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Researchers' perceptions of automating scientific research

David M. Douglas[1]

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Abstract

Science is being transformed by the increasing capabilities of automation technologies and artificial intelligence (AI). Integrating AI and machine learning (ML) into scientific practice requires changing established research methods while maintaining a scientific understanding of research findings. Researchers are at the forefront of this change, but there is currently little understanding of how they are experiencing these upheavals in scientific practice. In this paper, we examine how researchers working in several research fields (automation engineering, computational design, conservation decision-making, materials science, and synthetic biology) perceive AI/ML technologies used in their work, such as laboratory automation, automated design of experiments, computational design, and computer experiments. We find that researchers emphasised the need for AI/ML technologies to have practical benefits (such as efficiency and improved safety) to justify their use. Researchers were also hesitant to automate data analysis, and the importance of explainability differed between researchers working with laboratory automation and those using AI/ML directly in their research. This difference is due to the different role AI/ML plays in different research fields: laboratory automation performs processes already defined by the researcher and the actions are visible or recorded, while in AI/ML applications the decisions that produced the result may be obscure to the researcher. Understanding the role AI/ML plays in scientific practice is important for ensuring that scientific knowledge continues to grow.

Keywords Laboratory automation · Computational design · Simulation · Science · Computer experiments

Scientific research and experimentation involve considerable human effort in performing experiments, collecting data, and data analysis (Sozou et al. 2017). The increasing capabilities of artificial intelligence (AI), machine learning (ML), and other forms of automation are increasing the opportunities to assist or even replace human scientists in performing research. AI/ML is already being used across various sciences for a variety of purposes (Hajkowicz et al. 2022; Simon 2022; OECD 2023). It may be used for managing research literature, interpreting data, and automating experiment design and practice (Hastings 2023). Automating science may also contribute to research reproducibility, as the digitalisation of research data enables more data to be recorded during the research process (Hastings 2023).

As automation may be as disruptive to science as it is to other domains, it is important to understand how researchers themselves see automating science as affecting themselves and their work. Previous research has examined how university academics perceived the potential impacts of AI on research in university settings (Chubb et al. 2022), and the impacts of adopting laboratory automation in the life sciences (Holland and Davies 2020). In this paper, we present a snapshot of how researchers working for a national science agency in several fields (automation engineering, computational design, conservation decision-making, materials science, and synthetic biology) perceive automation in their work, including its benefits and pitfalls. The forms of automation discussed include AI/ML, laboratory automation, and computational design. The participants include researchers who use forms of automation in their work and those involved in developing automation systems for scientific use. This diversity of research domains provides an opportunity to compare how researchers in different fields perceive automation and to identify common benefits and concerns that occur across research fields and automation technologies.

✉ David M. Douglas
david.douglas@csiro.au

[1] Responsible Innovation Future Science Platform, CSIRO, Canberra, Australia

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The paper begins with a brief overview of how AI/ML may be used to automate science, followed by a summary of the potential impacts that automating research practice may have on science itself. We then describe the methodology of our study into how researchers from several research fields perceived the impact of automation on their work. The fields represented by participants in our study are automation engineering, computational design, conservation decision-making, materials science, and synthetic biology. We then describe the findings from our interviews with these researchers. We then discuss two significant themes we identified in the participant interviews: the difference in importance given to the explainability of AI/ML given to its use in laboratory automation and in using AI/ML for prediction, and the emphasis participants placed on maintaining a 'human-in-the-loop' in scientific research. After a summary of the limitations of this study and potential directions for further research, the paper concludes with a summary of our findings.

1 Automating science

Automation is the application of technological devices to serve as substitutes for human actions and decisions (Nof 2009). We define science automation broadly as the use of automation to perform tasks that would otherwise require human researchers to perform. Science automation ranges from automating mundane research tasks such as pipetting to autonomous 'robot scientists' that automate the process of generating hypotheses, designing and performing experiments, collecting and analysing data, and updating its model of the phenomena being studied based on this analysis (Sparkes et al. 2010).

Automating science draws heavily on AI and ML. AI is the use of computer technology to make decisions and perform tasks that otherwise require a human to perform them (Mitchell 2019). ML systems are a form of AI that identifies patterns within training data and makes predictions about new data presented to them based on these patterns (Alpaydin 2021). Robots and cyber-physical systems use AI to monitor their surroundings and to make decisions about the appropriate action for that system to perform (Rajkumar et al. 2010; Jordan 2016). Specific applications of AI and ML that may be used to automate science include (but are not limited to):

- Computer experiments (or 'in silico' experimentation): using simulations to test models and designs.
- Design of Experiments (DoE) with ML: systematically performing experiments and analysing experimental results to determine where further experiments are required.
- Data analysis: analysing data to classify samples, identify patterns, or highlight unexpected features.
- Generative AI: using AI/ML to generate new text, images, designs, and data based on a set of specified requirements.
- Robots: remote-controlled or autonomous systems used for scientific applications.
- Laboratory Automation: the use of robots and cyber-physical systems to perform laboratory work that would otherwise require humans to perform.

Simulations are representations or models of target systems, which may be empirical, theoretical, or imaginary (Durán 2018). Computer simulations may be used to represent and communicate knowledge, predict future events, or gain a better understanding of the simulated system (Winsberg 2022). They may also be understood as primarily a means of finding solutions to the system model within the simulation (the problem-solving perspective) or as a means of describing the simulated system (the description of patterns of behaviour perspective) (Durán 2018). From the problem-solving perspective, a simulation is a means of solving formal models that cannot be solved using analytic methods (Durán 2018). From the description of patterns of behaviour perspective, a simulation may be studied as a proxy of the simulated system, and insights gained from studying the simulation are applicable to the original system (Durán 2018).

