Chapter 4 Transformation of Science by the Use of AI

Given the development and dissemination of high-performance computing resources and the publication and sharing of research data in line with the progress of AI technology, initiatives have been made to use advanced AI in scientific research in various fields, including biotechnology and material science, under titles such as "AI for Science" and "AI in Science." Expectations are rapidly growing for AI technology to accelerate resolution of scientific problems and improve research productivity, etc..

One of the pioneering cases is the high-accuracy prediction of three-dimensional (3D) structures of proteins by Google DeepMind's machine learning model "AlphaFold" in 2018 (see Section 1).

In addition, the number of papers mentioning AI and machine learning terms in fields other than information science is also increasing (Figure 1-4-1).

Under such circumstances, the OECD released a report titled "Artificial Intelligence in Science: Challenges, Opportunities and the Future of Research" [1] in June 2023. EU also requested the Group of Chief Scientific Advisors to provide advice on the strategy for using AI in science[2] in June 2023, and released an policy brief in December 2023, [3] pointing out the need for strategic initiatives. Meanwhile, the U.S. National Academies of Sciences, Engineering, and Medicine gathered leaders from industries, universities, and governments inside and outside the United States, and held an international workshop on "AI for Scientific Discovery" in October 2023, [4] and discussed the future response measures.

Use of AI in R&D has also started in Japan, with the National Institute for Materials Science (NIMS) succeeding in designing new materials by using machine learning [5] under the MEXT's "Material Research by Information Integration Initiative (FY2015 to FY2019)." Due to the recent further advancement of AI technology, RIKEN started the development and shared use of AI foundation models for scientific research (Advanced General Intelligence for Science Program of the Transformative Research Innovation Platform of RIKEN platforms; TRIP-AGIS) [6] in April 2024 (see Section 2), and initiatives of "AI for Science" are about to be accelerated.

While use of advanced AI in scientific research has attracted attention and research aiming to achieve a paradigm shift in scientific research has been accelerated inside and outside Japan, in a survey conducted by journal *Nature*, [7] many researchers anticipated that the use of AI as research tools will continue to be increasingly important in the future, but also indicated concerns

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1 OECD, "Artificial Intelligence in Science: Challenges, Opportunities and the Future of Research." https://www.oecd.org/publications/artificial-intelligence-in-science-a8d820bd-en.htm

2 European Commission, "Scoping Paper : Successful and timely uptake of Artificial Intelligence in science in the EU." https://research-and-innovation.ec.europa.eu/system/files/2023-07/Scoping_paper_AI.pdf

3 European Commission, "Harnessing the potential of Artificial Intelligence in science to boost Europe's global competitiveness." https://research-and-innovation.ec.europa.eu/news/all-research-and-innovation-news/harnessing-potential-artificial-intelligence-science-boost-europes-global-competitiveness-2023-12-13_en

4 The National Academies of Sciences, Engineering, and Medicine, "AI for Scientific Discovery - A Workshop." https://www.nationalacademies.org/event/40455_10-2023_ai-for-scientific-discovery-a-workshop

5 Material Research by Information Integration Initiative, NIMS, "Use of Machine Learning to Design Optimal Nanostructures to Control Heat Current in Materials." https://www.nims.go.jp/MII-I/news/d53p8f000000639k.html

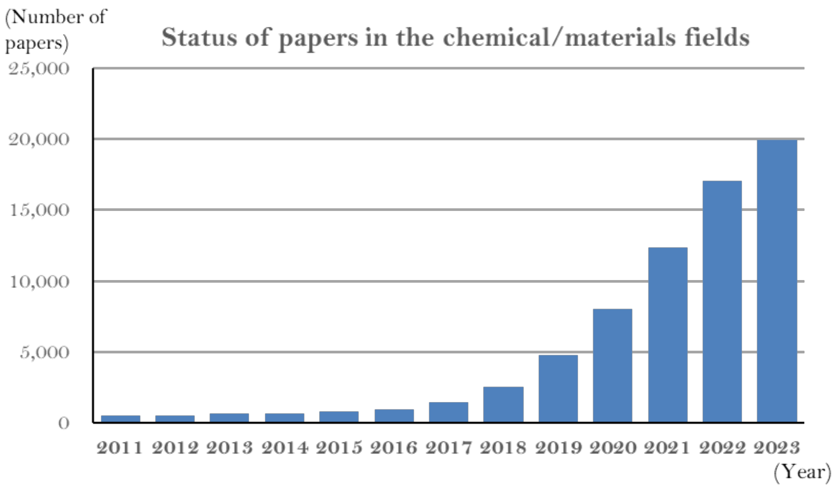
6 RIKEN, "Advanced General Intelligence for Science Program." https://www.riken.jp/research/labs/trip/agis/

7 Van Noorden, R., Perkel, J.M., (2023), "AI and science: what 1,600 researchers think," *Nature* 621, 672-675. https://www.nature.com/articles/d41586-023-02980-0

about misuse and abuse of AI tools, etc. The issues of the reliability and safety associated with the characteristics and limitations of AI are common issues also in the use of AI in scientific research, and responsible use is required.

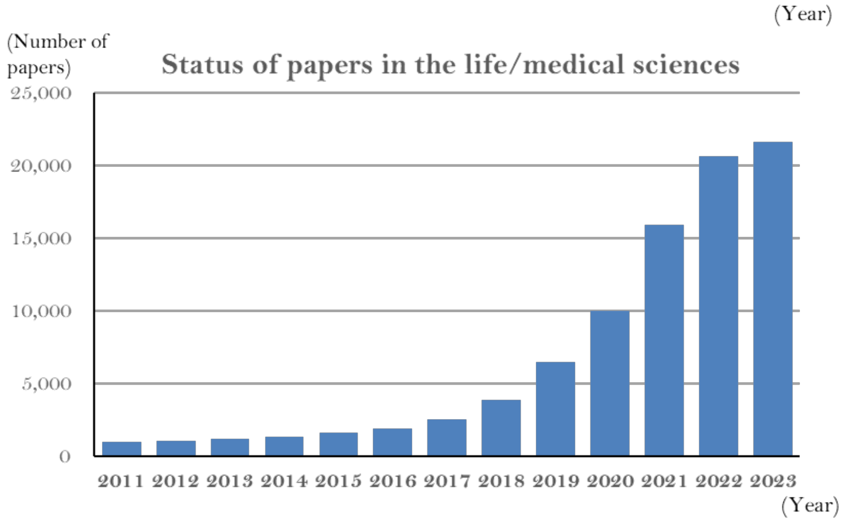
In light of such circumstances, this chapter explains the impacts and issues of the use of advanced AI in R&D, while introducing specific initiatives inside and outside Japan.

