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The digital lab manager: Automating research support

Simon D. Rihm [a,b,c], Yong Ren Tan [a], Wilson Ang [a], Markus Hofmeister [a,b,c], Xinhong Deng [a], Michael Teguh Laksana [a], Hou Yee Quek [a], Jiaru Bai [b], Laura Pascazio [a], Sim Chun Siong [a], Jethro Akroyd [a,b,d], Sebastian Mosbach [a,b,d], Markus Kraft [a,b,d,e,f,*]

[a] CARES, Cambridge Centre for Advanced Research and Education in Singapore, 1 CREATE Way, CREATE Tower, #05-05, 138602, Singapore
[b] Department of Chemical Engineering and Biotechnology, University of Cambridge, Philipppa Fawcett Drive, Cambridge, CB3 0AS, United Kingdom
[c] Department of Chemical & Biomolecular Engineering, National University of Singapore, 4 Engineering Drive 4, 117585, Singapore
[d] CMCL Innovations, Sheraton House, Cambridge, CB3 0AX, United Kingdom
[e] School of Chemical and Biomedical Engineering, Nanyang Technological University, 62 Nanyang Drive, 637459, Singapore
[f] The Alan Turing Institute, 2QR, John Dodson House, 96 Euston Rd, London, NW1 2DB, United Kingdom

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ABSTRACT

Laboratory management automation is essential for achieving interoperability in the domain of experimental research and accelerating scientific discovery. The integration of resources and the sharing of knowledge across organisations enable scientific discoveries to be accelerated by increasing the productivity of laboratories, optimising funding efficiency, and addressing emerging global challenges. This paper presents a novel framework for digitalising and automating the administration of research laboratories through The World Avatar, an all-encompassing dynamic knowledge graph. This Digital Laboratory Framework serves as a flexible tool, enabling users to efficiently leverage data from diverse systems and formats without being confined to a specific software or protocol. Establishing dedicated ontologies and agents and combining them with technologies such as QR codes, RFID tags, and mobile apps, enabled us to develop modular applications that tackle some key challenges related to lab management. Here, we showcase an automated tracking and intervention system for explosive chemicals as well as an easy-to-use mobile application for asset management and information retrieval. Implementing these, we have achieved semantic linking of BIM and BMS data with laboratory inventory and chemical knowledge. Our approach can capture the crucial data points and reduce inventory processing time. All data provenance is recorded following the FAIR principles, ensuring its accessibility and interoperability.

1. Introduction

Scientific advancement and breakthroughs often depend on the integration and collaboration of various systems, disciplines, and institutions [1,2]. Conventional workflows therefore entail complex manual coordination of researchers, operations, experiments, and resources across multiple laboratories. To accelerate scientific discovery, those need to be improved. Digitalisation and automation in research laboratories are essential to increase their efficiency and productivity and minimise human error, which improves experimental reproducibility, precision, and accuracy [3,4].

Conventionally, laboratory automation in scientific research and development (R&D) has been focused on experimental automation and the development of “self-driving laboratories” – specifically to plan, execute, and optimise scientific experiments in an autonomous loop [5]. However, to fully automate processes or even achieve autonomy, a more general view is necessary that includes the influential peripheries of experimental research, often related to managerial duties [6,7]. The ability of key stakeholders (*e.g.* laboratory managers, technicians, and principal investigators) to focus on core tasks that require sophisticated decision-making, creativity, and problem-solving is pivotal to accelerating scientific discoveries and, more importantly, addressing urgent global challenges through R&D [8].

Realising the digital transformation of R&D in science laboratories requires the adoption of cutting-edge technologies such as artificial intelligence and cloud-based platforms [3]. Automated laboratory data capture systems were recently shown to support harmonising siloed laboratory data from analytical instruments, reporting systems, and operational platforms [9]. However, the sole implementation of digital solutions alone is not sufficient as increasing data complexity

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[*] Corresponding author at: Department of Chemical Engineering and Biotechnology, University of Cambridge, Philipppa Fawcett Drive, Cambridge, CB3 0AS, United Kingdom.

E-mail address: mk306@cam.ac.uk (M. Kraft).

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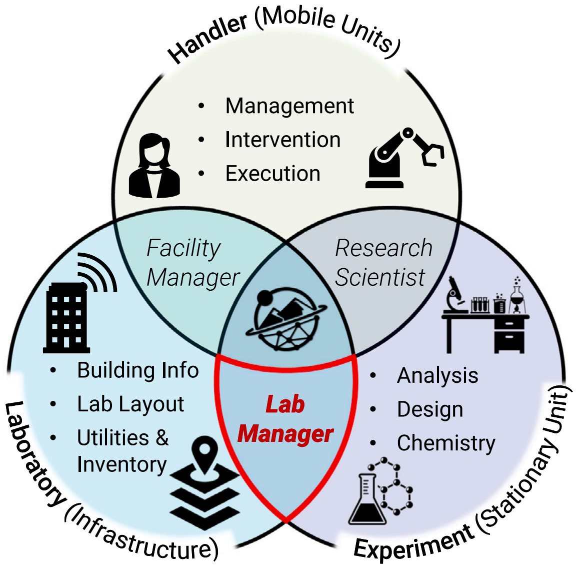


Fig. 1. An illustration of interconnected features of a scientific research laboratory that need to be represented by a comprehensive digital twin . The current work will focus on the automation of laboratory management tasks.
Source: Adapted from [6].

and volume requires stored information to be accessible and interoperable. Unfortunately, existing digital tools are limited, isolated, and fragmented [4]. Solutions are constrained by proprietary vendor data formats and hampered by siloed storage platforms that are case-specific.

Semantic Web technology has been identified as a promising solution to address these challenges and enable interoperability of data across scales and domains [10,11]. The World Avatar, for instance, is an ongoing project that uses the Semantic Web technology for laboratory automation (see Fig. 1) [6,12] within a “Digital Laboratory Framework” (DLF). This is achieved through the development of a sufficiently generic and all-encompassing digital twin (DT) that reflects every aspect of the physical laboratory accurately and enables seamless orchestration of experimental setups and resources. Software agents are developed and involved in continuously incorporating new concepts and data into the knowledge graph while maintaining connections to existing data. The knowledge graph captures the data provenance of experimental procedures as “knowledge statements” when it expands, thereby functioning as a dynamic representation of the actual world.

This work is part of a series of articles that argue for holistic laboratory automation encompassing all aspects of experimental research within a dynamic knowledge graph [6]. Fig. 1 illustrates these aspects: the laboratory which provides all relevant infrastructure and resources; the moving handlers carrying out the actual work; and the experiment itself. The **purpose of this paper** is to demonstrate a network of synchronised and connected digital twins based on Semantic Web technology, that can transform and automate laboratory operations. Particularly, we aim to overcome challenges posed by the traditionally manual workflows in laboratory management, allowing key stakeholders to focus on essential activities that demand complex reasoning, innovation, and creativity. Common standards and ontologies are used to semantically represent and link laboratory data on chemical properties, asset information, users, and related real-time data in a machine-readable and interoperable format. We also present platform-independent interfaces that allow for digital visualisation and operation of the laboratory, leading to a more connected and intelligent system that enhances the efficiency, quality, and innovation of scientific research.

2. Background

The management of research laboratories encompasses a diverse array of tasks that span many domains and scales to provide a safe and efficient work environment for researchers. Many of the tasks are of administrative nature and peripheral to the research itself. They have an enabling effect on users of lab facilities, providing relevant resources and monitoring ongoing research. To the authors’ best knowledge, there is a gap in the current literature body on comprehensive reviews of lab managers’ responsibilities and their potential for digitalisation and automation. We therefore identified 25 tasks in a strategic assessment of laboratory management duties at the Cambridge Centre for Advanced Research and Education in Singapore (CARES). We consolidated these tasks as listed in the Supplementary Information and categorised resulting problem spaces into asset management, inventory tracking, and resource allocation. For an accurate analysis of suitability for automation, we ranked them in Fig. 2 according to the relative expected cost of automation (ordinate) and the relative expected impact with the implementation of automation (abscissa). For context, a high relative impact means a considerable improvement in productivity and/or reduction of error in the execution of a tasks is to be expected.