Computer simulations may be considered a form of research automation if the simulation is used as a substitute for physical experimentation, as the description of patterns of behaviour perspective suggests. This may also be called in silico experimentation (Winsberg 2010). The simulation effectively automates both the system or phenomena under investigation and the data collection from experimenting on it.

Two approaches to experiment design are One Factor at A Time (OFAT)[1] and statistical Design of Experiments (DoE) (Gilman et al. 2021). OFAT experiment design changes one variable in a process or system and then measures any differences in that process or system (Gilman et al. 2021). DoE is a statistical methodology that systematically and simultaneously changes multiple variables in a process or system to observe how these variables interact (Gilman et al. 2021). The empirical data gained from these experiments may then be used to develop statistical models that suggest new experiments to further optimise the output of the tested process or system (Gilman et al. 2021). ML may be used

[1] One Variable At a Time (OVAT) is another name for this approach (Antony 2023).

to further analyse the data collected using a DoE approach (Fontana et al. 2023).

A challenge in modern science is processing the volume of data collected by digital instruments (Hastings 2023). In astronomy, for example, catalogues of astronomical data contain terabytes of data, and modern instruments such as the Square Kilometre Array (SKA) can collect petabytes of data per year (Sen et al. 2022; Scaife 2020). AI/ML methods make it possible to gain insights and make predictions from this volume of data (Fluke and Jacobs 2020). AI/ML has similarly been applied in sciences ranging from archaeology (Mantovan and Nanni 2020) to wildlife conservation (Tuia et al. 2022).

Generative AI uses AI/ML methods to create new text, images, data, designs, and other artefacts based on input data. Large Language Models (LLMs) that use statistical patterns identified in large amounts of training data to generate new data for a specific purpose are the most prominent form of generative AI (Morris 2023). Scientific applications for LLMs include creating educational materials, creating synthetic data (data that shares the attributes of actual data without being actual data itself), performing literature reviews, generating software source code, and assisting in writing scientific papers (Morris 2023). Another form of generative AI are evolutionary algorithms, which use models of evolutionary processes to generate a range of potential solutions to a specific problem, compare how well the potential solutions solve the intended problem, and combine the most effective solutions to create a new set of potential solutions (Eiben and Smith 2015). Evolutionary algorithms are particularly suited for solving optimisation problems, such as creating designs for physical objects with specific performance characteristics (Eiben and Smith 2015).

Robots are machines with sensors that make decisions to perform physical actions based on the input of these sensors (Jordan 2016). Robots may be either stationary (fixed in one location and capable of performing work within a defined area) or mobile (able to move around) (Thurow and Junginger 2023). Mobile robots, including drones and autonomous underwater vehicles (AUVs), may be used for environmental monitoring (van Wynsberghe and Donhauser 2018; Bogue 2011).

Stationary robots and other cyber-physical systems may be used for laboratory automation, where they perform roles such as sample processing, liquid handling, and controlling and analysing laboratory processes (Thurow and Junginger 2023). The degree of laboratory automation may be described as a series of levels, ranging from no automation to full automation, as listed in Table 1 below (Holland and Davies 2020). Note that these levels of automation (except level 7) concern the physical functions of the laboratory process. Human researchers still perform the design of experiments and data analysis.

Level 7 laboratory automation systems may be called autonomous experimentation platforms or 'self-driving laboratories'. These systems use ML algorithms to select experiments which it then performs using the laboratory hardware connected to the platform (Abolhasani and Kumacheva 2023; Martin et al. 2023). The platform gathers data from its experiment and this data is used to update its ML model, and the updated model is then used to select new experiments to perform (Abolhasani and Kumacheva 2023).

Autonomous experimentation platforms are intended to perform autonomous scientific discovery and to serve as 'robot scientists', where automation technology can perform every step of the research process (Sparkes et al. 2010). Autonomous scientific discovery systems would be able to create hypotheses that explain observations, test these hypotheses by designing and experiments, interpreting the results of these experiments, and repeating this process in light of the new data it has acquired (King et al. 2018).

2 Automation and science

The potential impact of adopting automation into scientific practice may be considered by reflecting on the purpose of science itself. Science has two complementary goals: epistemic and practical. The epistemic goal (or intellectual view) of science understands its purpose as gaining

Table 1 Levels of Laboratory Automation (from Holland and Davies 2020)

Automation Level	Description	Examples
1	Fully manual work	Glass washing
2	Manual work with a static tool	Screwdriver, scalpel
3	Manual work with a flexible hand tool	Adjustable spanner, pipette
4	Manual work with an automated tool	Power tool, handheld dispenser
5	Machine designed for a single task	Lathe, centrifuge
6	Machine that may be reconfigured to perform different tasks	CNC (Computer Numerical Control) machine, motorised stage microscope
7	Fully automatic system	Autonomous system

knowledge and understanding of the world (Resnik 1998; Humphreys 2020). The practical goal or view sees science as offering the means for predicting and manipulating the world (Resnik 1998; Humphreys 2020). These goals will often overlap as research may be intended to satisfy both these goals.

A concern about automating science is the potential epistemological impact: human scientific knowledge and our ability to use it effectively will be negatively affected if human researchers no longer perform scientific practices (Humphreys 2020). This is particularly true if we accept the intellectual goal of science as being our best means of gaining knowledge and understanding the world, which places an anthropocentric constraint on scientific explanations (i.e. explanations must be capable of being understood by humans) (Humphreys 2020). To illustrate this point, consider the difference between scientific discovery and scientific understanding: new discoveries made possible by opaque ML systems may be scientific discoveries, but as the ML system is opaque, these discoveries do not (on their own) provide new scientific understanding (Krenn et al. 2022).