■ Figure 1-4-1/Status of papers using AI and machine learning



Cumulative top 15 countries/regions during 2011 to 2023 (integer count)

China	24,934
U.S.	11,181
ROK	6,477
India	3,914
Germany	3,301
UK	3,230
Saudi Arabia	3,194
Japan	2,829
Spain	2,483
Italy	2,211
Taiwan	2,102
Iran	2,091
Canada	1,909
Australia	1,780
Pakistan	1,730



Cumulative top 15 countries/regions during 2011 to 2023 (integer count)

China	26,591
U.S.	25,904
UK	6,325
Germany	6,087
India	6,001
ROK	4,210
Canada	4,057
Italy	3,654
Japan	3,439
Australia	3,210
France	2,942
Netherlands	2,719
Spain	2,672
Switzerland	2,221
Taiwan	2,123

Note: The number of papers (articles and reviews) in the chemical/materials fields and life/medical sciences fields containing any of the keywords “artificial intelligence,” “machine learning,” “deep learning,” “Neural Network,” “Bayesian optimization,” “Large language Models” or “Natural Language Processing” was aggregated using Web of Science.
Source: CRDS, JST

Section 1 Use of advanced AI in diverse scientific fields (AI for Science)

The methods of using AI in scientific research have become diversified and sophisticated according to the field and purpose, and the foundation models, etc. being used have also advanced further. Generally, scientific research is conducted by generating a hypothesis, and then verifying it through experiments, observations, etc. In this series of processes, advanced AI is expected to be used, for example, for analyzing research or observation data, generating or inferring hypotheses, and automating research, and various studies have been carried out on this matter.[1]

This section introduces examples of major initiatives inside and outside Japan.

Column 1-4 Nobel Turing Challenge[2,3]

In 2016, Dr. KITANO Hiroaki, Director of Sony Computer Science Laboratories, proposed the "Nobel Turing Challenge," which sets a bold goal: to develop AI capable of making Nobel Prize-level or even greater scientific discoveries autonomously by 2050.

This challenge consists of two components: the Challenge and the Question. The Challenge is to develop AI that can achieve Nobel Prize-level scientific discoveries. The Question revolves around whether such AI will behave indistinguishably from humans (i.e., passing the Turing Test) or evolve into an entirely different form of intelligence.

To advance the automation of the scientific discovery process, numerous technologies and methodologies have been discussed and developed. International workshops have been held several times in locations such as the UK, Japan, the U.S., and Sweden, with ongoing discussions and efforts surrounding this initiative.

This ambitious goal is also gaining traction internationally. In January 2021, the UK's Alan Turing Institute launched the "Turing AI Scientist Grand Challenge Project," inviting Dr. KITANO as one of the key participants. Similarly, the government of Singapore has also begun significant efforts and plans to host an international conference and launch a research project in July 2024.

1-1. Improving scientific data and extracting information by using AI

By using advanced AI for analyzing massive scientific data, it is hoped that information and relationships that would have been overlooked by conventional research methods can be clarified, bringing new discoveries and innovative insights.

- Removal of noise in space observation data

In 2021, a research team of the Institute of Statistical Mathematics in ROIS and National Astronomical Observatory of Japan in National Institutes of Natural Sciences succeeded in mapping dark matter that had been buried in noise, by removing noise that occurs when creating a map of dark matter distributions from actual galaxy data by using deep learning technology (generative adversarial networks).[4] As a result of using AI and becoming able to investigate the low-density regions of dark matter, which had been difficult to do by observation alone, it may be possible to obtain information concerning the mass of elementary particles that are thought to be candidates for dark matter and the forces that act

1 Wang, H., et al., (2023), "Scientific discovery in the age of artificial intelligence," *Nature* 620, 47-60. https://www.nature.com/articles/s41586-023-06221-2
CRDS, JST (2023), "New Trends in Artificial Intelligence Research: Impacts of Foundation Models and Generative AIs."
CRDS, JST (2024), "Research and Development on Next-Generation AI Models."

2 Kitano, H., (2016), "Artificial Intelligence to Win the Nobel Prize and Beyond: Creating the Engine for Scientific Discovery," *AI Magazine* 37, 39-49. https://doi.org/10.1609/AImag.v37i1.2642

3 Kitano, H., (2021), "Nobel Turing Challenge: creating the engine for scientific discovery," *npj Systems Biology and Applications* 7, 29. https://doi.org/10.1038/s41540-021-00189-3

4 The Institute of Statistical Mathematics, ROIS, "Digging up a buried map of dark matter: observation, simulation, and AI join forces to reveal a clear universe."
https://www.ism.ac.jp/ura/press/ISM2021-06/pr0702.pdf

between dark matter particles, and it is hoped that this will accelerate the elucidation of the mysteries of the universe.

- Ultrasound image diagnosis support

In 2022, the Cancer Translational Research Team of RIKEN Center for Advanced Intelligence Project (AIP) developed a new technology that visualizes the basis for AI's determination when applying AI technology to ultrasound examination, and assists the examiner in making a diagnosis.[1] While ultrasound image diagnosis support technology using AI is expected to be introduced even further in a wide range of medical domains, including obstetrics and gynecology, it is hoped that this technology will enable medical service providers and patients to use AI-mounted medical care devices with a greater trust, in clinical settings.

