reconfigurable platforms have distinct modules that can be moved around and connected together usually with the use of tubing. Most reconfigurable laboratory automation platforms focus on handling low-viscosity, low-density liquids,

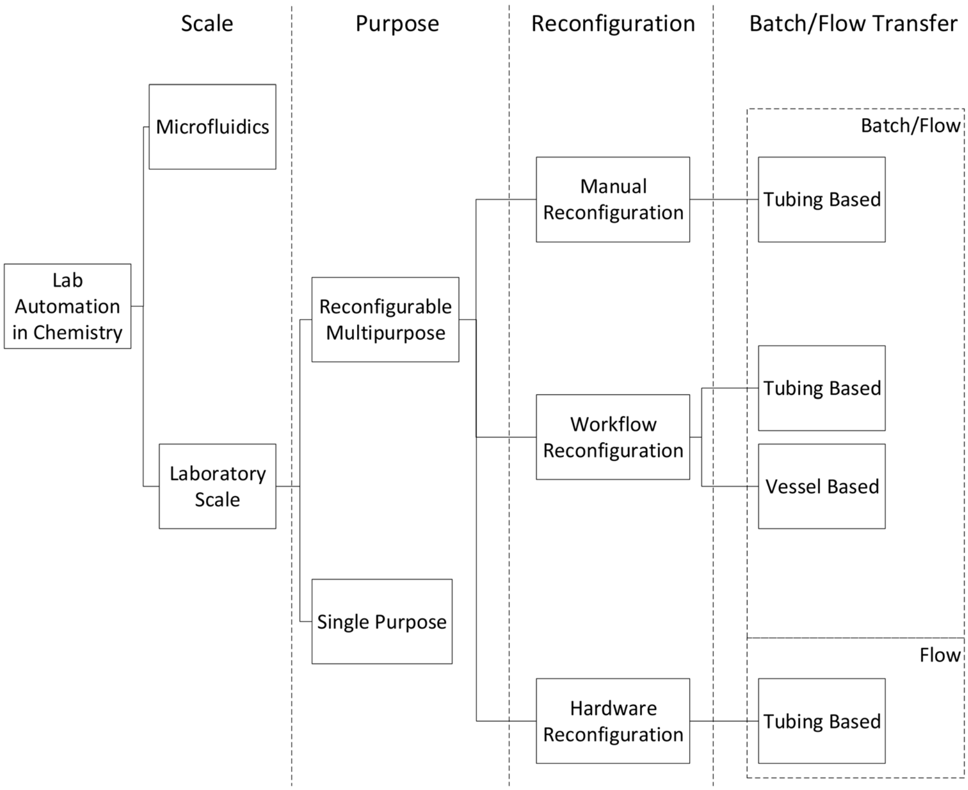

Fig. 5 Taxonomy of reconfigurable multi-purpose laboratory automation systems as part of the general category of laboratory automation.

similar to water, as there are many existing tools for this purpose.[5,38] Tubing systems often make use of plastic (made or coated) flexible hoses, that can be easily adapted to a variety of pump and valve types,[39] and combined them with glass apparatuses for operations and reactions at different pressure points. Tubing systems can be very precise when dispensing (*e.g.* by using syringe pumps). Yet, plastic materials are not as universally resistant as glassware to solvents and heat. It is also difficult to keep hoses, pumps, and valves completely clean, so most systems ultimately discard the parts that can be contaminated and replace them with new ones for a new experiment. An example of a system that uses tubing is the pharmaceutical compact reconfigurable system.[40] Using external pumps, the system modules are packed in a portable cabinet in which they are connected through hoses with standard fittings and selection valves (Fig. 6). Following the main goal of the platform, crystallization and suspension modules have been developed as part of the downstream processes available (Tables 1 and 2). The system in ref. 41, the Plug-and-play, reconfigurable, continuous-flow chemical synthesis system, shows a step further in organising the module connections in the system. Modules performing different flow operations are connected to a central backbone using matching connections that can be quickly connected and disconnected to different bays in the backbone. Pressurised liquids are transported through the central backbone and to the modules. Reagents are added to the backbone and to the modules using standard injection and selection valves. This allows the process to be quickly reconfigured by manually changing the sequence of modules connected to the available bays and makes the system small enough to fit a laboratory bench (Fig. 7).

Pumps can also be fitted inside the modules, making them able to independently transferring liquids to the other modules, eliminating the need for an external transfer system. This is the case of the MODEX modular synthesis system, which is described in ref. 42 and is composed of decimeter scale modules that perform a single unit operation and that connect to each other using standard luer connectors. However, connectors cannot carry energy and communication is done wirelessly, which can be unreliable. Each module is composed of a dry side for housing electronics and a wet side for handling liquid chemicals, both encased in 3D printed standard frames. The system can be quickly and manually assembled and calibrated and has a small enough footprint to be mounted next to a synchrotron beamline detector (Fig. 8). The module's small, easy to assemble design allowed the authors to program and test the system beforehand and then disassemble, transport, and reassemble it on-site.

Liquids can also be moved around using vessels. Traditional laboratory materials like glass are used for vessels, which offers a number of benefits because glassware, which chemists typically rely extensively on while doing experiments, can withstand high heat, solvents and is relatively cheap and easy to clean. However, to manipulate glass vessels, automation systems introduce multiple specific tools and adjustments that make them bulky and add multiple points of failure. In addition, the

Table 1 This table summarizes key features of the system and is not exhaustive. For a comprehensive understanding, please consult the detailed articles published on this system