Humphreys (2020) identifies four concerns relating to the impact of automation on science:

- Understanding: if researchers do not understand how automated science works, it may reduce our understanding of the world.
- Error: the likelihood of errors will increase if humans do not understand the science they are using.
- Application: the applications of science may be reduced if humans do not understand science.
- Creativity: science requires creativity that is impossible to reproduce in automated systems.

The first three aspects relate to the significance of human involvement in scientific practice: the benefits of science are reduced if human involvement in scientific practice is reduced or removed. A useful parallel can be drawn here with the interest in explainable AI (XAI), which is often motivated by concerns about trustworthiness and accountability (Mittelstadt, Russell and Wachter 2019). Like the use of AI/ML in other contexts, scientists may be less likely to trust the output of AI/ML systems if they do not understand how the system operates.

The concern about creativity can be traced back to early work in computation and the question of whether computer systems would be able to produce creative work (Turing 2004; King et al. 2018). Generative AI itself is a response to the objection that computer systems cannot be 'novel' or 'creative'. For example, evolutionary algorithms often provide surprising and non-intuitive solutions to specified problems (Lehman et al. 2020).

3 Methods

3.1 Participant selection

We used purposive sampling to identify researchers using forms of research automation within a national scientific research organisation. We initially sought participants from the fields of industrial design, synthetic biology, and conservation decision-making, as these fields incorporate a range of science automation methods (computational design, laboratory automation, and computer experiments, respectively). The industrial component design incorporates various fields, such as materials science and generative AI. Synthetic biology is the deliberate creation of new living systems (Davies 2018). It uses AI/ML to design experiments to develop and refine new biological systems and components. Conservation decision-making uses simulations of environmental conditions and wildlife populations to test different approaches to managing environmental risks.

Potential participants were invited to participate in this study via email. We used snowball sampling to expand the pool of potential participants by asking participants if they could recommend others whose work might be relevant to this study (Patton 2015). As a result, our sample also included researchers in materials science with experience in using laboratory automation, and automation engineers who implement laboratory automation systems for researchers. This reflects the prominence of 'in-house' development of laboratory automation (Holland and Davies 2020; May 2019).

We conducted 18 interviews with researchers between November 2022 and May 2023. The distribution of participants between application areas was automation engineering (4), computational design (3), conservation decision-making (4), materials science (4), and synthetic biology (3).

3.2 Data collection

The interview questions covered the participant's experience, how automated science affects the role responsibilities of researchers, the trade-offs and risks of automating science, and the broader impacts of automated science.

The questions were arranged into four groups: *experience*, *science role responsibilities*, *role trade-offs and risks*, and *impact responsibilities*. The experience questions asked participants to describe their current role and how long they had been active within their research field. The science role responsibilities questions asked participants to describe the applications of research automation they were involved in, what they believed to be the purpose of this automation, and how it affected their role as a researcher. The role trade-offs and risks questions asked participants to explain how decisions about whether to use automation in their research were made, whether there were any trade-offs that accompanied the use of research automation, and what they believed to be the risks of adopting such automation. Finally, the impact responsibilities questions asked participants about other applications of research automation that they were aware of or could foresee, and how research automation affected the end-users of research.

Each participant gave informed consent before the interview. Interviews were conducted using the Webex videoconferencing platform (Cisco 2023). If the participant gave permission, the interview was recorded and transcribed for analysis; otherwise, the interviewer took notes which were used for analysis. Interview notes and transcripts were anonymised before analysis by assigning a number to each participant interview (P1-P18).

Interview transcripts were analysed using reflexive thematic analysis (Braun et al. 2019). To code the data, portions of the interview transcripts were assigned to codes describing a specific theme within the text (Braun et al. 2019). NVivo software (released in March 2020) was used for coding the data (QSR International Pty Ltd. n.d. 2020). 343 codes were identified in the data. Similarities in the content of the codes were used to group them together into broader themes. After the initial reviews of the data, the responses from participants P10 (materials science) and P11 (conservation decision-making) were removed as their responses focused on commercial applications of automation rather than the use of automation in scientific research or did not refer to research automation methods or AI, respectively.

4 Findings

The applications of research automation discussed by the participants are automation engineering, computational design, conservation decision-making, materials science, and synthetic biology. Automation engineering is the development and implementation of laboratory automation systems. Materials science investigates the relations between the properties of materials and their molecular structure and composition (Mercier et al. 2003). Table 2 presents the distribution of participants between these applications, and the participants' responses are described below.

4.1 Automation engineering

The participants categorised as automation engineers are researchers who develop and implement methods of laboratory automation for their own use or for other researchers. They saw their role as increasing the efficiency of laboratory researchers, without necessarily requiring them to adopt complete laboratory automation systems. P3 explained that they seek to "provide the ability to have things run in an automated fashion, in a safe and automated fashion, and then have them report to a centralised place so [the researcher] can log in from any location and control and watch the system". P5 described their goal as "being to try to create an ad hoc ecosystem where chemists and material scientists […] can set up a robot with minimal effort to automate some of the tasks that they need to on an as-needed basis rather than having a bespoke million-dollar platform to do things."