1-2. Increasing the sophistication and speed of simulations using AI

Initiatives to create models that predict 3D structures and candidate substances, etc. from massive scientific data by using deep learning technology, etc., and to increase the efficiency and speed of the identifying processes are also accelerating.

- Prediction of 3D structures of proteins

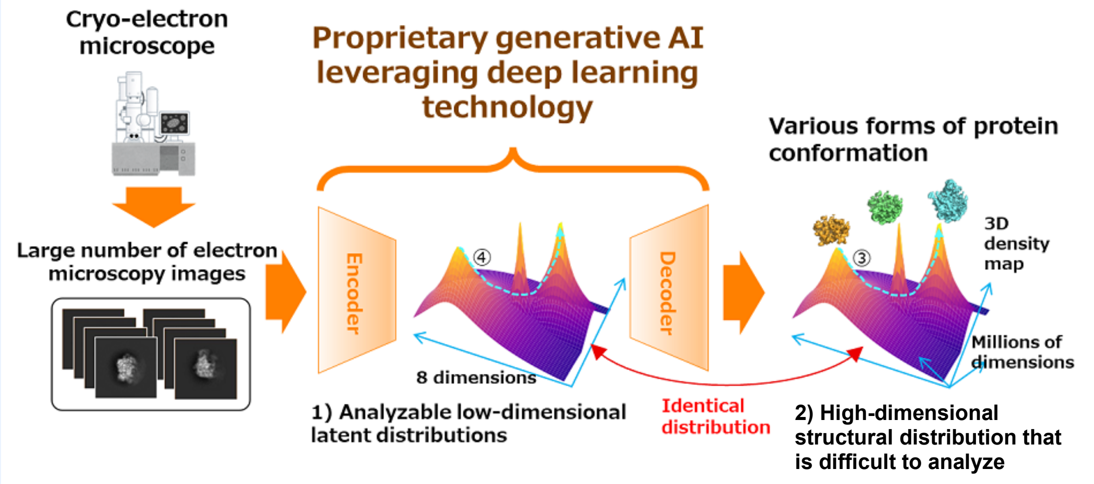
More than 200 million kinds of proteins have reportedly been discovered. In order to understand their functions and use them for treating diseases or developing new drugs, it is important to know their 3D structures. The structures have been studied through experimental techniques, such as X-ray crystallography, cryo-electron microscopy, and nuclear magnetic resonance, but the time and cost required have presented issues. In such a situation, AlphaFold, a machine learning model developed by Google DeepMind, which predicts 3D structures of proteins, won the first place in CASP[2] 13, an international competition to predict protein structures, held in 2018. In CASP14 held in 2020, an improved model AlphaFold2 demonstrated an even more dramatically higher accuracy. Then in July 2021, its source code was published, and in July 2022, Google DeepMind announced that structural prediction was performed for approximately 200 million kinds of known protein sequences.[3] Although some problems have been pointed out for the model, such as the fact that it does not support shape changes caused by mutations or interactions with other proteins, it has brought about a major change in the way in which research in the structure prediction field is carried out.

- Prediction of structural changes in proteins

In order to predict a wide range of structural changes, or conformational changes, in proteins, it is necessary to first estimate the proportions of the possible conformations and then accurately estimate the time changes of the conformation. In 2023, Fujitsu Limited and RIKEN developed new technologies "generative AI technology that accurately estimates the various forms of protein conformation and their proportions" and "technology for predicting conformational change based on the low dimensional feature of protein conformation" by using Fujitsu's proprietary generative AI technology "DeepTwin" and a large amount of image data processed by supercomputer "Fugaku." These two technologies reduced the time for prediction of conformational changes in a target protein from one day to two hours[4] (Figure

1 RIKEN, "Doctors diagnosing fetal heart disease benefit from explanatory AI." https://www.riken.jp/press/2022/20220322_2/index.html
2 Critical Assessment of Protein Structure Prediction
3 Google DeepMind, "AlphaFold reveals the structure of the protein universe." https://deepmind.google/discover/blog/alphafold-reveals-the-structure-of-the-protein-universe/
4 Fujitsu Limited, "Fujitsu and RIKEN develop AI drug discovery technology utilizing generative AI to predict structural changes in proteins" https://pr.fujitsu.com/jp/news/2023/10/10-1.html

■ Figure 1-4-2/Prediction of structural changes in proteins



Source: Fujitsu Limited

1-4-2).

● Acceleration of atomistic-level simulations

In developing new materials in a wide range of fields, it is important to be able to not only deal with diverse elements, but also accurately predict the properties of a substance, such as its atomic structure, density, and bonding state, which affect the character of the material. In the past, however, time-consuming simulation calculations were required for studying the electronic state of a material. Through joint research with ENEOS Corporation, Preferred Networks, Inc. developed "Matlantis," a universal atomistic-level simulator incorporating deep learning technology, which realizes atomistic simulations for material discovery, and launched its service in 2022.[1] By incorporating deep learning technology in a conventional physical simulator, the calculation speed could be increased by tens of thousands of times, and it became possible to apply the simulator to a variety of substances without limiting the domains.

● Discovery of materials and reactions with desirable properties

In the materials field, R&D is conducted on the use of AI in efficient discovery of new materials having specific characteristics, such as searches for high-performance battery materials or superconducting materials, and prediction of physical/chemical characteristics or reaction properties of materials.

For example, in September 2023, NIMS announced that it succeeded in increasing the high-temperature strength of alloys through collaborative efforts with AI.[2] While the number of possible thermal aging condition patterns for nickel-aluminum alloys is enormous, with approximately 3.5 billion patterns, 110 patterns that produce better results than conventional processes were identified by using an AI algorithm that efficiently searches optimum patterns from a huge number of combinations. The researchers further analyzed this result, and designed thermal aging processes that can further increase the high-temperature strength of alloys than the patterns identified by AI. The

1 Preferred Computational Chemistry, Inc., "Matlantis™: Core Technology and Mechanics." https://matlantis.com/ja/product
2 NIMS, "Increasing High-Temperature Strength of Materials Through Collaborative Efforts of AI and Materials Researchers—Optimizing Thermal Aging Schedules by Analyzing the Unconventional AI-driven Outcomes—." https://www.nims.go.jp/eng/press/2023/09/202309250.html

performance is better than the results of the search by AI alone, and it can be considered as a collaboration model between AI and researchers.