Tasks related to procurement and finance are expected to show a high impact on automation but related systems are usually predefined or highly entangled with other departments. Meanwhile, inventory management is a crucial aspect of laboratory management and operation with a consistently high expected impact of automation. These tasks are highly manual and repetitive which applies in particular to fixed asset and equipment auditing, requiring users to track items and update different systems when new assets are purchased [13]. This can lead to inconsistent and error-prone data, which can compromise the quality and integrity of the experimental metadata. Moreover, the tracking of hazardous chemicals lacks standardisation, and the conventional approach of using a physical log book is prone to human errors. Thus, automating these tasks could potentially enhance the productivity of research facilities and accelerate scientific discoveries by maximising managers’ available time for supporting researchers on actual scientific research and discoveries. Whilst the implementation of automation processes using digital tools is crucial, security concerns are of utmost importance as well, especially when managing sensitive research projects. Therefore, an authentication system also needs to ensure that sensitive data or information is safe and secure [14,15].

2.1. Digital tools in laboratory management

Digital solutions exist in laboratory management to address some of the actionable problem spaces shown in Fig. 2. However, they are often fragmented, and lack interoperability and specificity [6]. This is especially evident in attempts to integrate diverse systems within a unified framework that allows smooth collaboration and communication. The integration of different software, equipment, and monitoring systems from various suppliers, as well as tracking their usage, occupancy, and maintenance schedules remains a critical challenge [13]. Many research laboratories have adopted a plethora of digital tools and platforms in the management of their labs that need to be maintained separately. This section will present some of these solutions and the challenges involved [15].

Laboratory Information Management System (LIMS) can digitalise the management of laboratory inventory such as equipment, chemicals, and consumables. It is used for automating tasks and workflows, handling data entry and import from external sources, facilitating inventory purchase and scheduling, as well as monitoring and tracking inventory levels, usage, location, and status [16]. Meanwhile, Enterprise Resource Planning (ERP) software unifies every element of corporate operations and presents a consolidated overview of the organisation on a single platform, which supports supply chain, human resources, operations, finance, and other key organisational tasks [17].

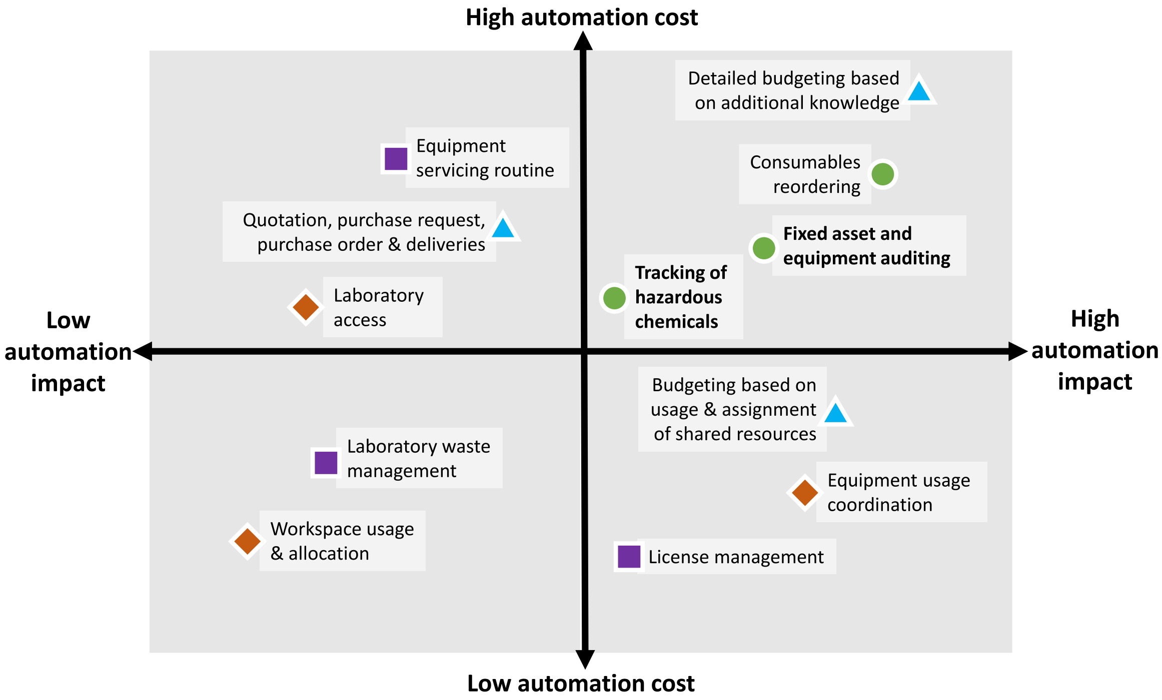


Fig. 2. Cost-impact analysis of challenges in laboratory management. The highlighted problem spaces are the focus of the current work. Legend: ● Inventory management; ▲ Procurement and finance; ■ Maintenance; ◆ Access management.

ERP gives laboratory managers access to crucial information related to stock levels, operating costs, and expenses. It can be coupled with LIMS which allows the synchronisation of internal and external laboratory activities as well as enhanced quality control and resource allocation.

An Electronic Laboratory Notebook (ELN) allows the digital collection and management of laboratory data. A typical ELN offers various functionalities such as workflow automation, documentation, data management, and collaboration tools [18]. Similarly to ELN, the Laboratory Execution System (LES) also facilitates electronic processes and automates the interaction with methods, instruments, and supplies in routine laboratory procedures to ensure compliance and quality control [16]. ELN and LIMS are often integrated to improve laboratory productivity; examples are SLIMS, LabCollector, LabWare, openBIS, and Labguru [19]. A key difference between ELNs and LIMS is that ELNs store and record unstructured research data (*e.g.* R&D stage experimental data), while LIMS stores structured and repetitive data that follow patterns and templates (*e.g.* diagnostic results from a testing lab). LES is also often integrated with LIMS, or ELN when there are parts of the LES workflow that are not supported [16,20]. As such, LIMS-LES integration was shown to improve the quality of data acquisition and sample turnaround time [16].

The Scientific Data Management System (SDMS) is a centralised document management system, that collects, stores, and exports scientific data generated by and in a laboratory. SDMS is designed to capture, store and manage a variety of unstructured data formats integrated with systems such as LIMS, ELN, LES and ERP [15]. It also allows for direct interaction with laboratory instruments, systems, and databases. With an SDMS, laboratory managers and other laboratory personnel can generate reports on laboratory activities, speed up workflows and approval processes, and optimise collaboration using data from LIMS and ELNs.

Meanwhile, Chromatography Data Systems (CDS) are digital tools that specifically acquire, manage and report test results from experiments involving chromatography [15,21,22]. CDS acts as an instrument coordinator with devices to send work schedules, receive measured data, and analyse the data [22]. CDSs are useful for laboratories that perform routinised and regulated testing for quality control, pharmaceutical development, or manufacturing [21]. Mazzarese et al. [21] provided a review of the main CDS providers with some smaller or niche market CDS providers that are often linked to the products of the chromatography products.

Typically, all these software can be classified into commercial and open source. Commercial models are usually platform-based and popular among large corporations because they are particularly designed to be good at managing high-throughput data and preventing data loss. They offer a well-organised support system, frequent maintenance and upgrades, regulatory compliance, and smooth integration capabilities. They do, however, incur significant costs owing to licensing, implementation, customisation, and technical training for users [18]. Open-sourced software is therefore more attractive to small and medium-sized businesses and academic institutions. These solutions have little or no licencing, maintenance, and external service expenses, yet often provide competitive features as their commercial equivalents [23]. However, inactive updates may result in long-term security and maintenance problems [18]. They can be easily customised to suit the unique needs of different laboratories but they may require a higher level of technical expertise to implement and maintain.