The benefits of adopting laboratory automation included automating tedious tasks (P3), greater efficiency (P3), allowing multiple experiments to be performed simultaneously (P5), increased throughput (P7 and P8), and the greater speed with which research may be performed (P8). As P8 observed, *"robots can work 24/7 and a human scientist can't"*. Laboratory automation also allows for experiments

Table 2 Distribution of participants and forms of research automation across automated science applications

Application	Description	Participants (N = 16)	Forms of research automation discussed
Automation engineering	Developing automated systems for use by researchers	P3, P5, P7, P8	Laboratory automation, automated data analysis
Computational design	Using AI and ML to create novel designs of physical objects	P6, P9, P15	Computational design, simulation experiments
Conservation decision making	Using AI and ML to simulate the effects of potential environmental decisions	P2, P4, P12	AI/ML, Automated Design of Experiments (DoE)
Materials science	Using laboratory automation to perform experiments in material development	P13, P14, P17	Laboratory Automation, Automated Design of Experiments (DoE)
Synthetic biology	Using laboratory automation to perform experiments in developing new living systems	P1, P16, P18	Laboratory Automation

to be performed at scale (P5 and P8). As P8 explained, *"instead of having a scientist in a fume hood that's maybe doing one or two reactions in a day, we can set up tens or hundreds"*. Reproducibility was also mentioned as another purpose for adopting laboratory automation (P5 and P7).

Laboratory automation was also perceived by automation engineers as being about making the best use of the researcher's skills. Laboratory automation allows researchers to spend more of their time and effort in planning experiments and planning the analysis of the experiment data (P3 and P5). Similarly, P7 noted that laboratory automation has the potential to move research bottlenecks from conducting experiments to analysing data.

P5 and P8 mentioned safety as a motivation for adopting laboratory automation. The safety benefits described included reducing repetitive strain injuries (P5), reduced exposure to hazardous materials (P8), and performing monotonous tasks for long periods of time (P5).

P7 noted that laboratory automation creates a need for more diverse technical expertise in research teams and that researchers require more technical knowledge to use the technology effectively and to possess skills for equipment maintenance. As P8 observed, *"just having to manage these big pieces of kit as opposed to just in a lab environment where it's really quite simple stuff, […] that was a big change for us"*. P8 also observed that automation has brought them into greater contact with experts in ML.

P8 observed that explainability is not necessarily required for AI to be used for automating science:

> *…philosophically a lot of scientists still have trouble with the concept of doing robotics and high throughput experimentation because their argument is, well, you don't understand what you're doing, so you're just randomly trying to do things. That's their perception, which isn't the reality. There is a lot of science that we do where you can't empirically predict what you are going to find and see (P8).*

All four automation engineers (P3, P5, P7, and P8) noted that laboratory automation had to provide a practical benefit to be worth adopting. Researchers may have unrealistic expectations of what laboratory automation is capable of, and part of the automation engineer's role is working with researchers to determine where adopting automation in laboratory processes will be most effective (P5). P5 described, *"[i]f it makes more sense to do something manually as part of the process, then we'll do that"*. P8 noted that the time and effort needed to implement automation must be considered against the benefits it will bring. P3 made a similar point: *"the classic trade-off is the time, energy and money put into a new, novel process […] and whether the payoff is worth it, or whether you're automating for the sake of automating"*. Researchers may also be reluctant to adopt laboratory automation as they are satisfied with their current methods (P8). The cost of laboratory automation was also an important factor in deciding whether to adopt it (P8). P5 also noted the costs of the necessary infrastructure for laboratory automation.

P7 and P8 mentioned technical risks with laboratory automation. P7 noted that the technical risks of automating research procedures mean that the benefits may be uncertain. As P8 explained, *"The biggest risk is that we fail, that we should be able to do something and then we just go, no, we just can't get this to work in the robot. That's the biggest risk is that a task that they want to do won't work"*. Errors in the automated process may also compound (P7).

Both P3 and P5 mentioned the importance of maintaining a 'human-in-the-loop' in laboratory automation. P5 observed that *"they're not going to completely replace our base level technicians and chemists"*. However, they also noted that automated laboratory processes may reduce the opportunities for researchers to make serendipitous discoveries during these tasks:

> *[T]he robots allow us to speed things up, explore a particular experimental space very quickly, but they're not always able to see the minute changes that might occur. […] I guess the limitations are that sometimes you could miss quite minute but incredibly important details by automating the process (P5).*

Automated laboratory equipment may fail (P5). P8 also noted that laboratory robots may not be as accurate as human experimenters. Nonetheless, P5 observed that the risks of automation are outweighed by their benefits.

In addition to laboratory automation, two automation engineers (P7 and P8) also discussed automated data analysis. P7 mentioned data analysis as one part of research practice that they would be unwilling to automate. P8 also raised concerns about the quality of automated data analysis: *"when you have automated data analysis, a lot of algorithms, you get some information out of them but how biased are they, how accurate, how reproduceable are they?"* False positives and false negatives are another concern (P7).

4.2 Computational design

The use of computational design and simulations offers researchers and engineers the capability to automate the design of physical items (P6 and P15). Computational design allows researchers and engineers to *"investigate designs that quite possibly a human wouldn't think of"* (P9). P15 explained the methodology using a hypothetical example:

> *Our algorithm spits out 10 designs for wind turbine blades, we put them into a fluid dynamic simulator which simulates the airflow and the effects of the*

airflow on those blades as they rotate and generate energy. At the end of that simulation, we can gather a load of statistics about how those blades have performed. (P15)

This information is used as input for the AI algorithm to generate a new set of possible designs, which can also be assessed for performance, and so on until the designs meet the desired performance requirements (P15).