- Weather prediction

As extreme weather events are becoming more frequent and severe around the world in recent years, faster and more accurate predictions are becoming increasingly important. In November 2023, Google DeepMind released "GraphCast," an AI model that can deliver 10-day weather predictions at unprecedented accuracy in under one minute. [1] While conventional weather forecasts had used numerical prediction models based on physical equations and algorithms, designing these equations and algorithms was time-consuming and required deep expertise, as well as large-scale computing resources to make accurate predictions. This GraphCast was trained on decades of historical weather data to learn a model of the cause and effect relationships that govern how Earth's weather evolves, from the present into the future, by using deep learning technology instead of physical equations. The model has already been open sourced, and its high-accuracy predictions of the tracks of cyclones and flood risks are hoped to lead to improvements in warnings and countermeasures.

- Plasma behavior prediction for fusion energy

To realize fusion energy through the magnetic field confinement method, it is necessary to control high temperature plasma that exceeds 100 million degrees Celsius over a long period. However, the prediction and control of its complex behavior are a challenging issue. Therefore, institutes such as the Naka Institute for Fusion Science and Technology of the National Institutes for Quantum Science and Technology and the National Institute for Fusion Science of the National Institutes of Natural Sciences conduct research on predictions of plasma density/temperature behaviors[2] and on changes in plasma that lead to radiative collapse[3], by using machine learning. In addition, Google DeepMind announced in February 2022 that, through joint research with the Swiss Federal Institute of Technology, it developed an algorithm that autonomously controls magnetic coils, for maintaining the inherently unstable plasmas stable at high temperatures inside a tokamak reactor, by using deep reinforcement learning.[4] It is hoped that advanced AI will further contribute to realizing fusion energy.

- Shortening the computational fluid dynamics simulations

In automotive design, computational fluid dynamics (CFD) simulations are performed to study factors such as the aerodynamic drag experienced by the car body, from the viewpoint of improving fuel efficiency. However, a large amount of computing time and resources are required for analyzing the complex fluid phenomena. "NeumaticAI" developed by Araya Inc. has managed to reduce the overall design cycle time with a hybrid technology of AI and

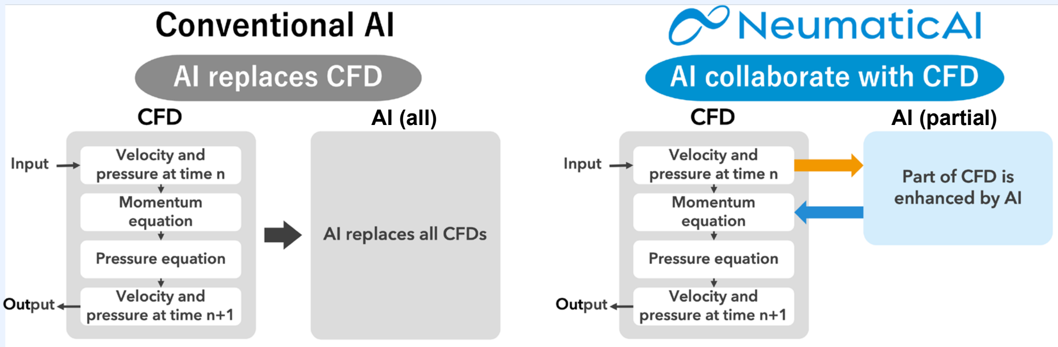
1 Google DeepMind, "GraphCast: AI model for faster and more accurate global weather forecasting." https://deepmind.google/discover/blog/graphcast-ai-model-for-faster-and-more-accurate-global-weather-forecasting/

2 National Institutes for Quantum Science and Technology, "Making the future with quantum science and technology: Nuclear fusion power generation Part 15, Increasing speed and accuracy with AI." https://www.qst.go.jp/site/fusion/nks-rensai-15.html

3 National Institute for Fusion Science, National Institutes of Natural Sciences, "Predicting the occurrence of plasma collapse and capturing the changes in the plasma that heads towards collapse." https://www-lhd.nifs.ac.jp/pub/Science/Paper_PFR16-2402010.html

4 Google DeepMind, "Accelerating fusion science through learned plasma control." https://deepmind.google/discover/blog/accelerating-fusion-science-through-learned-plasma-control
Degrave, J., et al., (2022), "Magnetic control of tokamak plasmas through deep reinforcement learning," *Nature* 602, 414-419. https://www.nature.com/articles/s41586-021-04301-9

■ Figure 1-4-3/Mechanism of NeumaticAI



Source: Araya Inc.

CFD.[1] As it makes maximum use of available CFD technology, and keeps the role played by AI in CFD to a minimum, high generalization performance and reliable analysis results can be expected even with a small amount of training data (Figure 1-4-3).

1-3. Realtime prediction and control by using AI

In current robotics, it is extremely difficult to develop a robot that can do various types of work from housework, such as cleaning and cooking, to nursing care, such as assistance with transfers, in the same way as humans. It is hoped that, by using AI, technology will be developed to perform various tasks in the same way as humans while making predictions according to the environment. For example, in Moonshot Goal 3 "Realization of AI robots that autonomously learn, adapt to their environment, evolve in intelligence and act alongside human beings, by 2050," a research team led by Professor SUGANO Shigeki and Professor OGATA Tetsuya at Waseda University conducts research on the AI-driven Robot for Embrace and Care (AIREC), the world's highest-level robot that coexists with humans, with an aim to realize robot intelligence that supports human manual labor, especially housework, by utilizing a technology that applies deep learning technology to predict high-dimensional changes in sensation and motion in real time and minimize prediction error (the deep prediction learning technology).

1-4. Generation and inference of scientific hypotheses using AI

Interest is also growing in the fact that generating and finding hypotheses from large-scale data by using AI can lead to scientific discoveries that transcend the limits of human cognition and bias.