It is clear that the laboratory management digital tool ecosystem is quite fragmented, which can hinder collaboration within or between institutions and organisations. These solutions are highly specific and lack **interoperability** hampering **orchestration** of operations. Moreover they are often unable to represent actual **knowledge depth** [6]. Critically, the data from these platforms are often not FAIR (Findable, Accessible, Interoperable, Reproducible) compliant [24]. For example, some software can monitor chemical usage, but not transfer data to other platforms for budgeting or inventory. Similarly, some platforms can manage laboratory assets, but require slow and error-prone manual input and updating. This makes it a challenge to fully utilise the available software solutions as they often need to be consolidated manually via spreadsheets [13]. Furthermore, information on equipment availability, risk assessments, or manuals is often scattered and poorly documented, making it difficult for laboratory users to access and use them. Therefore, a more integrated and automated solution for laboratory management and operation is needed to enable FAIR data practices across organisations.

To address these challenges, an innovative solution lies in the creation of digital twins for lab equipment. These digital replicas comprehensively capture a wide range of relevant information — from financial aspects and purchase history to servicing schedules and measurement data. In theory, these data do not have to be on a single platform but can be accessed from different dedicated systems as long as an appropriate Application Programming Interface (API) exists. This approach not only streamlines information access but also aligns with the need for more integrated and automated laboratory management. To ensure accuracy and real-time consistency, digital twins rely on continuous synchronisation with their physical counterparts through sensor data, facilitating shared instrument use, monitoring operations, and scheduling maintenance [14,25]. Integrating these elements into an Internet of Things (IoT) framework enhances the overall lab automation and resource management system [25,26]. Currently, there have been limited efforts towards establishing a "smart lab" environment that leverages these technologies [27].

2.2. Leveraging semantic web technology for lab management

The adoption of digital solutions, either commercial or open-source, varies across different laboratory settings. Although laboratories in large corporations tend to use them extensively, university-based laboratories exhibit a lower rate of adoption due to the lack of flexibility of most solutions, which are customised for specific workflows and require sophisticated training and investment for any modification [26]. Laboratories based in universities face numerous challenges, such as limited budgets, outdated equipment and software, and heterogeneous vendor equipment. Consequently, they are reluctant to adopt digital solutions that are not interoperable with various vendors. Some vendors have attempted to address this issue by integrating different digital tools (*i.e.* SDMS, LIMS, ELN and LES) to offer more holistic solutions, such as STARLIMS and SampleManager LIMS. However, these solutions still encounter difficulties in terms of vendor-agnosticism, data ingestion, and "lock-in" effects [6].

Semantic Web technology is a promising approach to achieving the required data interoperability and vendor-agnosticism for laboratory automation. It enables the development of ontologies that span across different domains, facilitates the integration of different systems, and more importantly provides human- and machine-readable data [28]. An ontology is a comprehensive and structured representation of knowledge, such as concepts and relationships within a specific domain [29]. These representations provide a shared understanding and a standardised definition of knowledge to align both the human and machine perspectives [28]. Machina and Wild [15] recently suggested a new ELN-centric laboratory informatics tool based on Semantic Web technology that integrates LIMS, ELN, CDS, and SDMS semantically. There have also been attempts to develop an ontology-based ELN for microscopy workflows [30]. However, this domain-specific solution has limited interoperability of data across different experiments and domains and did not address laboratory management issues [30]. Recently, the "Open Semantic Lab" project used Semantic Web technology to build a comprehensive online platform capable of semantically capturing and linking laboratory data and concepts, resulting in machine-readable and human-operable data [31]. While the platform aims to support the integration of complex procedures, software, and data, it is still in the early stages of development and currently does not include many of the peripheral aspects and infrastructure relevant to lab managers.

Given the intrinsic complexity related to the Semantic Web technology, a brief explanation will be provided to describe some of the ideas essential to the subject. The terminological component (TBox) and the assertional component (ABox) are the two basic components of an ontology [32]. Through a taxonomy or classification system for domain knowledge, the TBox establishes concepts, their hierarchical relationships, and associated attributes. The TBox concepts are instantiated by ABoxes to represent real-world entities as instances. These instances are all online resources identified by unique internationalised resource identifiers (IRI) and provide meaningful attributes and relationships about a subject. The data of the instances are typically recorded and stored in the form of a "Resource Description Framework" based on subject–predicate–object triples. By extending the representation capabilities of ontologies through the use of knowledge graphs new cross-domain knowledge can be derived. A knowledge graph consists of "nodes" referring to entities of interest and "edges" representing the relationships between two nodes which eventually form a directed graph with the use of ontologies [33]. Such a representation enables a standardised form of human- and machine-readable data model that can be further processed in applications. Notably, the existing ontologies in the data model can be reused and connected with each other to further encapsulate expanding domain knowledge. Knowledge graphs can therefore play a crucial role in facilitating the creation and management of evolving digital twins, enabling continuous integration of information representing the real-time state of laboratory equipment [6].

2.3. The world avatar digital laboratory framework

This work is part of the larger "The World Avatar" project. Its objective is to develop an all-encompassing digital twin that can connect data and computational agents in real-time to create a living digital "avatar" of the real world, inclusive of abstract concepts and processes [12]. DTs are realistic digital representations of assets, processes, or systems in the built or natural environment that create the opportunity for providing feedback into the physical world [34]. The TWA approach differentiates itself from traditional Semantic Web implementations through the seamless holistic integration of real-time dynamic data, knowledge, models, and tools (*i.e.* dynamic knowledge graph, dKG) in a distributed architecture through an ecosystem of autonomous agents [12].

TWA project was initially developed to address the challenges of decarbonisation in the chemical industry of Singapore [35]. Since then, it has expanded to cover a broad range of domains, such as chemistry, chemical processes, laboratories, power systems, as well as various "smart city" applications [36–38]. By acting on real-time data through the agents, TWA describes the behaviour of complex systems and performs tasks such as updates, analysis, decision-making and control of real-world entities [12]. To ensure constant error correction and synchronisation of the digital twin with the real world, TWA captures metadata of derived values and ensures the propagation of new data through the knowledge graph by making derivations and agents an inherent part of the knowledge graph [39].

In the following sections, we present the implementation and application of the TWA-based Digital Laboratory Framework (DLF) to supporting the role of laboratory managers and users. DLF uses a multi-agent system to create the comprehensive laboratory DT, which inherently incorporates and considers human and infrastructure aspects [6]. The use of modular ontologies facilitates **interoperability** between scales and domains beyond the capabilities of monolithic ontologies. For example, we recently demonstrated the integration of data collected by distributed IoT sensors with a commercial building management system (BMS) and building information management (BIM) data [40]. By leveraging APIs of different proprietary or open-source software, autonomous agents retrieve and exchange data to enrich the laboratory digital twins. This enables TWA to support **orchestration** in monitoring and controlling efforts between separate systems. Moreover, TWA includes chemistry domain knowledge [37] which facilitates the **knowledge depth** required for complex lab management tasks.