Systems	Pharmaceutical compact reconfigurable system[40]	Modular science factories[44]	Plug and play reconfigurable synthesis system[41]	MODEX[42]	ORGANA[23]
System-type	Continuous flow	Batch	Continuous flow	Batch flow	Batch
Footprint	$1.0 \times 0.7 \times 1.8$	$3.4 \times 2.25 \times 2$	$0.61 \times 0.86 \times 0.41$	$0.375 \times 0.3 \times 0.64$	—
Min temperature	−20 °C	3 °C	−20 °C	—	—
Max temperature	180 °C	99 °C	120 °C	—	—
Max pressure	17 bar	—	6.9 bar	—	—
Software interfaces	—	YAML recipe files	Minimal GUI, scripts	Python scripts, OpenAPI docs	Instructions in natural language, object recognition
Operational capabilities					
Flow reactions	✓	✗	✓	✗	✗
Heated reactions	✓	✓	✓	✗	✓
Packed bed column processes	✓	✗	✗	✗	✗
Mixing	✓	✓	✗	✓	✓
Separation processes	Gravity	✗	Membrane	—	✗
Filtration	✓	✗	✗	✗	✗
Evaporation	✗	✗	✗	✗	✗
Other	Sonication, adsorption, dissolution, crystallization	PCR, pippeting, plate handling, plate sealing and unsealing	Fixed bed catalytic reactions, photochemical reactions	White, UV irradiation	Solid dispensing, electrode polishing, crystallization
Analytics					
Spectroscopy	IR[a]	UV-vis	IR[a], Raman[a]	✗	✗
Chromatography	✗	✗	HPLC-MS	✗	✗
Process monitoring sensors	Ultrasonic probe	✗	Pressure, flow meters, pressure, phase sensor, infrared temperature sensor	UV-vis and near-infrared sensors	Camera
Other	—	Camera, plate readers	—	Temperature, humidity	Camera, voltammetry, ph

[a] In-line.

emptying and filling of vessels can be very imprecise unless specialized types of vessels or mechanisms are used. Vessels are also used for transporting powders and solid samples. In ref. 23 the authors propose ORGANA a system that combines vessels and tubing. Modules are comprised of different devices and containers (beakers) that can be rearranged around a robot arm. The robot arm automatically detects the position of the containers and it is mainly in charge of transferring materials between the different devices by handling and pouring liquids or powders from some of the vessels (Fig. 9). A syringe pump and tubing can transfer liquids between vessels, enabling parallel execution of certain workflow steps. The main difference with a level 2 system is that the robot arm is considered as a module itself and can also be used to perform certain processes, including handling electrochemical solid samples, polishing them and submerging them in a liquid solution, in a similar way as in ref. 43.

In contrast to the MODEX and plug-and-play systems, the module boundaries in the ORGANA system are not completely defined, this can be an advantage because chemists can use familiar devices however this also makes reorganization difficult, for example in the case of the syringe pump, as engineering skills are needed. The modular science factories system presented in (ref. 44) proposes to remedy this problem by using a uniform hardware form factor. Collections of devices or vessels containing reagents, called modules, are placed on top of the cart. Carts can be spatially arranged by attaching them to each other using mechanical attachment parts, and using a way to transport vessels or well-plates from one cart to another (*e.g.* using a robot arm) they can form "workcells" in the author's words. By manually attaching carts in different ways (see Fig. 10), different experiments can be performed, making them the next step towards reconfigurability from systems like Syncar and ASL. Although carts currently cannot transfer material or data/energy to each other, the authors envision using mobile robots beneath the carts or pushing them to automatically reconfigure workcells and developing connectors from cart to cart in the future.

Table 2 This table summarizes key features of the system and is not exhaustive. For a comprehensive understanding, please consult the detailed articles published on this system

Systems	CityScape[50]	ARChemist[25,29,51,52]	Chemputer[45,46]	C3PU[47,48]	Robot arm assisted plug and play platform[13,53]
System-type	Continuous flow	Batch	Batch	Batch	Continuous flow
Footprint	3.9 × 1.7	Whole room	—	0.25 × 0.66 × 0.39	2.5 × 1.5 × 2
Min temperature	0 °C	4 °C	−30 °C	−13 °C	—
Max temperature	185 °C	450 °C	160 °C	120 °C	150 °C
Max pressure	—	—	—	—	13.8 bar
Software interfaces	Workflow GUI, scripts	Custom recipe definitions, command line interface	χDL scripts	χDL scripts	CRF scripts, database connections
Operational capabilities					
Flow reactions	✓	✗	✗	✗	✓
Heated reactions	✓	✗	✓	✓	✓
Packed bed column processes	✓	✗	✗	✗	✓
Mixing	✗	✓	✗	✓	✓
Separation processes	Gravity	✗	Membrane	✗	Membrane
Filtration	✗	✓	✓	✓	✗
Evaporation	✗	✓	✓	✓	✗
Other	Gas–liquid separator	Solid dispensing, grinding, inertization, crystallization, drying	Reactor with condenser	—	—
Analytics					
Spectroscopy	✗	✗	✗	✗	FT-IR[a]
Chromatography	HPLC-MS[b]	✗	✗	✗	HPLC-MS[b]
Process monitoring sensors	Flow, pressure, temperature	✗	Flow conductivity	Pressure	Pressure, temperature
Other	DART-MS[b], flow-NMR[b]	XRD	—	—	—

[a] In-line. [b] On-line.

3.2 Workflow reconfiguration

In workflow reconfiguration systems, the system design still allows modules to be manually reconfigured by an user. However, taking advantage of a central transfer system that allows materials to automatically reroute through itself and that can serve many modules, multiple experiments can be executed by automatically changing the order in which materials visit modules. For example, in the chemputer[45,46] different module inputs and outputs are connected through hoses to a central distribution system called a backbone (Fig. 11). The backbone is composed of a series of syringe pumps and selection valves that can route liquids around in the system. The flow of materials through the modules and the backbone determines the kind of experiment that is being performed. A smaller version of the chemputer[47] (C^3PU in Tables 1 and 2), following similar operational principles has also been developed (Fig. 12). In an effort to make the module designs more accessible, they are built using 3D printed vessels[48] that perform different operations and can be connected through standard connector hoses to a central commercial syringe pump and selector valve platform that acts as the backbone. A more recent addition to the chemputer family, the autonomous nanomaterials discovery platform, introduces a distinct approach.[49] Centered around a Geneva wheel, this system features a suite of components including a dispensing unit, sample and seat transfer mechanisms, and integrated analytics such as UV spectroscopy and a pH controller. However, the absence of evidence demonstrating the system's reconfigurability for different experiments makes us consider it to be closer to a HTS system than to a modular reconfigurable experimentation system.