For simulations, there are trade-offs to be made between the complexity of the model needed to simulate a system, and the time and computational power available to run it (P9). As P9 elaborated:

it just might be too complex a system, and you've always got to simplify your model to reality. So always your model will not be an exact digital twin or replica of the reality, and you've really got to understand what are the important things you are modelling, what are you missing out on? And those things that you are missing out on, will they actually affect […] the computational solution? (P9)

Determining the variables in a system that are important to model requires collaboration between experimenters and computational modellers:

[w]e [computer modellers] try to understand what their [the experimenters'] process involves, and they will try to explain to us what are the limitations, what are the variables, what are the parameters that control the particular application they're looking at (P9).

During the process of creating designs and testing them in simulations, the researchers will occasionally create physical replicas or scale models of the designs to physically test them, and this information can be used to make the simulation models more accurate (P15). This is necessary as designs created using computational design and tested in simulations may not perform as expected in physical testing (P6). Experimental verification is necessary to mitigate this risk and to ensure that the simulation results are valid (P9). P15 also explained that the physical handling of the replicas or scale models for testing could also be automated, but that this would be expensive and have little research benefit. P15 observed that there would be significant startup costs to establish the necessary infrastructure to combine computational design and simulation with physical experimentation for verification.

It is also important for researchers to be able to trust the automated systems they use:

The main change in automation is we need to be careful of, or we need to question - always be wary of the results that are coming out of automation. But not necessarily just discard […] what might seem contradictory or contrary results, but understand […] whether they are correct or not, and really understand what is coming out of the automated workflow (P9).

P6 stated that computational design does not change the responsibilities of researchers:

Since you're still doing the experiment anyway, in that sense we are still responsible for the final design, because now there is the computer playing a part as well. But humans still take the full responsibility that this is indeed doing the job as intended (P6).

4.3 Conservation decision-making

The researchers involved in conservation decision-making discussed how they used AI and ML as decision-support tool. *"I use AI to suggest methods that we can […] better plan conservation decision-making actions. But they're not really replacing; they're really designed to augment or support people rather than replace the decision maker or take humans out of the process"* (P4). AI is used as a forecasting tool to predict the expected costs of managing the population of endangered species or the costs of managing the land where endangered species can be found (P12). The larger scale of data gathered also makes it difficult for researchers to process and understand without machine learning (P12).

P4 and P12 raised efficiency as a benefit of using AI and ML. As P4 explained, *"we have limited resources for conservation and we want to use them as efficiently as possible"*. P12 observed that *"[p]rocesses can be made quicker and more efficient and more accurate and I have especially seen this in AI and machine learning"*.

Researchers also mentioned the potential risks of using AI and ML. As P2 explained: *"I think we are limited in our ability to model everything in an AI system. That's the danger. We need humans at every step, to check"*. Biases may also exist in the data that may compromise AI/ML decisions based on that data (P12). AI/ML models where sufficient data is unavailable may rely on expert opinions in developing their models, and biases may be present in these opinions (P4 and P12).

P4 and P12 both observed that explainability was important to researchers who use AI in their work. P4 emphasised the importance of explainability for fostering trust in the recommendations of the AI/ML model:

The other challenge we have is the optimisation spits out a complicated thing that's really easy for a machine to run through, but it looks like gobbledygook for a human and it's really hard to produce a sensible outcome from it. So we often have spent time trying to build heuristics or rules of thumb that peo-

ple will go, oh yeah, that looks about right, because without that they don't trust the outputs (P4).

However, there is a trade-off between the explainability or interpretability of an AI/ML model and its performance:

In our research, we ask, how interpretable do you want the solution to be? Once we have this information, we tell the managers, okay, that level of simplicity means that should be 10 per cent less performance; you'll perform 10 per cent less well than the optimal version. But, for 10 per cent, this is the best we can do. For this loss of performance, this is the most interpretable (P2).

Working with environmental managers is also important to encourage them to adopt the recommendations produced by the AI/ML model:

…they [environmental managers] don't like having something that they're told is optimal. They don't like having their agency taken away. You can only include certain assumptions in your models, that usually you're solving for one objective, for example. But there's always competing objectives and things that are not in the model, so you really need a person as well. We've been trying […] to incorporate different values, multiple objectives, and just make our optimisation algorithms more flexible over time so that we can better incorporate what people actually want from them. Because in practice often they don't use the results, they'll just say, oh that's good and they sort of take the vibe, which is not really very satisfying when you've done a whole bunch of work to optimise something (P4).

Another trade-off is between the cost of developing and using AI and the benefits of using it:

Using AI and using machine learning involves some initial investment; in hardware, in software, not only hardware and software, not only material things, but also in expertise and training, like having experts of people who works and understands about machine learning and artificial intelligence but it can also result in a long-term cost saving (P12).

P12 discussed the importance of having a human-in-the-loop in using AI as part of the research process:

[H]umans can handle unexpected situations better than an automatic process or an AI can do. Although an AI system can be highly reliable, which if a model has been well-trained and secured and studied, AI can be highly reliable, but on the other side can be less – maybe less flexible than the manual processors and less adaptable to changing conditions, or to unexpected results (P12).

P12 also noted that human researchers may bring greater creativity to research than AI systems.

The participants working in environmental decision-making (P2, P4 and P12) stated that using AI and ML does not change the responsibilities of researchers. This is especially the case if the researchers are developing automated systems themselves: *"I feel like the responsibility, still, is on us, for doing the science as well as possible, and creating that automation as well as possible"* (P2). Researchers have a responsibility to use AI and ML well and to critically evaluate what it produces (P4).