This offers a holistic approach to goal-driven automation of research laboratories. The framework is aligned with the vision of achieving a fully autonomous "AI scientist" [41]. Within a united framework, tasks relating to laboratory management are incorporated and automated

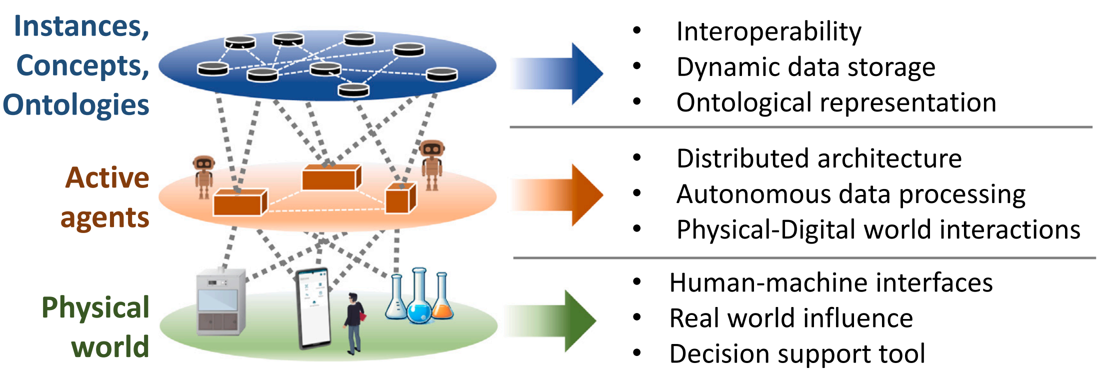


Fig. 3. Trilayer structure of TWA as employed in this work for enhanced management and automation of a research laboratory. The three layers are interconnected, creating a distributed and connected DT in order to address the challenges in managing research laboratories.

to create a distributed and connected DT. Such a “Digital Laboratory Manager” (DLM) can support, assist, and manage all aspects of the research laboratory which are captured by the dKG. The operation of so-called self-driving laboratories as well as non-automated or hybrid research laboratories is also enabled through the development of dynamic human–machine interfaces, coupled with the underlying use of the dKG within the DLF. Going forward, TWA-based agents can operate with an increasing degree of autonomy by re-evaluating their own goals, performing distributed optimisation tasks [5], considering its direct and indirect environment, and taking over managerial tasks related to inventory and chemical management.

3. Developed methodology

In order to automate lab management tasks – and particularly those related to inventory management which were highlighted in Section 2 – the challenges faced by currently available solutions need to be overcome. Based on the DLF, we developed appropriate methodology using Semantic Web technology in three areas. The first area is asset tracking where we employed radio frequency identification (RFID) technology to tag hazardous (*e.g.* explosive) chemicals, enabling automated safety measures using **deep domain knowledge**. The second area is asset management where we employed “Quick Response” (QR) code technology to tag assets in the laboratory and uniquely identify them for better planning and **orchestration** of experiments. Lastly, a flexible human–machine interface was established to facilitate constant availability of information, **interoperability**, and applicability of automated procedures: a mobile application that communicates directly with the dKG, enabling real-time access and interaction with underlying data models. The underlying TWA structure follows a trilayer concept as illustrated in Fig. 3.

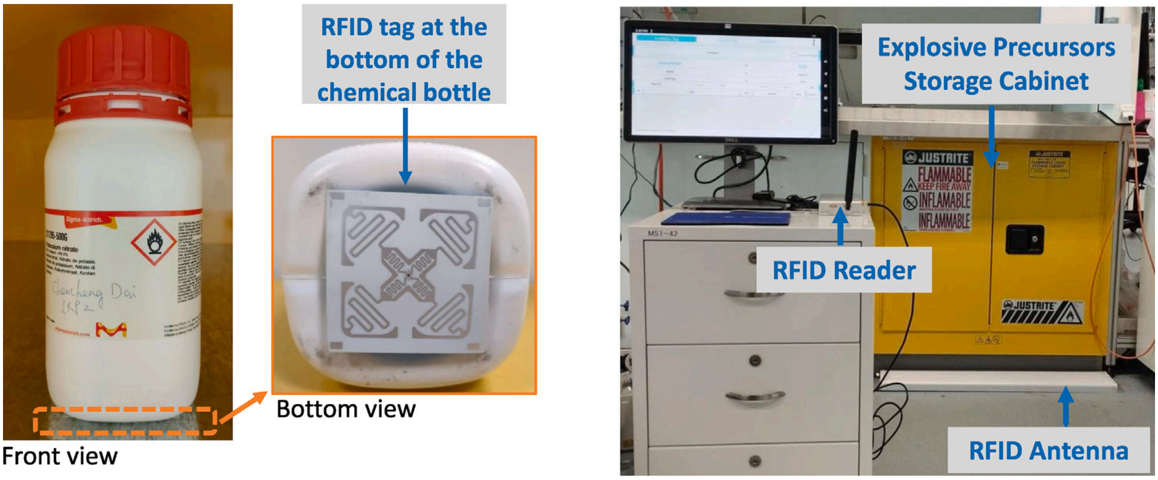
The top layer represents the ontological models used in the development of the laboratory digital twin. With the development of different ontologies, the resulting dKG can then be used to describe various objects of interest and their connections. The middle layer represents active agents that keep the knowledge graph up-to-date, coordinate data exchange between different servers, and automate various tasks related to lab management. Agents on distributed cloud-based or local servers can interact autonomously with the dKG to instantiate, create, access, and modify data as well as perform simulations, forecast time series, and even control physical objects. The main mode of communication between agents and the dKG is through HTTP requests. The bottom layer consists of physical entities in the real world which interact with and are orchestrated by active agents to carry out certain tasks or achieve certain goal. In the context of the current work, this would include for example fume hoods, temperature sensors, chemical containers, analytical equipment, flow reactors, liquid handlers, other laboratory assets, and even laboratory users. Furthermore, multiple digital interfaces and decision support tools are also included in this layer which can assist in communicating and interacting with active agents.

3.1. *Tracking assets*

In a research laboratory, many critical assets are often either highly valuable or dangerous and must be closely tracked. As included in Fig. 2, the need to closely track the location of critical assets (especially explosive chemicals) is imperative to ensure the laboratory operates in accordance with safety regulations and compliance. To ensure accurate knowledge on whereabouts of these assets, RFID tags can be employed to track the location of relevant containers. RFID is a key enabler of Industry 4.0 and is a versatile tool for automatic identification and tracking in various domains such as logistics, clothing, agriculture, food, and manufacturing [42,43]. It is based on a low-cost and accurate sensor that requires minimal or no power consumption and offers wireless power transfer, flexibility, and non-line-of-sight communication [42]. As such, it can be applied to digitise chemical inventory management, resulting in reduced chemical search time and increased efficiency of inventory checks, chemical refills, and safety management [44]. Moreover, integration with a cloud computing platform and a wireless sensor network has been shown to improve efficiency in supervision and utilisation of equipment, and maintain its life cycle accurately [27].