The chemputer systems work with a batch approach to liquid based experiments but workflow reconfiguration systems can also work with flow chemistry. The CityScape platform described in (ref. 50) uses a Swagelok® Modular Component system as a base (A frame with slots in which different flow components, such as reactors, valves, and pipes, can be fitted). Custom flow components are inserted to create a “subway map” through which different kinds of liquids can flow (Fig. 13). Different layers allow the liquid to be directed through alternative fluid paths. Manual and automatic valves can be actuated to redirect the flow and reconfigure the system for different

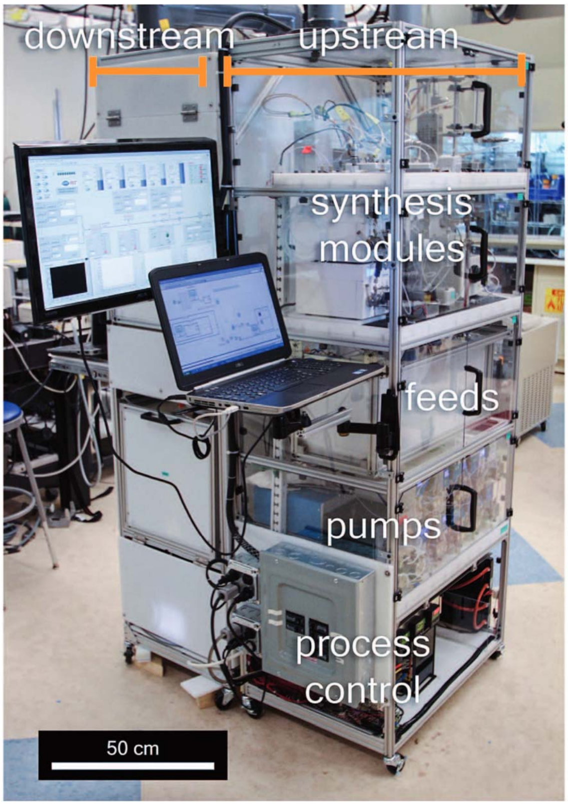

Fig. 6 Pharmaceutical compact reconfigurable system, all modules are contained in a single cabinet, reconfiguration can be done manually by swapping hose connections between modules. Reproduced/modified from Adamo *et al.*, *Science*, https://doi.org/10.1126/science.aaf1337 [2016], AAAS.

synthesis experiments with the same components attached to the modular base. Moreover, components can be rearranged spatially in the base, and special components, like reactors, can be placed in different paths to account for different reaction times and temperatures. This is one of the few systems in which samples are taken after each component for performing analytics and temperature and pressure sensors are integrated inline and in the flow components (Tables 1 and 2).

The system in ref. 51 uses a mobile robot arm platform as a central transport mechanism for vessels between different stations or modules (Fig. 14). These stations perform different operations including solid powder and liquid dispensing,[52] photolysis and gas chromatography using standard laboratory

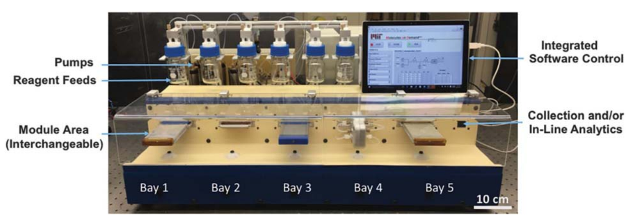

Fig. 7 Plug and play reconfigurable synthesis system, using matching interfaces, modules can be easily and quickly swapped by and operator from a central tubing backbone. Reproduced/modified from Bedard *et al.*, *Science*, https://doi.org/10.1126/science.aat0650 [2018], AAAS.

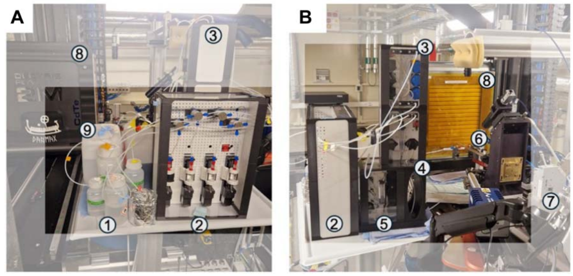

Fig. 8 MODEX system, decimeter scale modules perform one unit operation each and connect to other modules using standard connections. Modules can independently push liquids to other modules using internal pumps. Reconfiguration is achieved by manually rearranging module positions. (A and B) Photographs of the system as deployed next to a synchrotron beamline detector. (1) Chemicals (2) syringe module (3) pumping module (4) mixer module (5) UV illumination module (6) capillary (7) synchrotron X-ray beamline (8) detector (9) waste container. Reproduced/modified from Anker *et al.*,[42] arXiv under CC BY 4.0.

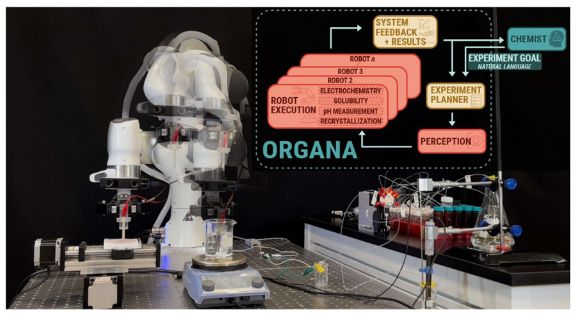

Fig. 9 Organa system, vessels and other modules in the experiment are automatically detected when defining a experiment workflow. Large language models are used to capture the instructions from chemists. Reconfiguration is achieved by giving new instructions to the system. Reprinted (adapted) with permission from ref. 23 Copyright 2025 Elsevier.

devices and robot arms. Some of the devices have been modified to interact with the mobile robot arm platform.[29] Grasping problems[27,28] are reduced by using a custom gripper for

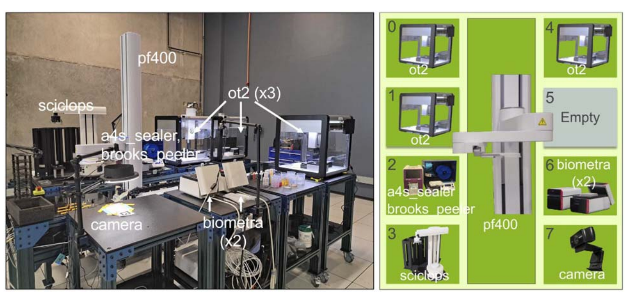

Fig. 10 Modular science factories system, carts are used as a uniform form factor for modules, which can be collections of devices. Robot arms are used to move materials between modules. Reconfiguration is achieved by manually rearranging cart positions. Reproduced from ref. 44 with permission from the Royal Society of Chemistry under CC BY-NC 3.0.