One researcher working on conservation decision-making (P2) also had experience working on automating the design of experiments. P2 distinguished between two types of automated experiments, knowledge discovery and problem-solving: *"there's the experiments just to discover new knowledge, so you're just trying to better understand all the interactions, everything. […] The other type is the one where it's not so much about knowledge, but it's about maximising an outcome"*. With automated experiments for knowledge discovery, *"the risks are not as high; if you're failing – it's like, when you try to gain new knowledge, failing can give you a very high reward, you can learn a lot from that"* (P2).

4.4 Materials science

P17 described improving reproducibility through the consistent performance of processes as a positive factor in favour of adopting laboratory automation. Standardising the preparation and labelling of samples was another benefit (P17). Greater amounts of data that can be recorded about experimentation processes due to laboratory automation, and there is a reduced risk of lower data quality due to human error in recording it (P13). As P17 explained, *"we've got automatic logging for humidity, temperature not only just in the reactor or in the fume hood or in the environment of the sample but actually in the room itself. […] We've got cameras now that automatically take photos when things change and can post those updates."*

Greater throughput was noted by P13 as an important change that automation makes to research practice. Laboratory automation also gives researchers more time to think about future experiments (P17). Similarly, P14 and P17 also noted the reduction of repetitive work due to laboratory automation.

Variations in research practice may pose a difficulty for laboratory automation. P13 noted that since researchers *"usually do something new every day"*, many of their tasks cannot be easily automated. Human operators may also be better at performing certain laboratory tasks than automated systems (P14).

P14 mentioned cost as an important factor in deciding whether to adopt laboratory automation. P13 also noted the startup and maintenance costs of adopting laboratory automation.

A key safety benefit of laboratory automation is reduced exposure to hazardous materials (P14). Laboratories can be isolated so when the materials have been prepped for processing, researchers do not need to be physically in the laboratory once the automated system begins operating (P17).

An important safety precaution is to incorporate redundancy in automated systems (P14). Existing laboratory safety protocols also need to be updated when automated systems are introduced (P14). Risk assessment procedures can also assist in managing the risks of laboratory automation (P14). One noted change in the researcher's responsibilities from laboratory automation is the integration of safety protocols into the automation system (P14).

P17 observed that *"there's more risks around not automating in the labs, not getting ahead of the curve on this. Because it will be very easy to be left behind if you are solely reliant on not having an automated/digital lab. I can see there being a bigger risk in not automating"*.

Automating experiment design also offers efficiency benefits:

What that means is you have a feedback loop so you've got evaluation with online monitoring from your system telling you this last experiment was better than the ones that came before or worse. Then, the algorithm will say, I'll change parameter X-Y-Z to try next iteration. Again, this is taking out a very laborious optimisation protocol out of the hands of a human and making it more efficient by using a machine learning algorithm (P14).

However, P14 also noted using an ML algorithm to optimise the repetition of experiments with minor changes in conditions requires a high level of laboratory process automation to be effective.

Automating experiment design also creates the possibility of autonomous discovery of materials (P7). P5 (a participant working in automation engineering, but with a background in materials science) described how automated experimentation might be used in materials science:

> *… you want a material which has these properties. They're final properties or the starting properties because you want to limit it to the types of raw materials that you think are available, or are environmentally friendly, or such and such. Or if you flip that around the other side and say we need a material that has these properties on the end but we're restricted by these starting points. Go and iterate until you can produce a material that has these properties (P5).*

4.5 Synthetic biology

P16 described some of the automated processes in synthetic biology:

> *A lot of it is liquid handling, moving things into [micro]plates […]. Doing things like plasmid assembly which involves […] mixing liquids and heating them, so robots are quite good at that for us. Things like plasmid construction, your basic molecular biology, setting up PCRs [polymerase chain reactions], that kind of thing. [Doing] things like assay work, so miniaturising assays into that larger plate format, and that takes a little bit of time, optimise and adjust for smaller scale (P16).*

Researchers working in synthetic biology noted several benefits of laboratory automation: the ability to perform experiments at scale (P1 and P16), reproducibility (P1 and P16), increased throughput (P1 and P16), increased speed (P18), the automation of tedious tasks (P16), and new capabilities (P16). P18 also noted that laboratory automation has *"freed up our brain space, we're not doing all these repetitive tasks, we can actually think more about what we are trying to achieve […]—that's how it benefits the researchers"*. Laboratory automation also allows researchers to perform experiments that would be impractical or impossible with it, as P16 explained: *"[t]here's a limit to how small a scale a human can move liquids accurately and that kind of thing, so we've got a few robots that work down into the nanolitre scale, which is much, much smaller that I would ever be able to do reliably"*.

The increased scale of experimentation also requires robust data management systems to track and manage the samples being tested (P18). Researchers also need to adjust to thinking about how to best use the larger amounts of data available and the greater number of possible experiments (P16). The scale of experimentation made possible by automation may also make it inefficient for research clients who only need to perform a small number of experiments (P1).

Laboratory automation also affects the skills researchers require. P1 observed that more training is required for researchers to configure automated platforms to accommodate variations in experimental procedures. Maintaining the knowledge necessary within research teams to effectively use laboratory automation is also important: *"[b]ecause things tend to be on short contracts […], you don't necessarily transfer the knowledge to new people […], so we might have this great robot but nobody knows how to use it"* (P16).

Sometimes the changes introduced by laboratory automation follow broader changes within a research discipline. P16 observed that *"[t]here's been changes in synthetic biology anyway, with things like genomics and what's become possible sequencing-wise, which brought in a lot more of the* *programming/maths sides of things than there used to be"*. P16 also observed that automation has brought them into greater contact with experts in ML.