In Japan, "Foundation of 'Machine Learning Physics': Revolutionary Transformation of Fundamental Physics by A New Field Integrating Machine Learning and Physics" by a team led by Professor HASHIMOTO Koji was adopted as one of Grants-in-Aid for Scientific Research (KAKENHI) "Grant-in-Aid for Transformative Research Areas (A)" in 2022. The team conducts research to tackle the most important challenges in fundamental physics, such as the discovery of new laws and the exploration of new materials, by integrating machine learning methods with physics, with the participation of researchers from multiple universities and research institutes.[2]

1 Araya Inc. "NeumaticAI—Hybrid technology of CFD and AI: Reliable and fast aerodynamic prediction solution." https://www.araya.org/en/service/neumaticai/

2 MLPhys, "Grant-in-Aid for Transformative Research Areas (A): Foundation of Machine Learning Physics" (Grant-in-Aid for Scientific Research, MEXT). https://mlphys.scphys.kyoto-u.ac.jp/about/

1-5. Autonomous experiments and laboratories using AI

The use of AI in science has brought about the new advancement of automating a part or all of research and experiments by combining AI and robot technology. Initiatives are also under way to realize autonomous experiments and research, where robots not only perform high-speed compound screening and set up automated experiments, but can also utilize information from past research data and papers to optimize the design of new research, collect and analyze data from sensors and advanced measurement devices in real time, and evaluate and verify hypotheses (Table 1-4-4).

■ Table 1-4-4/Examples of initiatives for automated/autonomous experiments/laboratories

Name	University, etc.	Outline
Mobile robotic chemist	University of Liverpool, UK	A mobile robot that can conduct experiments to search for improved photocatalysts for hydrogen production from water. Reported to have performed 688 experiments over eight days in 2020.
Self-Driving Lab	University of Toronto, Canada	Accelerates discovery of new materials and molecules by combining AI, robot engineering, and high-performance computing
A-Lab	Lawrence Berkeley National Laboratory, U.S.	Accelerates the speed of materials research by 100 times through introduction of robots and AI
Autonomous materials search robot system	The University of Tokyo, the Institute of Science Tokyo (former Tokyo Institute of Technology)	An autonomous materials search system that combines machine learning with robotics. The system has multiple sample characterization apparatuses to collect large amounts of data.
Automated experimental robot	RIKEN, Osaka University	A collaborative robot with an AI system that can generate robotic motions for scientific experiments by combining a robotic arm with a camera and pipette attached with the hand and a 3D model of the experimental environment. This system can recognize plant shapes and automates detailed experimental procedures like adding solutions to individual leaves.

Source: Created by MEXT based on published information.

The University of Tokyo and the Institute of Science Tokyo (former Tokyo Institute of Technology) developed a system that autonomously searches materials (Digital Laboratory).[1] With the use of this robot system, thin films with optimal physical properties can be created without human intervention, with ten times the human throughput (Figure 1-4-5). The latest system has multiple sample characterization apparatuses to collect large amounts of data. The data is output in a Measurement Analysis Instrument Markup Language (MaiML) format, which became the Japanese Industrial Standard (JIS) in May 2024.

1 Institute of Science Tokyo (former Tokyo Institute of Technology), "Robot System Capable of Autonomous Materials Search Developed: How Automation Can Revolutionize Materials Research."
https://www.titech.ac.jp/news/2020/048276
Hitosugi Lab., School of Science, The University of Tokyo (Solid-state Chemistry Lab). https://solid-state-chemistry.jp/index

■ Figure 1-4-5/Autonomous materials search robot system (Digital Laboratory)

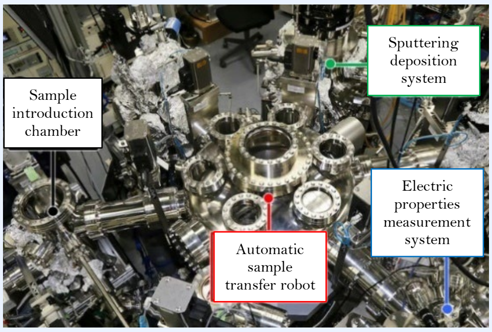


Photo courtesy of Prof. Taro Hitosugi

Meanwhile, in 2023, a joint research team from RIKEN and Osaka University developed an AI system that recognizes the unique characteristics of plants, non-standardized objects, on a sample-by-sample basis. The system autonomously generates robotic arm movements to conduct experiments without human intervention, enabling it to adapt flexibly to a wide range of experimental conditions[1] (Figure 1-4-6).

■ Figure 1-4-6/An automated experimental robot that can recognize environment, and flexibly dispense liquids to plants

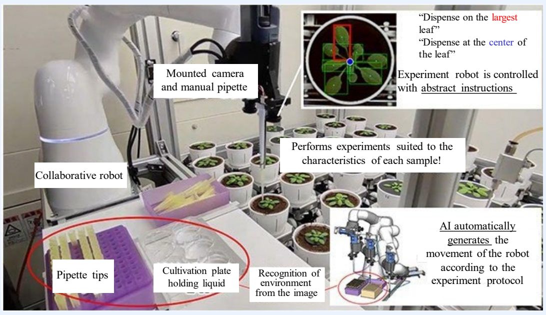


Photo courtesy of RIKEN

Such R&D efforts have already been made in industry. Chugai Pharmaceutical Co., Ltd. is improving processes of drug discovery research using lab automation and digital technology. In antibody discovery processes, hundreds and thousands of antibodies are prepared with lab automation technology, and multidimensional optimization of antibodies is executed through comprehensive data analyses. Furthermore, "MALEXA®," in-house developed AI-based technology, designs and proposes antibody sequences through machine learning approach with the vast amount of experimental data. Notably, its proposed sequences have more superior properties than those designed by researchers (Figure 1-4-7). In Chugai Life Science Park Yokohama that started its operation in 2023, a wide variety of automated systems contribute to drug discovery research, including a screening system that supports two different modalities -- small molecule compounds and antibodies--, and an automation system for antibody gene cloning (the process of making a genetically identical copy of DNA fragments). The company is also working on the automation of experiments for mid-size molecule drug discovery, an expected new drug discovery modality (methods and technologies for developing drugs).