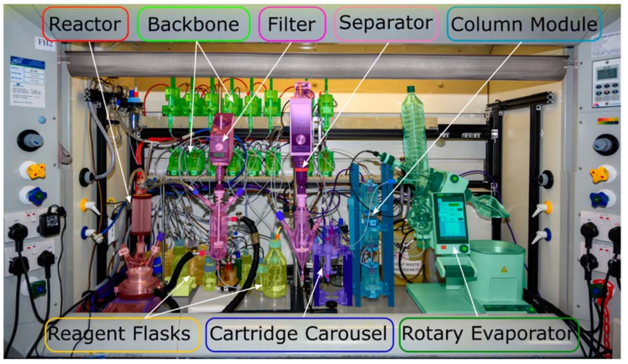

Fig. 11 The chemputer, modules are connected using hoses to a backbone of syringe pumps. The system is reconfigured by changing the order in which liquids are routed through the backbone, this order is defined in software. Reproduced/modified from Hammer *et al.*,[45] ACS Publications, under CC BY 4.0.

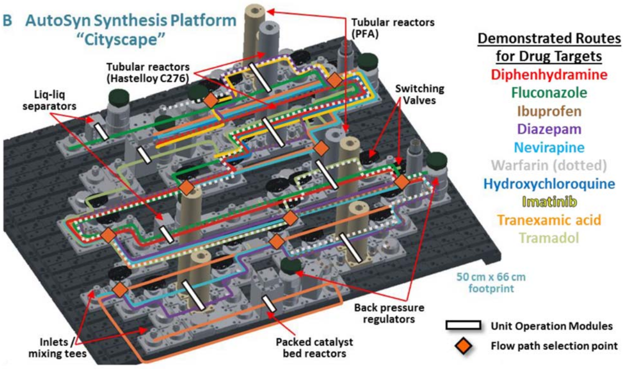

Fig. 13 CityScape, modular flow components are assembled using a Swagelok® Modular Platform Component system. Different experiment paths through the system can be configured by using manual or software controlled valves. Reprinted (adapted) with permission from ref. 50 Copyright 2020 American Chemical Society.

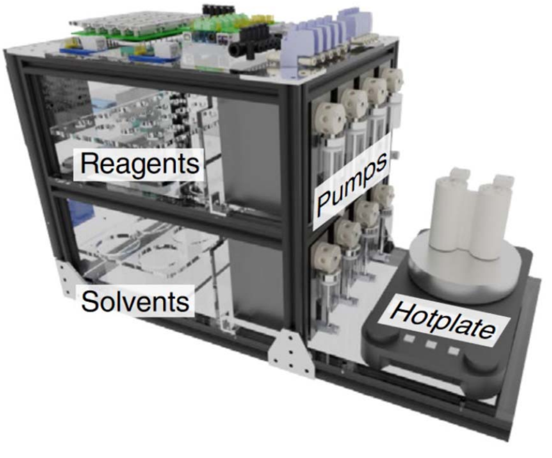

Fig. 12 The C^{3}PU system, modular 3D printed vessels that are connected to an array of syringe pumps backbone. Reconfiguration is done in a similar way to the chemputer. Reprinted (adapted), copyright belongs to Manzano, *et al.*, an autonomous portable platform for universal chemical synthesis,[47] *Nature Chemistry*, 14, 1114, 2022, Springer Nature.

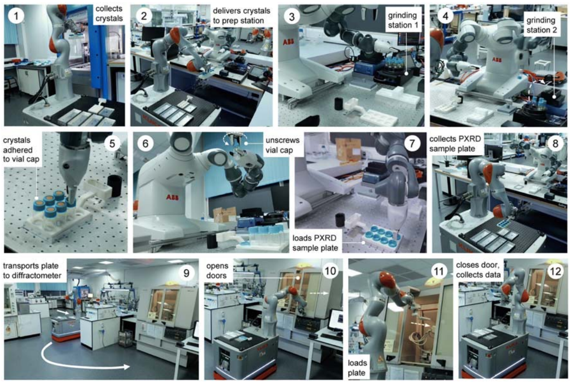

Fig. 14 ARChemist system, a mobile robot arm platform is used to move materials between stations. Markers and known positions are used to reduce errors in grasping and moving. Reconfiguration is achieved by changing the order of stations visited. Reproduced from ref. 52 with permission from the Royal Society of Chemistry under CC BY-NC 3.0.

handling standard vessels and solid dispensing cartridges, and by restricting the movement to known positions and recalibrating the robot at each station with a calibration cube. This ability to quickly recalibrate makes it easier to swap stations to reconfigure the system. Different processes have been demonstrated also expanding station functionality by adding smaller manipulators to some of them.[25] Although providing the same functionality as carts and racks in workcell/station systems like Syncar and ASL, the mobile robot provides more freedom to create different paths between stations, with the tradeoff of needing more space to maneuver.

3.3 Hardware reconfiguration

A way to have an always hardware-ready system for performing a wide range of different experiments is to automatically rearrange modules. The system in ref. 13 and 53 achieves this by using a robotic arm to move the modules in the plug and play reconfigurable synthesis system around (Fig. 15). In contrast to other platforms, in this system experiments that require different modules can be performed by physically changing them without human intervention.

The robot arm is also in charge of connecting tubes to inject reagents into the pressurized backbone, for this purpose different mechanisms have been implemented to prevent hoses from tangling when the robot moves them around. The robot arm increases the space used by the setup, but thanks to the modules standard connectors, form factor, and bays on the backbone, it circumvents most of the problems related to robot manipulation. At the same time it creates a more autonomous system that can perform multiple flow chemistry experiments without the need for a chemist technician.