A common safety benefit mentioned by synthetic biologists was reducing repetitive strain injuries (P1, P16 and P18). However, the movement of robotic parts in automated laboratories may pose a safety risk to researchers (P18). Laboratory robots may also incorporate safety functions to protect researchers: *"[m]ost of the robots that we have, have shields that contain them with interlockers that if that shield isn't there, it stops the robot"* (P18). Risk assessment procedures can also assist in managing the risks of laboratory automation (P18).

P16 stated that automation does not change the responsibilities of researchers: *"[t]here's always a responsibility to do science responsibly"*. P16 also mentioned cost as a restriction on the adoption of laboratory automation: *"every robot costs a fair bit […]—with a few exceptions, you tend to need a couple to be able to manage a whole pipeline to make it work"*.

P18 noted that laboratory automation may reduce the flexibility of research practice: *"If you want it to be efficient you don't want to have to be writing your protocols every single day. It's most efficient when you've got a standard process, that you know works, and then you can just run that."* P1 explained that.

> *"[w]e may be able to fully automate something with a bacteria but then if we want to do that same thing with a yeast because they have a couple of extra weird steps in there, it may not be as amenable to automation fully, there may be stages that we need to take off the platform and put back onto the platform"*.

P1 also observed that a blended approach where laboratory automation and manual experimentation are used together, minimised the need to make trade-offs due to automation.

5 Discussion

Two significant themes identified across the participants' responses that we will discuss further are the role of explainability in experimentation and the need for maintaining a 'human-in-the-loop' in scientific research. These themes directly relate to the epistemic and practical goals of science.

5.1 Explainability and experimentation

In the context of AI/ML, explainability (or interpretability) is the extent that observers can understand the cause of an AI/ML model's decisions (Miller 2019). It was discussed in the contexts of AI in laboratory automation (P8, automation engineering) and in using AI to assist in conservation decision-making (P2, P4, and P12). The researchers working in conservation decision-making perceived explainability as important; in contrast, the automation engineer stated that it was unnecessary for laboratory automation.

To better understand why explainability may be unnecessary in laboratory automation, note that there are two related claims in the automation engineer's comments on explainability:

1. Purposeful science experimentation requires understanding the processes involved in the experiment: "philosophically a lot of scientists still have trouble with the concept of doing robotics and high throughput experimentation because their argument is, well, you don't understand what you're doing, so you're just randomly trying to do things" (P8, who rejects this claim).
2. It is possible to perform scientific experiments without having a predicted outcome beforehand: "There is a lot of science that we do where you can't empirically predict what you are going to find and see" (P8).

In both claims is the perception that scientific experimentation is *theory-dependent*: experiments are performed to provide evidence for or against some theory that predicts their outcomes (Chalmers 2013). The first claim states that experimentation must be theory-dependent as this dependence makes experimentation scientific. The second claim is a rejection of the first: there are valid scientific experiments where there is not a theoretically predicted outcome that will be confirmed or rejected. This claim is consistent with the 'new experimentalist' view of science, where experimental results may be confirmed and supported independently of a scientific theory (Chalmers 2013).

If scientific experiments do not have to be theory-dependent, could a lack of explainability of the system's decisions affect the scientific understanding of the experiment? Consider an example where part of a laboratory process may be performed by a human experimenter or a laboratory robot. The actions of the human or robot experimenter are described within the laboratory protocol the researcher defines. Human experimenters would be expected to follow the laboratory protocol unless there is some overriding factor, such as recognising and reacting to a potential safety hazard. The laboratory robot is not acting autonomously: it will not deviate from the laboratory protocol unless there is some overriding factor that affects its operation (such as a system error or mechanical failure). In both cases, deviations from the laboratory protocol would be recorded. If the laboratory robot performs part of the process instead of a human experimenter, the researcher in charge of the process can determine whether it has successfully performed its role, either through direct observation or by reviewing data it has recorded. While the automated system may employ AI/ML to determine how to physically perform its role, how the AI/ML system decides to act is not part of the epistemological process of experimentation: there is no *loss of understanding* for the researcher about the process by automating a process they have defined. While it may be useful to understand how the automated system performed a laboratory task (especially if it did not act as expected), this understanding does not contribute to the researcher's understanding of the process itself.

In contrast, consider P4's comments that the explainability of how the AI/ML systems they used for conservation decision-making reached their decisions was important for the audience of their research to trust their recommendations. As in other domains, opaque ML models may have significant consequences when used in conservation, such as incorrectly identifying wildlife in collected data (Wearn et al. 2019). P4's comments reflect the commonly drawn connection between the explainability of an AI/ML system and the willingness to trust it (Mittelstadt, Russell and Wachter 2019). In these cases, the justifications for the decision are as important as the decision itself.

In the laboratory robot example, the scientific knowledge is in defining the laboratory protocol that describes the robot's actions. What is being tested is whether the laboratory protocol produces the expected results. When AI/ML is used to produce recommendations for conservation decisions, scientific knowledge is applied to developing and training the AI/ML model: *the AI/ML model itself is being tested*. If the AI/ML model is opaque to the researcher, they are unable to understand what characteristics of the input data are significant for making that recommendation. If the model makes a surprising recommendation, the researcher is unable to determine whether it is an error or an unexpected result that nevertheless is derived from the input data. There is a loss of understanding compared to an alternative where the researcher used an explainable ML model.