1 RIKEN, "An automated experimental robot that looks around, thinks and moves its hand: Development of generative AI that recognizes the experimental environment and generates robotic motions."
https://www.riken.jp/press/2023/20231225_1/index.html

■ Figure 1-4-7/ Gene cloning system and AI technology that support antibody discovery research

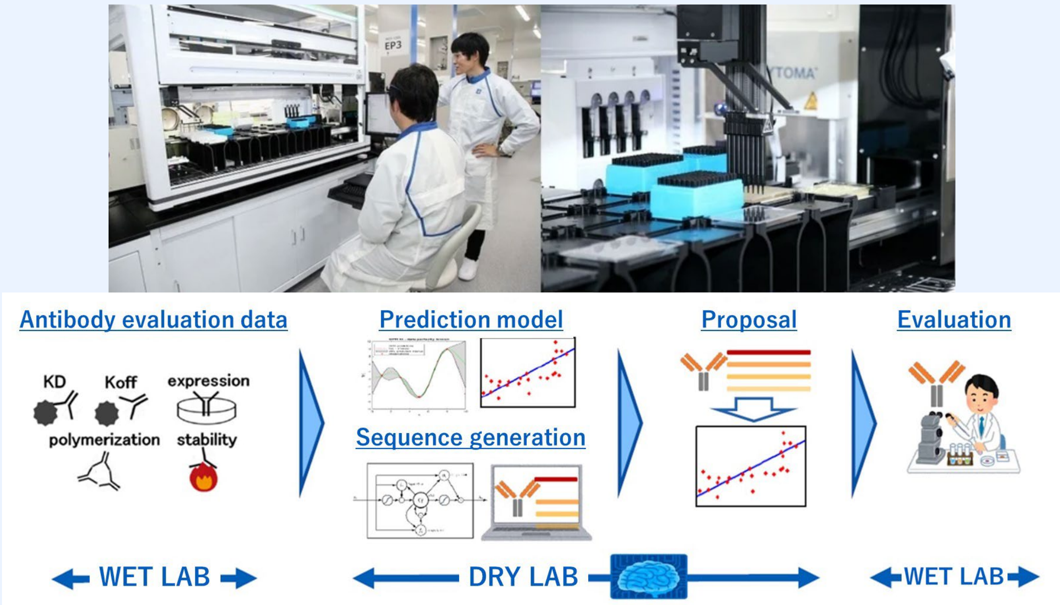


Photo courtesy of Chugai Pharmaceutical Co., Ltd.

Through such automation and autonomy of research, researchers will be freed from the repetition of simple tasks in experiments, and will be able to spend more time on creative work. It is also hoped that the analysis of large amounts of research data will lead to new discoveries and resolution of scientific issues.

In addition, with the aim of achieving a paradigm shift in the very nature of research activities, MEXT has set "Research innovation through autonomous-driven research systems" as a strategic objective for FY2024. In the future, MEXT will publicly solicit and support research projects on methodologies to autonomously drive research processes through appropriate processing, even when information is lacking, by integrating knowledge from AI, simulation, robots, data, and each research field, and on creation of an environment for using such methodologies, etc.

■ Figure 1-4-8/History of domestic projects on AI robot driven science[1]

FY (2018–2030)	
AI/robot	MS Goal 3 "AI & Robots that Harmonize with Humans to Create Knowledge and Cross Its Borders" (2023–)
AI/robot	MS Goal 3 "Co-evolution of Human and AI-Robots to Expand Science Frontiers" (2021–)
Life science	CREST "Innovation of Life Science through Digital Transformation Focused on Data-Driven and AI-Driven Technologies" (2021–2028)
Life science	Institute for Chemical Reaction Design and Discovery, Creative Research Institution, Hokkaido University (2018–2017)
Life science	JST-Mirai Program "Accelerating Life Sciences by Robotic Biology" (2018–2025)
Nanotech / materials	Data Creation and Utilization-Type Material Research and Development Project (DxMT) (2021–)
Nanotech / materials	Advanced Research Infrastructure for Materials and Nanotechnology in Japan (ARIM) (2021–)
Nanotech / materials	JST-Mirai Program "Materials Exploration Platform; Expanding Search Space by high-throughput technology" (2019–2026)
Platform	Exploration of "future science for prediction and control" through establishment of a next-generation research DX platform (Transformative Research Innovation Platform of RIKEN platforms (TRIP)) (2023–)
Platform	Developing a Research Data Ecosystem for the Promotion of Data-Driven Science (2022–)
Platform	NIMS materials data platform (MDPF) (2021–)

Source: CRDS, JST (2024), "Research and Development on Next-Generation AI Models."

1 CRDS, JST (2024) "Research and Development on Next-Generation AI Models."

Column 1-5

Moonshot Goal 3
"AI & Robots that Harmonize with Humans to Create Knowledge and Cross Its Borders"

● Project Manager USHIKU Yoshitaka
Vice President for Research, OMRON SINIC X Corporation

In this column, we interviewed Mr. USHIKU, the project manager who leads an AI robot project toward Moonshot Goal 3.

In innovation, deductive thinking is necessary for continuous performance improvement, while paradigm disruption requires knowledge creation through inductive thinking and abduction, as well as knowledge cross-border migration between fields (transilience). This project aims to first realize a form of AI that understands researchers' ideas based on their research papers, and then develop AI robots that can conduct research in a loop of assertion, experiment, analysis, and description while interacting with human researchers by 2030. We aim to create a world in which researchers and AI can harmonize and produce Nobel Prize-level research results by 2050.