3.4 Modular software

Software is a vital part of any automated experiment. Automatic hardware actions are controlled using firmware that receives

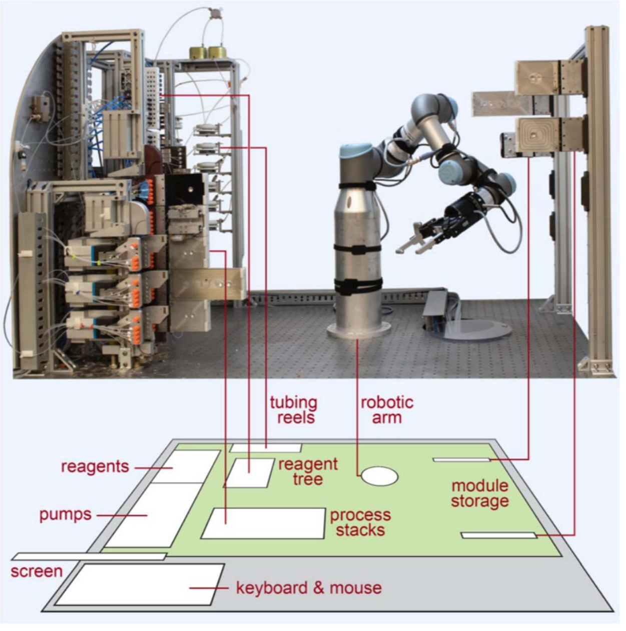

Fig. 15 Robot arm assisted plug and play platform, modules are moved from connector to connector using a robot arm. Unused modules can be stored in a different place. The robot can also change the input hoses connected to the modules in the central tubing backbone. Reproduced/modified from Coley *et al.*,[54] *Science*, https://doi.org/10.1126/science.aax1566 [2019], AAAS.

commands and exchanges settings and measurement data with external controllers and orchestrators using different communication interfaces.[5] With the development of distributed software applications, thanks to highly interconnected systems like the internet, software has become modular in itself and the barriers to use it have diminished. Nevertheless, due to the absence of standard programming interfaces and closed off protocols, communication with different vendor devices is still a challenge.[29,55,56]

This has not prevented efforts to develop modular software tools on top of vendor drivers; frameworks like HELAO,[57] WEI,[44] ChemOS,[58] and standards like SILA 2 (ref. 59) allow devices to connect to automatic workflow planners, data and laboratory management systems[8] and machine learning tools[60] to perform seamless concurrent orchestration; existing automation frameworks like ROS[21] and OPC-UA[61] are also often used. Some architectures[62] have even enabled the possibility of performing experiments asynchronously in different laboratories with different capabilities across the globe.[63] Languages like χDL,[45,56] used in the chemputer systems to specify recipes, modular protocol scripting languages like. The Laboratory Automation Protocol (LAP)[64] and graphical user interfaces[34] make it easier for chemists to describe recipes without having to deal with machine languages. Tools like Prisma[65] and MOCCA[66] help to automatically interpret result data from spectroscopy and chromatography results. Software in both of these ends is also essential to connect laboratory automation platforms to optimization and learning algorithms that can explore and exploit chemistry compound libraries and molecule features for accelerating material and drug discovery.[8] Different learning strategies have been used for the automatic discovery and synthesis optimization of compounds[56] including Bayesian optimization.[67] Other learning models including large language models are used for capturing natural language inputs[23] for specifying recipes and creating workflows,[68] or obtaining recipes from scientific literature.[53] More general architectures like ChemOS, AresOS or the one in ref. 23 include one or more of these tools to enable self driving laboratories.[6]

Surprisingly, among the systems reviewed, software and framework reuse in level 3 modular platforms is low. Only the ORGANA platform reuses a software tool created for another platform: in ref. 23 a Large Language Model (LLM) system converts natural language instructions into χDL instructions. Large language models are used to interpret input in natural language from a chemist and a workflow is then devised using planning algorithms. Almost all other systems use ad hoc solutions that implement graphical user interfaces,[41,50] recipe representations,[45,51,53] use base communication and workflow planning libraries from Python[42] and Matlab, tools like Labview[40] for reimplementing concepts like planners, schedulers, and optimization algorithms, as well as for drivers that talk to different devices. In particular, the modular science factories system[44] uses the concept of adapters to define code made particularly for talking to devices with different communication protocols like ROS or plain serial, and YAML markdown files are used to specify modules and workflows. In this platform, ROS was initially considered for interconnecting devices, but was later discarded as it was complex to setup for instruments running windows and that generated large amounts of data.

Still, even with the sleuth of advances on the software side, hardware remains the core of lab automation tools, and although many devices exist today to perform processes and experiments automatically, different challenges remain for creating level 4 modular laboratory automation platforms. On the one hand, we can take the lessons learned in software (language agnostic interfaces, compartmentalization, extendability) and apply them to hardware devices. For example, a module in a modular laboratory automation system can be built by grouping different devices that talk to a controller in the module; this controller can then appear as one entity to an orchestrator through a standard interface, simplifying much of its work. On the other hand, making modules more self-contained from the point of view of material transfer, communication and energy, using physical standard interfaces, makes them easier to abstract/represent as part of learning and orchestration systems and could open the way for different approaches to perform these tasks (*e.g.* multi-agent systems, cellular automatas, graph neural networks *etc.*…)

4 Navigating the modular landscape

In Section 2 we describe different advantages that modular design has for improving the implementation of automated laboratory experiments. Now with a background in the reviewed systems, this section discusses the extent to which the different platforms practically realize these features and also their