In computational design, both the ML model that creates new designs and the process of creating and testing them are being tested. Like laboratory automation, AI/ML is used to fulfill a role that a human researcher would otherwise perform: in this case, designing new physical items. While a human designer may be influenced by their expectations of how the optimised design might appear, the computational design system creates a variety of potential designs that are tested against a set of target specifications for the design. While the individual designs may differ in each use of the ML model, the researcher knows the process through which these designs are created and the criteria used to evaluate them. A theory of how that design meets these criteria is not the purpose of using the ML model itself: such a theory may be developed in retrospect by computer and physical simulation testing of the design. There may be an initial loss of understanding in using computational design compared to traditional theory-led design, but this understanding will be gained retrospectively through testing. Traditional theory-led design may also be misleading: simulation and experimentation results may show that the theory guiding the design does not produce the expected outcomes.

Computer simulations may also need to be explainable as they are simplifications of physical phenomena that necessarily will be an incomplete representation. As P9 (computational design) noted, some aspects of the physical system being simulated will necessarily be left out of the simulation. However, as P2 (conservation decisions) observed, explainability comes at a cost to performance: a more complex simulation that better reflects reality may be less explainable than a simpler but less accurate one.

5.2 Maintaining a 'human-in-the-loop' in scientific research

A frequent theme across application domains (automation engineering, computational design, conservation decisions) and technologies (AI/ML, generative AI, laboratory automation, and automated data analysis) is the importance of maintaining a significant role for human researchers within the research process.

An automation engineer (P5) did not see the laboratory automation systems they developed as fully replacing human researchers. A justification P5 gave for this was the possibility that a human researcher may make a serendipitous discovery by noticing something unusual while performing an experiment. While the greater collection of data made possible by laboratory automation might be seen to make this a moot point (since anything unusual would be recorded in the data), it is possible that the researcher's intuition may direct them to notice something unusual while performing an experiment that would not occur while they are reviewing the data collected by an automated system.

A response to this argument is that automated data analysis would identify anything unusual occurring during an experiment that a researcher might notice, and a lot more besides. However, the participants who discussed automated data analysis (P7 and P8, automation engineering) were weary of using it. The justifications they gave for this reluctance (algorithmic bias, false positives and false negatives, accuracy, and reproducibility) reflects common concerns about errors in AI/ML systems (Mitchell 2019).

P12 (conservation decisions) explicitly mentioned the possibility that human researchers may be more creative than automation systems used in research. This contrasts with the reasoning behind computational design, where AI/ML is used specifically for its capability to develop designs that human researchers would be unlikely to develop on their own (P9, computational design). This contrast may be due to the different purposes in which AI/ML is being used. Consider the distinction P2 (conservation decisions) made between experimentation for knowledge discovery and experimentation for optimisation. The creativity of human researchers may be necessary for some experiments for knowledge discovery, while the creativity of generative AI is suitable for optimisation experiments.

The significance participants placed on maintaining a 'human-in-the-loop' highlight the importance for researchers to be able to trust (or rely on) automated systems.[2] As P9 (computational design) noted, the output of automated systems cannot necessarily be relied upon without confirmation. As discussed earlier, simulations and models are necessarily limited in their representations of the phenomena they simulate. However, this does not mean that such output should be dismissed, only that it should be tested and verified if possible.

This is further supported by several participants (P2, P4, P6, P12, and P16) who also note that automating science does not affect the responsibilities of researchers. The role responsibilities of scientists are those that assist them in fulfilling the goals of scientific research (Douglas 2009). As described earlier, the goals of science are to gain knowledge and understanding of the world (the epistemic goal) and to provide the means of predicting and manipulating the world (the practical goal). As shown in the previous section, maintaining the epistemic goal of science justifies the need for explainability when an AI/ML model is part of what is being tested in an experiment. Achieving the practical goal of science using automation requires these systems to be trustworthy: the outputs of these systems should provide usable predictions about the modelled phenomena. The usability of these predictions may be confirmed by verifying the computer simulation with physical experiments (as in the example of confirming computational design with physical experimentation) or by having explainable AI/ML models that allow researchers to understand what is (and what is not) represented in the simulation. Here the epistemic and practical goals of science support each other: experimental validation and explainability allow for scientific understanding to support the decisions made by AI/ML models.

[2] There is debate over whether it is possible to 'trust' AI systems as trust requires the trusted party to be held ethically responsible for maintaining that trust (Ryan 2020). It may be more accurate to say that AI systems are *relied upon* rather than *trusted*.

6 Limitations and further research

A limitation of this study is the limited range of scientific fields represented by the participants. Having participants from an even wider range of scientific fields may identify additional effects of automation on scientific practice. The participants also belonged to the same research agency. Having participants from a variety of institutions may reveal differences in how automation is perceived within different types of research institutions.

The participant interviews were also conducted around the time that ChatGPT was first released which brought widespread awareness to the power of LLMs and generative AI (OpenAI 2022). As a result, the potential impact of using LLMs in research practice is not present in the participants' responses. The participants' responses can therefore be read as a snapshot of how researchers perceived the impacts of automation on research before they had gained experience of the capabilities of LLMs.

7 Conclusion

This paper described how researchers in several fields (automation engineering, computational design, conservation decisions, materials science, and synthetic biology) perceived the benefits, risks, and trade-offs connected with adopting various forms of automating science. We found different perspectives on the significance of explainability for AI/ML systems used in research. The need for explainability is reduced if the automated system is following procedures defined by human researchers, as there is no loss of scientific understanding in having an automated system perform a task that could otherwise be performed by a human experimenter. However, explainability is important when the automated system (such as an AI/ML model) is the subject of experimentation itself, such as where the AI/ML model is a simulation of a process or system. As models and simulations necessarily simplify or omit some aspects of the process or system they represent, it is important for researchers to understand what has been left out of the model or simulation. We also discussed how researchers often noted the significance of maintaining a 'human-in-the-loop' in automated system, and that maintaining a human role in scientific practice is important for maintaining the trustworthiness of results.

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