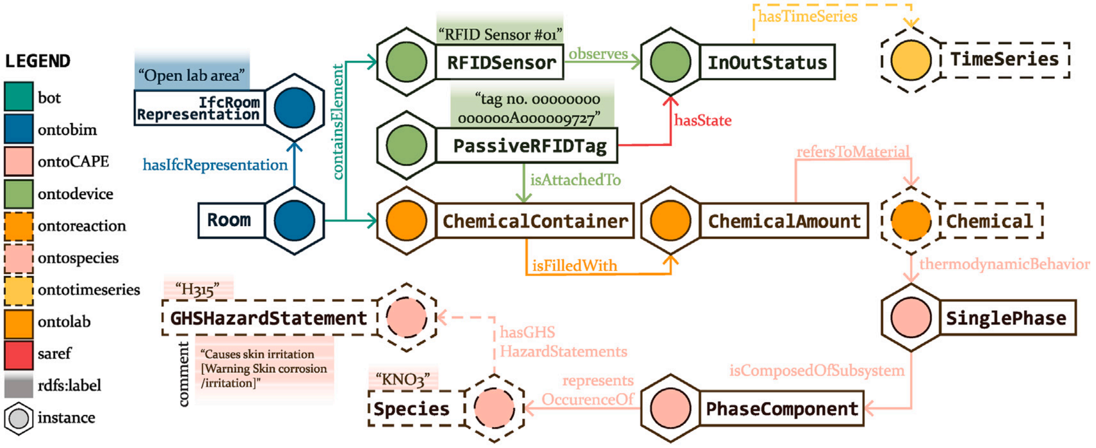
To implement and test location tracking of chemicals via RFID into the DLF, a sample setup was chosen as shown in Fig. 4: An Android `9.0` based 8-port UHF RFID Fixed Reader Writer, along with UHF 902–928 MHz 12dBi RFID Sector Antenna were installed outside of a specially designed metallic cabinet for explosive precursors (Fig. 4(a)). Each of the chemical containers in question were tagged with a UHF 860–960 MHz Frog 3D RFID Tag placed at the bottom of the chemical container (Fig. 4(b)). The reader sends radio frequency signals to the electronic tag through an antenna which receives and returns the signals. In operation, the reader decodes the information embedded in the electronic tag and sends it to the application system for further analysis [27]. If this application system has access to dKG-based digital twins, cross-domain information can be accessed, utilised, and updated in real time. An example is shown in Fig. 4(c): here, existing chemical information on KNO_3 such as the hazard statement (H315) is easily accessed [37] and combined with location data and status information collected by sensors. Additional information on the surrounding facility such as the room the chemical (KNO_3) is located (open lab area), its tag name (RFID Sensor #01), and 3D BIM models of cabinet and facilities [40].

Four key ontologies that were previously developed have been interlinked as part of the development process, namely `OntoLab` [5], `OntoDevice` [40], `OntoBIM` [40], and `OntoSpecies` [37]. This enables the combination and connection of relevant knowledge about location, container, and chemical risk — for example by utilising the previously developed `Email` agent [40] in combination with newly developed RFID agents. The synchronisation between the digital twin and the real world is facilitated through a seamless collaboration



(a) Sample arrangements of the RFID components.

(b) RFID labelling on a chemical container.



(c) ABox snippet for tracking a hazardous chemical container's location with RFID tags.

Fig. 4. Sample setup and corresponding digital twin of the asset tracking use case for explosive chemicals in a laboratory.

among the various agents. At the heart of this synchronisation lies the interplay between the `RFID` and the `RFID Update` agent, working in tandem to ensure real-time data flow and responsiveness. The `RFID Update` agent serves as the bridge between the physical environment and the digital twin by periodically querying the `RFID` agent which receives and manages the continuously streamed data from the RFID reader. This constant influx of data ensures that the digital twin remains updated with the latest information reflecting the state of the physical assets or entities it represents. Complementing this process, the `RFID Query` in turn queries the knowledge graph and retrieves relevant contextual information that serves as the basis for decision-making, in turn triggering desired changes in the real world.

3.2. Managing assets

In a typical research laboratory, there are a huge number of assets, including laboratory equipment, instruments, chemicals, consumables, and samples. Most of them incur a high cost of acquisition. Additionally, recurring mandatory inventory audit exercises can take many hours or even days to check all assets. To improve productivity and ensure optimal use of resources, lab managers and users need to be able uniquely identify these assets and access relevant information quickly. In fact, as shown in Fig. 2, the topic of inventory management has been identified as a key challenge to potentially benefit from further automation. As the number of assets in the laboratory is high, there is a need to use a low-cost technology to label and identify each asset. We have therefore opted to incorporate QR code technology which is widely used in various settings – including laboratories – to improve management and operation [45].

QR codes have been reported in the literature for similar applications in laboratories, but they have been limited in scope and functionality. For example, Shukran et al. [46] used a QR code to tag chemicals for an inventory system but did not provide information on the location or history of the use of chemicals. In a different publication, researchers reported the use of a QR code to replace the spreadsheet-based inventory checking with a web-based application, but it did not allow data interoperability or new updates [47]. For this work, we combined QR code and Semantic Web technology to address inherent data interoperability issues of previous implementations. An `OntoAssetManagement` has been developed as an ontology for representing asset information such as the assignee, location, identifiers such as serial number, manuals, maintenance information, and related purchase documents. Fig. 5 illustrates an extract of these modular ontologies, represented concepts, and linked domains. An accompanying `AssetManagerAgent` has been developed to perform several key tasks involved in the management of assets, including instantiation, QR code printing, and data retrieval. Details of its implementation are given in the Supplementary Information.

In particular, the `OntoAssetManagement` ontology allows the representation of documents involved in the purchase and use of items such as purchase requests, invoices, and manuals. The elements are linked to their physical representations that are located in specific a

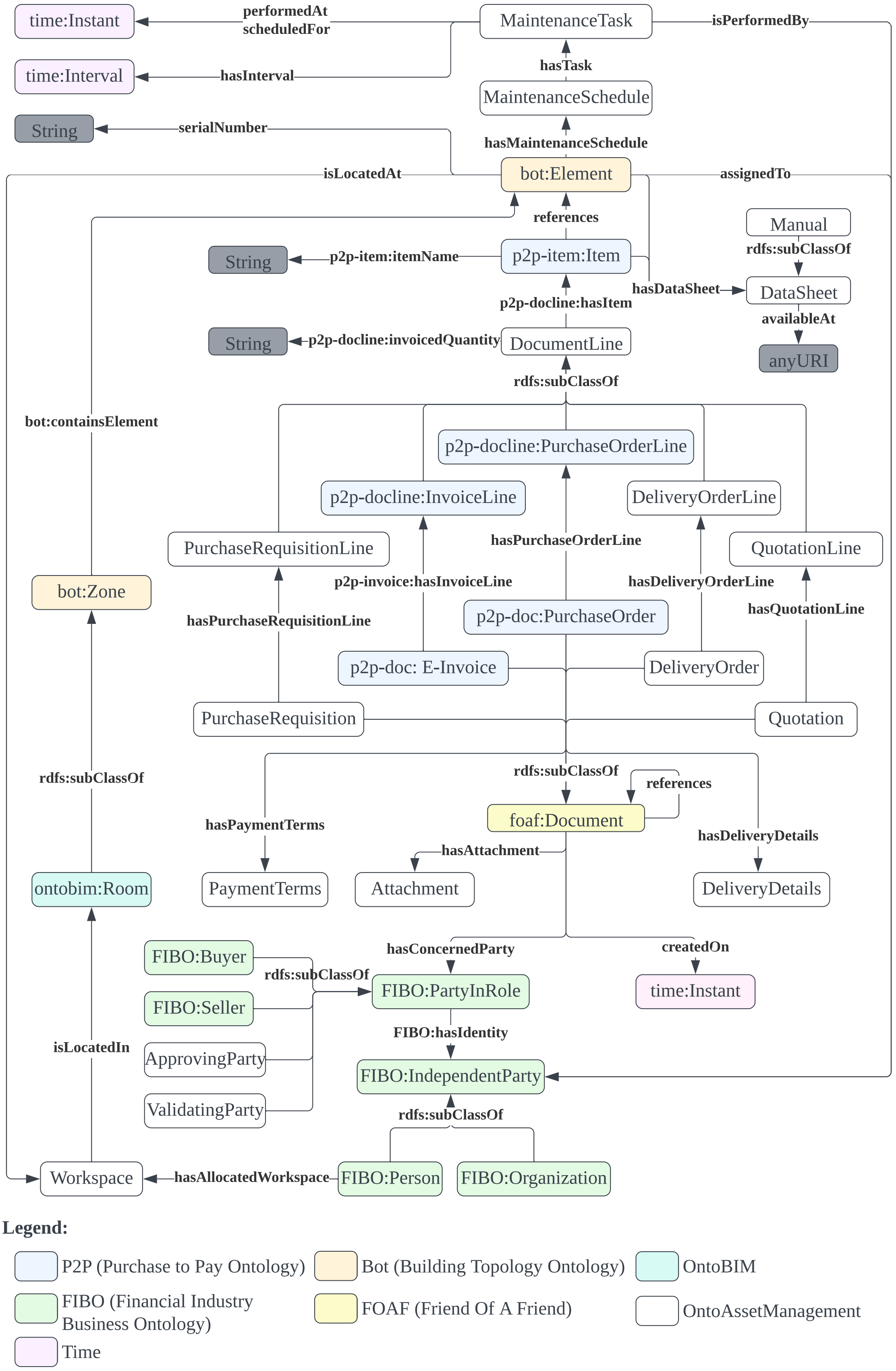


Fig. 5. An extract of the ontology design (TBox) for lab asset management, integrating geospatial, accounting, and research-related information.