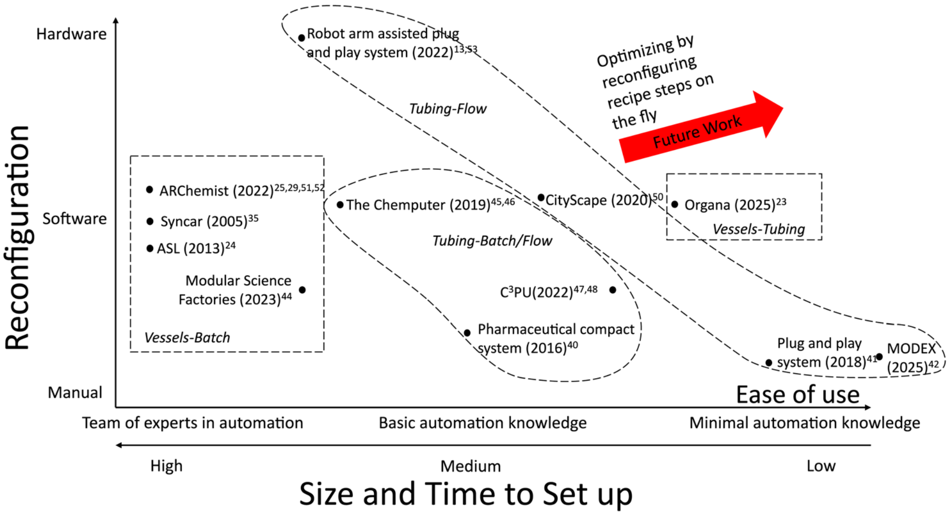

Fig. 16 Comparison of different reconfigurable laboratory automation platforms on their main way of reconfiguration, ease of use, time to setup and size.

limitations. Their individual design choices also impact their overall ease of use and other features including size. Fig. 16 shows a comparison of the different platforms reviewed in terms of their main reconfiguration method, how easy it is to use them based on the level of automation knowledge necessary, the time to set up and their overall size.

• Simple design: process step encapsulation in modules that can work separately from each other has been demonstrated in all reviewed platforms in varying degrees. For example, in ref. 23, module boundaries are not completely defined, this can be an advantage because chemists can use familiar devices, however this also makes reorganization difficult, for example in the case of the syringe pump, as engineering skills are needed. Scalability also suffers as connections can get very complicated as the number of modules increases and vessels and devices can be in arbitrary positions in the workspace of the robot. Similar issues arise in ref. 44 due to modules being able to house more than one device/operation. Other systems[41,42,45,47] provide a more distinct encapsulation of individual operations, making reconfiguration easier. Many platforms have modules that focus on similar process steps like mixing, heating, or liquid–liquid extraction, yet their capabilities present a significant challenge in direct comparison due to the lack of standardised testing across the different systems (see Tables 1 and 2). This lack of information needed for comparison has recently been discussed in.[55] The use of generalised and uniform benchmarks could help alleviate this problem.

• Extendibility: examples of design reuse can be seen in several platforms. In ref. 47 different 3D printed modules follow the same form factor and input–output arrangement. In ref. 13 and 53, modified versions of a base reactor design, that vary in size, can be used in different experiments. In ref. 44 case carts are used as a uniform form factor. In ref. 42, 3D printed frames are used as a base to implement modules. Some platforms provide extensive documentation which makes them easier to replicate and extend, this is the case of the chemputer systems[45,47] which make available drawings, fabrication files, and source code. Other platforms include schematic descriptions of the modules.[40,41,50,53]

Some platforms[23,51] do not follow a standard shape design for their modules and are thus more difficult to extend by creating new modules. Nevertheless, the ORGANA platform[23] alleviates this problem by relying on a human describing the different devices involved in an experiment and automatic object detection. However, this limits the experiments to devices that can be detected and reached by a robot arm. Lighting conditions must be controlled and there is no mention on the reliability of the approach. Markers were used in the first version to facilitate this process but may not be available for a mobile robot, leading to more restrictive transfer approaches.

• Flexibility: most platforms have demonstrated their capabilities in multiple and different experiments[40,41,46,47,50,53] (see Tables 1 and 2). However, most concentrate in the area of drug synthesis and production and material and nanoparticle synthesis.[42] In particular, the ARChemist platform[51] has performed experiments in the area of solid state material synthesis, taking advantage of using vessels to transport powders. Other systems[23,40] also have modules capable of handling solids, including crystallization and suspension modules.

• Reusability: the plug and play reconfigurable synthesis system[41] and its robot arm assisted version[53] use of uniform module frames makes modules quick and easy to swap around and reuse, even by a robot arm. This opens new ways to do experiments: AI-generated changing recipes can be executed automatically in a system.[69] However, specialised routing parts and robot arm and grippers still have to be implemented for the robot version. This makes the platform difficult to run by a lab technician and increases its size to around 3 to 4 square meters.

The system in ref. 44 also favors reusability by allowing the same carts to be rearranged in different ways. However, the technician must then perform the difficult task of reprogramming robot arms to transfer materials between carts. Similarly, some systems standard frame[42,50] imposes a physical constraint that makes modules quick and easy to swap around. Nevertheless, power should still be connected externally to each module.

Pressurised systems[13,41,50] are difficult to rearrange as the whole system or a big part of it must be stopped and drained before swapping modules around to make changes to the process. The most difficult to reorganize systems are the ones in which modules do not have frames encasing them.[23,40,45]

• Experiment reproducibility and debugging: most platforms only test the final result of the experiments. Only two works[13,50] have demonstrated automatically taking samples and performing analytics at different points of an experiment. Other platforms[47] measure process variables like temperature and pressure in reactors. Moreover, sensors are not usually included in all modules.

• Parallelization: glimpses of parallelization have been demonstrated in multiple platforms,[45,50] especially in managing concurrent experiments through solutions such as liquid manipulation heads with different functions and a geneva wheel.[49,70,71] Workflow orchestrators (see Section 3.4) can also organize steps to concurrently perform experiments. However, full parallelization with multiple replicated modules is still to be demonstrated.

• Environment control: no system has reported attempting to monitor or control the experiment environment in a per module basis. Only system in ref. 40 has implemented an integrated ventilation system. Better defined interfaces between modules could help isolate individual module environments.

• Reconfigurability: currently, only a couple of systems[13,41] implement matching module interfaces both for material transfer and for power and data connections. Additionally, in these systems, tubing is organized in a structured way inside the main system backbone. Tubing can also be organized inside modules[42] or as part of a frame system.[50] As a consequence of this organization, these systems require low mechanical and electronics expertise, time to setup, and space (Fig. 16). Alternatively, other systems[40,45,47] make also use of tubing and fittings but have no structured way of routing tubing around, they also do not have matching electrical connectors, which makes some technical expertise in electronics a must for using these systems (Fig. 16). This has the advantage of being flexible when arranging different experiments without moving modules and can be done manually by a human but, it can quickly lead to jumbled setups for high numbers of modules. Furthermore, materials must go back and forth through the same tubing in platforms with a central backbone[45] which has the potential for contamination in and between experiments. Platforms with robot arms[23,44,52] require reprogramming robot arm movements every time device positions inside modules change, which requires technical mechanical expertise.