We have been advancing research on AI and robots that achieve harmony between humans and machines. In that process, we have studied AI and robots that can understand and assist with research tasks, such as hypothesis discovery and experiments, to enable people engaging in research and development to enjoy more creative work. Our specific robot research includes studies on a robot that weighs and mixes powdered materials while grinding them and a robot that executes symbolic planning based on linguistic instructions from humans and visual data. As for AI, we have developed, for example, AI capable of conducting symbolic regression for discovering scientific laws from observed data, predicting the physical properties of materials, and generating new materials.

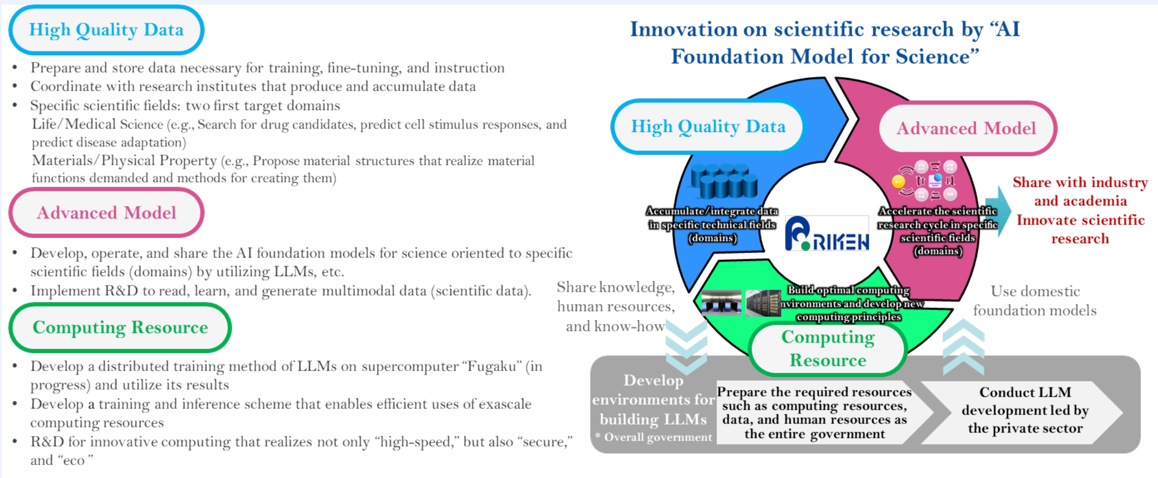
In the Moonshot project that started in January 2023, we first focused on AI's understanding of literature. We worked on the research and development of AI which, from among existing papers, understands the relationship between the research contribution claimed at the beginning and the experimental results of each paper, collectively understands multiple papers in a summarized manner, and reproduces experiments from papers. Going forward, we intend to elevate the technology to a level that allows AI scientists to generate new hypotheses together with human researchers, while automatically conducting and exploring a wider range of experiments. Also in collaboration with Ms. HARADA Kanako, a project manager working towards the same Goal 3, we aim to bring about a paradigm shift in AI robot-driven science in diverse disciplines, such as materials and biotechnology.

Section 2 Development of foundation models and algorithms for further use of next-generation AI

As described in the previous section, use of advanced AI in scientific research has brought about major changes in various aspects, such as acceleration of R&D, promotion of new discoveries, and improvement in research quality. In order to make further use of the ever-advancing AI, development of foundation models and algorithms is also progressing.

At RIKEN, development of AI foundation models for scientific research in specific scientific fields (domains) (Figure 1-4-9) started in full fledge in April 2024. In the same month, MEXT and U.S. Department of Energy revised their project arrangement, and newly placed AI for Science in the Japan-U.S. governmental collaboration framework. In addition, RIKEN and U.S. Argonne National Laboratory signed a Memorandum of Understanding for working in collaboration in the area of AI for Science.

■ Figure 1-4-9/Development and sharing of AI foundation models for scientific research (TRIP-AGIS)



Source: RIKEN.

In addition, under the strategic objective "Toward scientific discoveries through DX in life science research" set by MEXT, the JST's Strategic Basic Research Programs have made public solicitations since FY2021 for the research area "Innovation of Life Science through Digital Transformation Focused on Data-Driven and AI-Driven Technologies," and have adopted and supported a total of 17 research projects to date.[1]

- Quantum AI

Research in the field called quantum AI or quantum machine learning, where a quantum computer is used to conduct what has become possible with AI, is accelerating. In 2018, Associate Professor MITARAI Kosuke from Osaka University, together with Professor FUJII Keisuke and others, announced an algorithm called "quantum circuit learning" which hybridizes a quantum computer and a classical computer, and attracted attention.[2]

- LLMs that process biological information

LLMs have started to be used also in such fields as life sciences, by making them learn a large amount of information such as amino acid sequences, instead of natural language. For example, research is accelerating on "protein language models," which are deep learning models that deem the respective amino acids constituting proteins as "words" and primary protein sequences as "sentences," and learn the feature expressions of "sentences" and the probability functions of sentence generation.[3]

For example, ESM-2, developed by Meta in 2022, is a huge Transformer-based model with 15 billion parameters.[4] As it does not require input of multiple sequence alignments (MSA) that had been required for models such as Google DeepMind's AlphaFold2 (see Chapter 4, Section 1), its use as a tool for predicting protein 3D structures is rapidly

1 CREST, Strategic Basic Research Programs, JST, "[Bio-DX] Innovation of Life Science through Digital Transformation Focused on Data-Driven and AI-Driven Technologies." https://www.jst.go.jp/kisoken/crest/research_area/ongoing/bunya2021-3.html
2 Research at Osaka University, "Will quantum computers be commercialized in 2030? Algorithms will accelerate the 'dream device.'" https://resou.osaka-u.ac.jp/ja/story/2023/nl89_research02
3 Yamaguchi, H. and Saito, Y. (2023), "Tanpakushitsu no gengo moderu" (Protein language models), *JSBi Bioinformatics Review* 4 (1), 52-67. https://www.jstage.jst.go.jp/article/jsbibr/4/1/4_jsbibr.2023.1/_html/-char/ja
4 Meta, "ESM Metagenomic Atlas: The first view of the 'dark matter' of the protein universe." https://ai.meta.com/blog/protein-folding-esmfold-metagenomics/
ESM Atlas, "About." https://esmatlas.com/about

increasing.[1]

Meanwhile, the Medical Research Center for High Depth Omics of the Medical Institute of Bioregulation, Kyushu University started to develop, through joint research with BlueMeme Inc., language models in the biomedical field trained with a vast amount of biological data in that field by using quantum AI, in April 2023.[2] Such LLM is expected to become one of the tools for disease cause detection and pharmaceutical design.