room or facility within a building, represented by the `OntoBIM` developed previously. The `OntoAssetManagement` ontology extends and interlinks various existing ontologies, such as `Purchase-To-Pay Ontology` (P2P-O) [48] for the related purchase document concepts, `Financial Industry Business Ontology` (FIBO) [49] for concepts relating to persons and organisations, `Time Ontology` [50] for its time concepts, and `Ontology of units of Measure` (OM) [51] for the concepts relating to its measurable quantities. To the best of the authors' knowledge, this holistic interlinking of various domains has not been done before as the existing ontologies were designed discretely and used exclusively in their corresponding domains. For example, the FIBO is mainly used for the financial industry application while the OM is for the formulation of quantitative knowledge in scientific research. In this work, we interlinked these two ontologies to address requirements for representing an R&D laboratory and related managerial tasks: FIBO provides role concepts related to transactions (buyer and seller), roles in an organisation, and independent roles which are crucial to represent the transactional history of lab assets. Meanwhile, most of the assets in a laboratory are used for scientific research, and they will need to have a concept of what they measure and their units.

3.3. *Mobile interface*

In the management of a research laboratory which can span multiple rooms or even buildings, being able to access relevant information on-the-go helps to ensure ease of access and reduce "downtime". Moreover, many of the manual tasks involved are repetitive such as updating spreadsheets, printing labels, and checking for device information on site. A flexible mobile interface can therefore facilitate user access and interaction, as well as automate repetitive tasks. If this app has access to a dKG such as TWA representing comprehensive digital twins of relevant equipment as introduced earlier, complex tasks and decision-making can be accelerated and supported significantly.

In this work, an Android-based mobile application has been developed within the DLF to facilitate the management of the laboratory. The mobile application has two main functionalities: scanning QR codes to check the asset information and adding new assets along with printing the QR codes. Similarly to the BMS Query mobile application developed in a previous work [40], Keycloak – an open-source identity and access management solution – was used to authenticate and authorise access to the different users for the mobile application. The authorisation code and access token model are implemented by Keycloak based on the OAuth 2.0 authorisation framework (RFC 6749). Keycloak is crucial in the authentication of user login as well as the authentication of users that have rights to access, add, or edit assets, based on their respective role. For this purpose, we extended the ontology used for representing people and their roles based on FIBO [49].

The mobile application has been tested with lab users to ensure that the user experience is seamless, and modification of the user interface has been performed based on their feedback. The application can be adapted to other types of laboratories or organisations as long as the underlying ontologies ensure data interoperability.

4. Exemplary applications

This section presents specific use cases within the DLF that have been targeted to improve workflows related to laboratory management and, more specifically, the challenges identified in Section 2. The Cambridge CARES research laboratory has been used as the model laboratory for these applications. It supports interdisciplinary and cross-domain research initiatives in a variety of fields, such as combustion research, nanomaterial synthesis, electrochemistry, and pilot plants. Given the complexity of facilities, functions, and requirements, the chosen facilities are suitable to test the TWA methodology and devise strategies to manage laboratories across scales.

A generic and all-encompassing digital twin has been developed and applied to this laboratory, including dedicated agents that interact with both the chemistry and facility domains of the laboratory. This has enabled a number of transformation strategies to enhance operations, namely the orchestration of autonomous experimentation [5] and the integration of facility management aspects to ensure more sustainable operations [40]. The applications presented here are part of this work and extend the DT's capacity to represent knowledge and automate tasks relevant for laboratory management.

We present a system for automated tracking of explosive precursors to enhance safety and a mobile app for asset management to accelerate supporting tasks and increase productivity. Implementing these had significant impact on our lab. Table 1 lists some tasks related to lab management that have benefited from the TWA implementation. While these are separate from tasks traditionally associated with lab automation or facility monitoring, the underlying system of connected digital twins can also be used for these as illustrated in the Supplementary Information.

4.1. *Explosive chemicals tracking system*

One key responsibility of laboratory management is ensuring the safety of chemicals stored, especially those that are corrosive, flammable, or explosive. To tackle this challenge, a digital explosive chemicals tracking system has been developed and augmented with cross-domain knowledge from chemistry and facility management. This includes information on the explosive limit and conditions. The generic workflow and interaction between the components in the TWA trilayer for this use case is illustrated in Fig. 6.

The connected DTs mirror the real world situation and enable us to observe the agents and their actions autonomously, updating the dKG accordingly. As shown in Fig. 6, when one of the explosive precursor bottles is taken out of the cabinet, it is registered and recorded by the RFID system and the digital twin is updated by the `RFID Update` agent. If the bottle is not returned in due time, the laboratory manager will be notified by email or mobile application, depending on the hazard level of the respective substance. These interactions between `RFID Query` and `Email` agents for example are possible because all relevant chemical properties and safety data are accessible via chemical's `OntoSpecies` representation [37], which is linked to the bottle contents as shown in Fig. 4(c). The RFID tracking method is not limited to the tracking of just explosive precursors but can be used for any high valued assets.

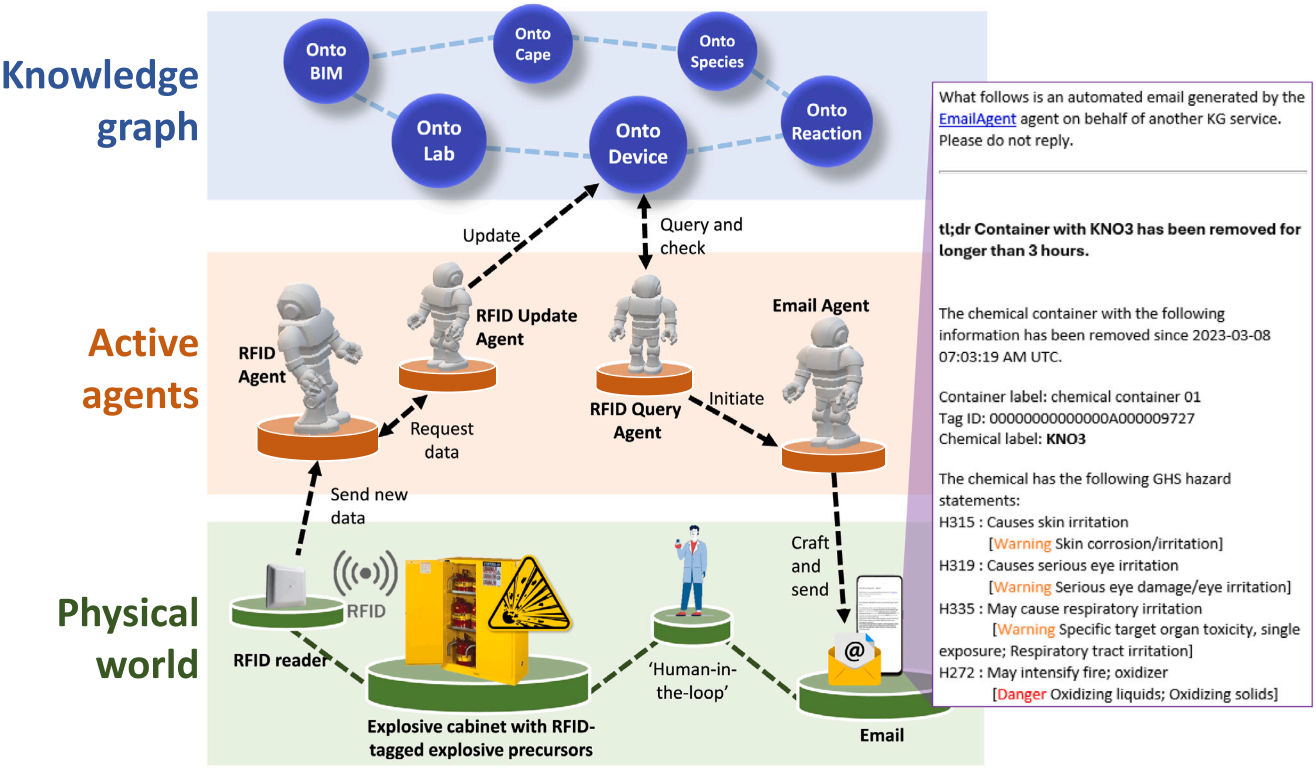
Automating and augmenting lab management tasks in this manner can help improve laboratory safety as it removes some of the potential hazards related to human oversight and forgetfulness. However, this application also presents some new challenges that require further consideration. For example current safety regulations do not allow the installation of electrical devices inside the cabinet,limiting the use of an omni-directional antenna. Another concern is the possible interference of liquids with the RFID signal. Hence, the introduction of self-correcting agents that can keep track of uncertainties and potential error sources is a key area of future development [6]. For the application at hand, this includes finding the best placement of a tag on the bottle as well as ensuring regular system checks to verify the information presented by the digital twin.