• Leaks: only a few platforms[40,47] report checking for leaks as a safety measure. It is noteworthy that most safety mechanisms are usually left to external devices.[22]

• Complex orchestration: all platforms implement software to orchestrate their different modules. See Section 3.4.

• Overhead: most of the platforms reviewed show significant overhead for performing basic actions, *i.e.* who needs a robot arm for mixing two reagents? As being able to perform complex multi step reaction routes is one of the main goals of the platforms reviewed,[13,45,47] most of them are not designed to perform simple procedures.

• Cleaning: cleaning is also important when reusing modules. For most of the platforms reviewed, cleaning considerations between and inside experiments are kept to the bare minimum, for example, by using a quick cleaning solution in tubing systems or by replacing all the tubing in the system between experiments.[42,45,46]

5 Addressing the slow adoption of modular laboratory automation: key barriers and solutions

Modular laboratory automation systems, with their potential to revolutionize experimental research, particularly in chemistry, face slow adoption due to a constellation of unresolved challenges.[29,55,56] Despite their significant flexibility these systems have not seen widespread implementation.[29] The barriers to their adoption are multifaceted, encompassing both general challenges inherent in lab automation and specific hurdles tied to modular systems.[5,72] A fundamental dilemma at the heart of this slow adoption rate is the mismatch between the driving force behind automation and the technical demands of robotics and system design. Chemists aim to streamline or optimize specific sets of chemical reactions,[5,6] not necessarily to develop universal robotic platforms. Vendors also usually concentrate around popular sets of processes. This focus, while essential for scientific progress inadvertently narrows the scope of automation efforts, limiting their broader applicability and adaptability. Moreover, level 3 modular reconfigurable laboratory automation platforms are concentrated in the area of drug synthesis and only a few have wandered in the area of solid state material and nanoparticle synthesis. This is mainly due to the drive the pharmaceutical industry has had in laboratory automation development and the difficulties of handling powders and other types of solid materials with different transfer systems.

• Financial and technical hurdles: the development of systems that automate and quickly adapt to diverse experimental setups requires substantial financial investment, not only in hardware but also in assembling interdisciplinary teams.[73] This represents a significant barrier, especially for smaller research groups with limited resources.

One practical strategy to ease these challenges is broadening the availability of modules capable of performing basic common processes. This can be done by developing modules that can be built using widely available techniques, like 3D printing, and off-the-shelf components so that they can be easily reproduced, and sharing not only software but also hardware designs openly. Smaller labs can take advantage of the modular design and replicate these modules multiple times and use them as a starting point for their experiments.[7] This still requires engineering skills for assembling the modules but allows researchers to focus more on their scientific objectives rather than on system design. Examples on modular systems that have released instruction on building their various modules include.[13,46,47]

Module kits could also be developed and distributed using different channels, with or without assembly, while keeping designs open. This would minimize the technical hurdle and would help to gradually familiarize chemists with common mechanical and electronic tools for automating experiments. It has been tried with relative success in other areas of robotics[74] and has been one of the driving forces in popularizing, adopting and modifying the current generation of 3D printing technology.[75] Of course, also including robotics and automation skills into chemistry courses and improving user interfaces[34] would help show chemists the possibilities of using modular systems in their experiments.

Materials are one of the highest costs when developing automated modules. To reduce these costs, another strategy would be taking advantage of new materials that are now becoming available to 3D print, including glass[76,77] and PEEK (Polyetheretherketone),[78] to completely 3D print chemical resistant modules, that can be directly fitted with electronic components and sensors.

• The importance of benchmarking for adoption and optimization: emphasizing safety and accessibility:

A major challenge in current practices is the lack of standard tests and metrics, which leads to difficulties in comparing systems effectively.[55] All the systems reviewed are evaluated based on their ability to produce specific compounds or achieve particular results in specialized applications. However, such assessments do not provide a clear, generalizable measure of system performance that is understandable across different disciplines. For example, the yield of a medical compound might demonstrate a system's capability in a specific context but offers little insight into its broader applicability or efficiency. Instead, defining physical specifications such as reactor wattage, maximum temperature, and pressure capacities (as detailed in Tables 1 and 2) provides clear, comparable metrics that are easier to use across various fields.

Standardized benchmarking is fundamental to advancing the adoption and optimization of modular laboratory automation systems.[29] By establishing uniform experiments and metrics, we enable effective comparisons based on system performance, compatibility, and operational parameters. Prioritizing non-toxic materials in these benchmarks not only enhances safety but also broadens participation.[7] This approach allows laboratories from diverse fields, such as robotics and electronics, and even smaller chemical laboratories, to safely engage in chemical research and development activities. By conducting standardized, simple experiments—as exemplified in Fig. 17—these labs can contribute significantly to the field without needing extensive chemical safety infrastructure.

• Addressing modular-specific challenges.

Modular systems also confront unique challenges. One particular example arises in the realm of analytics. Current

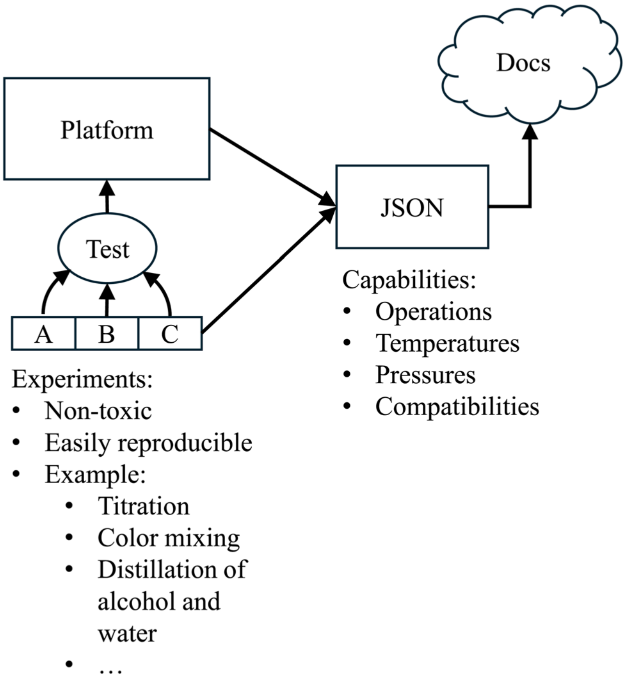

Fig. 17 A standardized set of benchmark experiments can be run in a platform in order to evaluate it against other solutions. Ideally these experiments should be easily reproducible and use non toxic materials, in this way other groups and specially roboticists can take this information to develop new systems. The capabilities of the system could be recorded then in an easy to process format (*e.g.* JSON) that can be disseminated and ontologized for other scientist to use.

analytic solutions are not designed with encapsulation in mind.[29] Many of the platforms presented connect to external analytical tools[42] or in some cases samples must be taken by a technician to perform different tests.[24] Although it may not be possible for all kinds of equipment, different tools can be miniaturized taking advantage of micro sensors and microfluidics[79] to be more easily integrated as part of different modules.

Safety also emerges as a significant concern in systems that can be quickly reconfigured. The inherent flexibility of these systems, allowing for numerous configurations, can inadvertently introduce errors.[55] Designing comprehensive safety procedures for a system with such adaptability is challenging, as the higher flexibility can increase the likelihood of accidents.

As can be seen from the span of time of the systems covered in this review (Fig. 16), novel hardware is slow to develop. This does not mean that new systems and automated devices for different kinds of experiments are not being developed all the time. Although not always in a modular way, this can be seen in the development of automation solutions for self driving laboratories in different application areas.[6] Easily extendable systems, interdisciplinary teams and standard form factors can help speed up this development. The proliferation of robot arms in different setups[8] is a good example of this speed up due to a standard form factor. This same concept can be expanded to other types of devices and forms of material transfer (*e.g.* analytic devices, solids transport).

Finally, orchestration of concurrent operations introduces unique challenges, particularly in the coordination and sharing of resources. Shared resources within modular systems, such as tubes, valves, or entire modules like heating or cooling units, can become bottlenecks. For instance, if multiple processes require the same cooling module at overlapping times, coordination becomes critical to prevent process delays and ensure smooth operation. This necessitates sophisticated orchestration to manage resource allocation efficiently, akin to how an operating system manages memory and processor time among programs.[44,45,56] Although many frameworks exist already for tackling these problems, they are seldom reused (Section 3.4) in level 3 modular platforms, and the complexity of managing these shared resources significantly heightens the entry barrier.

6 Outlook: towards a collaborative and open future in laboratory automation

Modular lab automation represents an evolution in laboratory technology, necessitating the collaboration of chemists, roboticists, engineers, and computational scientists to develop practical and versatile solutions. The establishment of partnerships across academic institutions, industry, and funding bodies is necessary for reducing financial constraints and integrating diverse expertise. Such interdisciplinary collaboration promotes the development of modular systems tailored to the needs of end-users, merging functionality with user-centric design.[7] This convergence of multiple disciplines is known to accelerate technological innovations, leading to more robust and applicable solutions.[6,80,81]

6.1 AI-guided experimentation: dynamic recipes

The integration of AI with laboratory automation is already creating a new era of scientific exploration. AI experiments can benefit from the capability of automatically reconfiguring modules to optimize a recipe by testing different sequences of physical steps on the fly, for different purposes, for example, reducing precursor consumption. This concept has begun to be explored in platforms such as the robot-assisted plug and play platform, indicating the potential for developing dynamic recipes.[35,45,50,56] This approach assumes that system modules can be rearranged as needed for any experiment, supported by software checks to reject implausible or unsafe runs, with some platforms already showcasing these capabilities.[13,24,35,47] Furthermore, the incorporation of simpler sensors for real-time monitoring could significantly enhance this dynamic recipe capability, allowing for on-the-fly course corrections and optimization based on sensor feedback.[5,47,82] Bridging the gap between innovative hardware solutions and, the experimentally focused literature in chemistry, we encounter the challenge of converting the predominantly natural language documentation of scientific discoveries into actionable insights. Here lies an intriguing exploration, where Natural Language Processing (NLP) and other techniques have been used to parse the literature and reaction repositories, transforming them into executable scripts.[83] Platforms like the ones in ref. 50 and 13 mark early forays into this domain. Additionally, the emergence of large language models opens a promising pathway to further advance this integration, potentially revolutionizing how chemical knowledge is interpreted and applied in laboratory automation.[23]

6.2 A call for open collaboration and standardization

As we look to the future, the advancement of modular lab automation hinges on a foundation of open collaboration and standardization. Sharing design files and developing universally accessible and interoperable modules will be a key to democratising innovation across the field. By fostering an environment where design files are openly shared and standard interfaces are established, we enable a broader spectrum of researchers to contribute to and benefit from the collective progress in lab automation. This approach not only facilitates the integration of diverse modules and systems but also encourages the pooling of expertise from across disciplines.

In the end, the journey towards realizing the full potential of modular lab automation hardware is a collective endeavor that transcends disciplinary boundaries. By embracing parallelism, leveraging AI, and committing to open collaboration and standardization, we can unlock the capabilities of modular hardware systems. In the future, modular reconfigurable laboratory automation system hardware could become as versatile, quick and easy to use as glassware. This collaborative future promises to make lab automation more adaptable, efficient, and accessible, benefiting chemists and the broader scientific community.

Author contributions

Rodrigo Moreno has contributed with the conceptualization, data curation, investigation, methodology, visualization and writing – original draft. Jonas Jensen has contributed with the conceptualization, data curation, investigation, visualization and writing – original draft. Andres Faina has contributed with supervision, and writing – review & editing. Kasper Stoy has contributed with supervision and writing – review & editing.

Conflicts of interest

There are no conflicts of interest to declare.

Data availability

No primary research results, software or code have been included and no new data were generated or analysed as part of this review.

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sustainable batteries of the future. This text has been refined using artificial intelligence tools to enhance clarity.

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