4.2. *Mobile app for lab asset management*

In the Cambridge CARES research laboratory and office, over 5000 assets need to be managed, necessitating a comprehensive digital solution to maintain the necessary overview. Furthermore, the processes of adding new equipment to the system and looking up existing equipment in the system need to be streamlined. Hence, we have developed a mobile application, which – together with the underlying `AssetManager`

Table 1
Impact of TWA methodology for three laboratory management tasks.

Scenarios	Conventional methods	New opportunities
Registration of a newly purchased item into the system.	New assets are added to an inventory spreadsheet without validation. An identification tag is then manually printed.	New assets can be registered through the mobile app or online interface. After validation, a QR code is automatically printed, enabling users to later retrieve their information immediately.
Monitoring the explosive chemical usage in a storage cabinet.	Users must manually register their usage in a physical log book which is checked in regular intervals.	RFID-enabled automated tracking system sends an email to the lab manager if hazardous chemical is removed from the cabinet for a prolonged time.
Searching for the manual of a certain lab equipment.	Users search online or look through the manual cabinet for the physical copy.	Using the mobile app to scan the QR code on the asset and retrieve a soft copy of the manual.



What follows is an automated email generated by the EmailAgent agent on behalf of another KG service. Please do not reply.

tl;dr Container with KNO3 has been removed for longer than 3 hours.

The chemical container with the following information has been removed since 2023-03-08 07:03:19 AM UTC.

Container label: chemical container 01
Tag ID: 00000000000000A000009727
Chemical label: **KNO3**

The chemical has the following GHS hazard statements:
H315 : Causes skin irritation
[Warning Skin corrosion/irritation]
H319 : Causes serious eye irritation
[Warning Serious eye damage/eye irritation]
H335 : May cause respiratory irritation
[Warning Specific target organ toxicity, single exposure; Respiratory tract irritation]
H272 : May intensify fire; oxidizer
[Danger Oxidizing liquids; Oxidizing solids]

Fig. 6. Interactions between TWA components within the RFID application.

agent and the `OntoAssetManagement` ontology – allows us to manage all assets via QR codes.

Three key functionalities are present in the mobile application, *i.e.* instantiate device, print code, and scan code. As shown in Fig. 7, all the functionalities for the management of the assets were enabled through the collaboration of the `AssetManager` agent, the `OntoAssetManagement` and the Asset Management mobile application. Fig. 7 illustrates the interactions between the involved components of each TWA layer when executing these key functionalities.

These features constitute a significant improvement compared to the existing Business-As-Usual (BAU) processes: As is common for a medium-sized research laboratory, assets were mostly tracked within a spreadsheet. While some platform-based solutions for special use cases such as equipment booking or maintenance planning were employed, the "master list" of all existing equipment needed to be maintained separately. When acquiring new equipment for example, a lab manager or user would need to manually add a row to the database with all relevant information, determine a new identification number based on naming conventions, accurately key in this code, and print a label. Within this process, numerous potential error sources exist: the rigid structure of a rectangular database might prevent recording an important property specific to an equipment; an edit in the "master list" might not be enough as the same asset needs to be added or updated across different systems; the unique identifier on the label might be erroneous; *etc.*. With the implementation of the presented solution, error sources are reduced and process time accelerated. For example, the dKG structure inherently ensures consistency of new or changed equipment properties throughout different applications and an automated agent takes care of printing a unique label.

One of the most tedious BAU processes was retrieving asset information such as purchase history, manufacturer specifications, or usage instructions. As shown in Fig. 8, this often included performing searches on the internet, manually checking the inventory list,asking other people, or searching documents in a cabinet to obtain information. With the asset management mobile application, it requires the user to scan the QR code and all the relevant information is made available instantly. The equipment queried in Fig. 8 is a liquid handling autosampler and part of an autonomous experimentation setup [5] with linked information about technical specifications, current location, and assigned lab users.

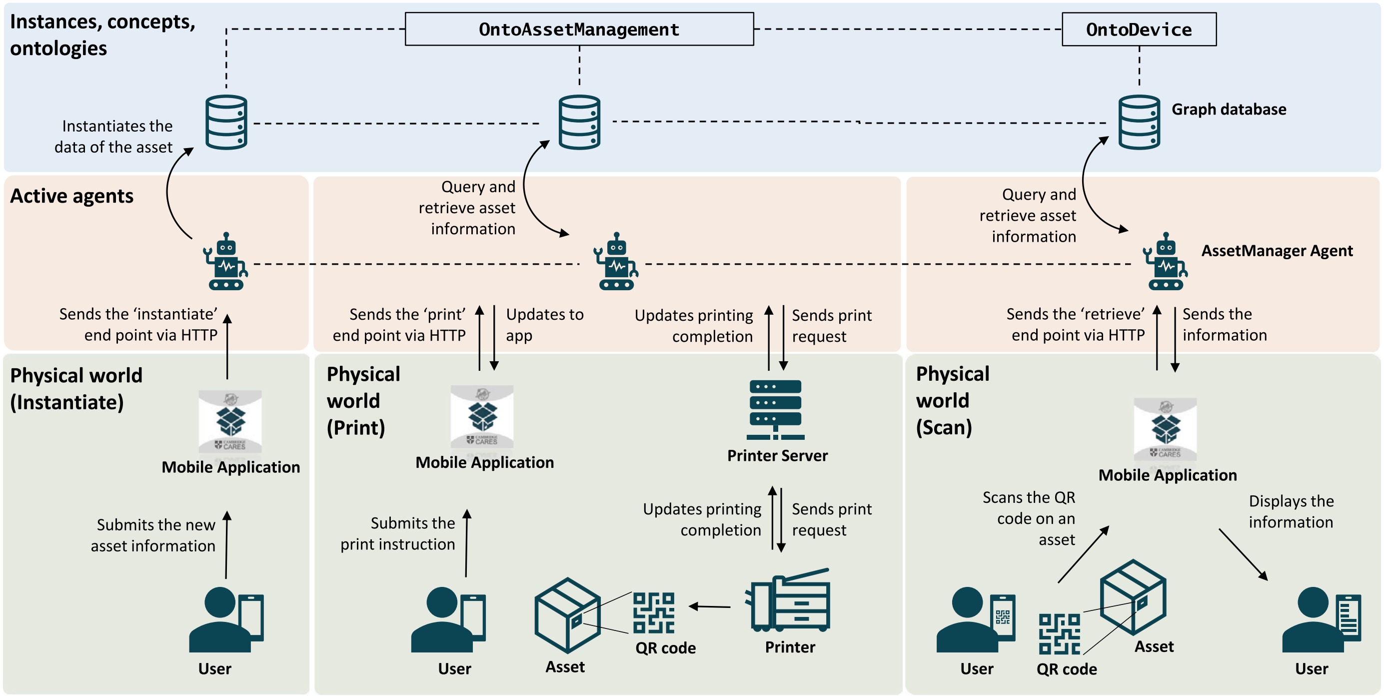


Fig. 7. Interactions between TWA components within the asset management application. The different coloured rows represent the TWA layers as introduced in Fig. 1 while columns represent a key functionality each.

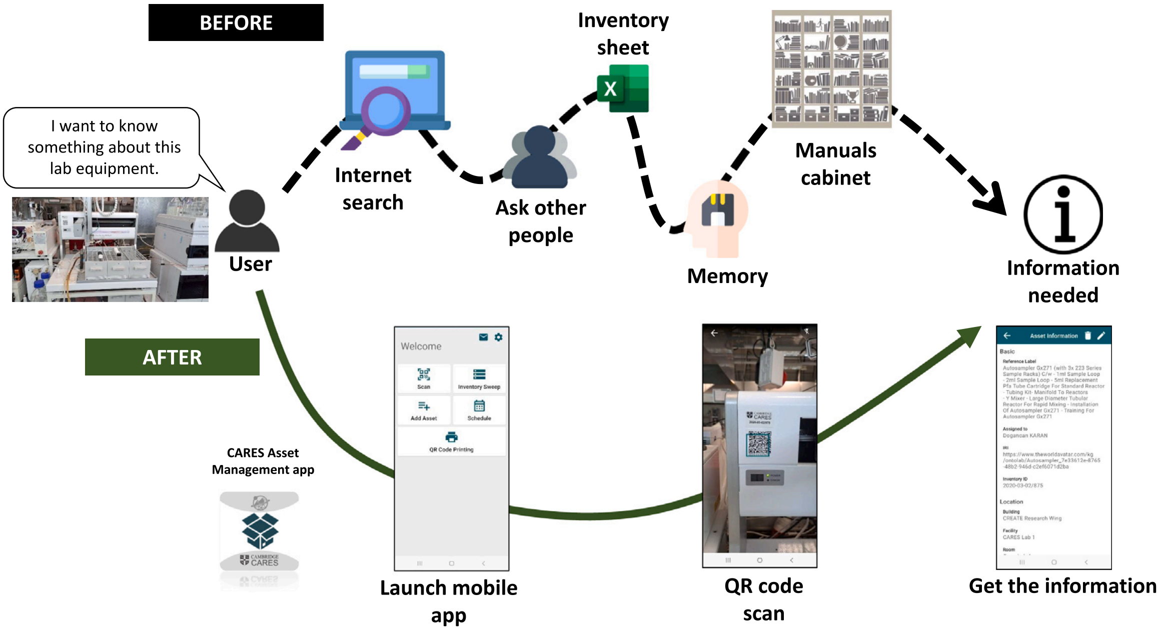


Fig. 8. A comparison of user flow for looking up equipment information before and after the implementation of the DLF-based asset management mobile application.

5. Conclusion

The advancement of automation in laboratory management is crucial to ensure lab users' safety while providing optimal research support. However, available digital solutions are often fragmented and kept separated from information and data around actual research. To and ultimately realise the vision of an "AI scientist"[41], we harnessed the power of the Semantic Web and developed ontologies, agents, and digital tools for the digitalisation and automation of laboratory management as part of The World Avatar, an all-encompassing digital twin. The modular flexible ontologies developed are able to link knowledge across domains and support data granularity across different scales from chemistry and molecules to lab equipment, room, and facility level. We have shown two use cases that address crucial challenges in the management of research laboratories, *i.e.* keeping track of hazardous chemicals such as explosive precursors and managing laboratory assets via a mobile application offering a unified user interface.

The gradual implementation of the proposed "Digital Lab Framework" [6] in our model laboratory demonstrates the value of interoperability between different technologies and systems that not only address existing challenges but also enhance the accessibility and convenience for laboratory management operations. Software systems and information can be connected within the agent ecosystem to enable new modes of interaction. The integration of RFID tracking with an autonomous email agent serves to automate tracking of critical assets, which is often still based on manual paper-based procedures. For the asset management use case, the unique resource identifiers of the dKG were coupled to QR codes with which relevant attributes, digitised documents, and environmental information of assets can be made instantly accessible. The accompanying mobile application provides a one-stop platform to support laboratory managers and users in their daily routines.

Further implementation of the DLF will continue to address different challenges of laboratory management such as access management, maintenance, and procurement. Consequently, key stakeholders in laboratory management can better focus on core tasks that require sophisticated attention such as decision making, innovation, and problem solving. This shift will be facilitated by the development of further sophisticated tools aimed at automating and simplifying researchers' workflows. For example, we aim to automatically provide researchers with Safety Data Sheets for the chemicals they are working with or exposed to. Expanding on the presented work on digital twins, a semi-automated system to track chemical inventories could even account for reagent loss when using certain equipment or processes.

Another integral aspect of future work will involve extending the resource planning capabilities within DLF. This expansion will entail integrating ERP systems and tracking changes in our asset management system, (e.g., via timeseries). In addition, this will enable automating regulatory compliance and certification processes, which are usually very time-consuming aspects of lab management. Consequently, by expanding the underlying knowledge model with more comprehensive and interoperable digital twins will facilitate collaboration between facility managers [40], laboratory managers, researchers, technicians, and robots [5]. Ultimately, a fully connected and intelligent system for holistic lab automation will enhance the efficiency, quality, and innovation of scientific research with Semantic Web technology.

CRediT authorship contribution statement

Simon D. Rihm: Conceptualization, Formal analysis, Investigation, Project administration, Visualization, Writing – original draft, Writing – review & editing. **Yong Ren Tan:** Investigation, Project administration, Supervision, Visualization, Writing – original draft. **Wilson Ang:** Data curation, Methodology, Resources, Software, Validation, Writing – original draft. **Markus Hofmeister:** Methodology, Software, Supervision, Writing – review & editing. **Xinhong Deng:** Methodology, Software, Visualization, Writing – original draft. **Michael Teguh Laksana:** Data curation, Formal analysis, Software, Visualization, Writing – original draft. **Hou Yee Quek:** Conceptualization, Methodology, Resources, Software, Visualization, Writing – original draft. **Jiaru Bai:** Formal analysis, Methodology, Validation, Writing – review & editing. **Laura Pascazio:** Methodology, Software, Supervision. **Sim Chun Siong:** Methodology, Validation, Writing – review & editing. **Jethro Akroyd:** Funding acquisition, Project administration, Supervision. **Sebastian Mosbach:** Conceptualization, Funding acquisition, Supervision, Writing – review & editing. **Markus Kraft:** Conceptualization, Funding acquisition, Methodology, Project administration, Supervision.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Declaration of Generative AI and AI-assisted technologies in the writing process

During the preparation of this work the authors used ChatGPT in order to enhance the readability and language of the manuscript. After using this tool, the authors reviewed and edited the content as needed and take full responsibility for the content of the publication.

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Appendix A. Supplementary data

Supplementary material related to this article can be found online at https://doi.org/10.1016/j.slast.2024.100135.

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