Section 3 Issues and attempts relating to AI for Science

As discussed in Section 1, further use of advanced AI in scientific research will bring about new hypotheses and viewpoints, and it will be possible to conduct research and exploration under conditions and in a scope beyond what can be considered or experimented by humans, which is hoped to lead to new discoveries and breakthroughs. In this manner, the use of advanced AI is expected to have a possibility of not only increasing the speed and efficiency of research, but also leading to changes in science itself. At the same time, however, the ideal forms of science and researchers have also come to be questioned. While advanced AI enables an increase in efficiency and speed of experiments and simulations as well as automation and autonomy of research activities, it will be important for researchers to focus on setting research agenda and designing research, etc. while using AI as a tool.

Meanwhile, issues relating to reliability and safety which are associated with characteristics and limitations of AI are issues common to use of AI in scientific research. Further, issues concerning sharing of research data and reproducibility of research, and issues relating to papers and patents, etc. have also been pointed out. As technology develops further in the future, it is possible that new risks will become apparent and require further action. While discussions and studies progress on the development of countermeasures and the establishment of an international framework, there is a need for governance and responses that can be adjusted quickly and flexibly while monitoring technological progress and risks.

This section explains the issues involved in using advanced AI in scientific research, as well as the initiatives being taken to resolve them.

(1) Sharing of research data and open science

For use of AI in scientific research, it is important to publish and share research data that is generated in the overall research processes. Based on the "Principle on Management and Utilization of Publicly Funded Research Data,"[3] the government specifies the initiatives and publicizes them. It also promotes building, sophisticating, and implementing the NII Research Data Cloud, and supports core institutions of Research Transformation that develop environments which contribute to the building and use of research data platforms and the development of systems and rules for research data management in universities.

In addition, to realize open science, the National Institute of Informatics (NII), ROIS, is conducting research on a secure computation platform to accelerate the utilization of university research

1 Lin, Z., et al., (2023), "Evolutionary-scale prediction of atomic-level protein structure with a language model," *Science* 379, 1123-1130. https://www.science.org/doi/10.1126/science.ade2574

2 Kyushu University "BlueMeme and Kyushu University start joint research for building large language models by using quantum AI." https://sdgs.kyushu-u.ac.jp/11206

3 Integrated Innovation Strategy Promotion Council (April 2021), "Principle on Management and Utilization of Publicly Funded Research Data." https://www8.cao.go.jp/cstp/tyousakai/kokusaiopen/sanko1.pdf

data while appropriately managing it. Also, in January 2023, NII and NTT jointly started to offer a trial for universities to use the world's first secure computation AI software capable of training and inferencing with key algorithms in four major categories of AI while keeping data encrypted.[1]

(2) Issues concerning the reproducibility of research

The use of AI in research is expected to relieve the problem of reproducibility by consistently automating the conditions and procedures of experiments and methods for analyzing the results. On the other hand, it is also important to ensure the transparency of AI models and pre-trained data in order to maintain the reproducibility of research.[2] In relation to this, guidelines for using generative AI in research have been developed at universities and research institutions, etc. In addition, in AI research, it has become increasingly recommended that the model architecture and trained models be made public in order to ensure reproducibility and promote sharing with other researchers.

(3) Impact on submission rules, etc. for research papers

The impact of AI on research is significant, and it has also brought about changes in the rules for writing and submitting papers. For example, AI models can automatically generate drafts and sections of papers. It can also assist with quality checks and proofreading of papers, such as by pointing out missing references or statistical errors. Although it is possible to write documents using AI models, scientific journal publishers such as Springer Nature and Elsevier do not allow AI models to be authors,[3] The main concern behind this is the issue of the responsibilities required of authors. AI models are not necessarily responsible for the content. In cases where the use of AI models is allowed, the authors are required to appropriately state in the paper that AI has been used. In addition, the journals indicate that images created by AI models should not be used in the paper. On the other hand, if appropriate disclosure is made, the authors are allowed to use AI models to improve the language and conciseness of their papers. This is very useful for researchers in Japan whose native language is not English, when searching for specified information in research papers, and it can greatly reduce the time spent writing papers.

Another concern is the confidentiality of the information provided in prompts (instructions or questions entered by the users). This is because most AI models store the information contained in prompts and use them as training materials for the AI model. Elsevier instructs editors to treat the manuscript of a submitted paper as a confidential document and not to upload it to a generative AI tool.[4] In addition, the U.S. National Science Foundation (NSF) also issued a notice in December 2023 to reviewers and proposers not to upload information on projects proposed for research funding to AI models.[5]

1 National Institute of Informatics, ROIS, "NII and NTT started offering a trial for universities: to use a secure computation system: offering the world's first 'secure computation AI software capable of training and inferencing with key algorithms in four major categories of AI.'" https://www.nii.ac.jp/news/release/2023/0123.html

2 Ball, P., (2023), "Is AI leading to a reproducibility crisis in science?" *Nature* 624, 22-25. https://www.nature.com/articles/d41586-023-03817-6

3 Springer Nature, "Nature Portofolio/Editorial Policies/Artificial Intelligence (AI)." https://www.nature.com/nature-portfolio/editorial-policies/ai

4 Elsevier, "Elsevier Policies/Policies - Publishing ethics." https://www.elsevier.com/about/policies-and-standards/publishing-ethics

5 NSF, "Notice to research community: Use of generative artificial intelligence technology in the NSF merit review process." https://new.nsf.gov/news/notice-to-the-research-community-on-ai

(4) Problems and responses related to AI and intellectual property rights, such as copyright

A problem has also surfaced regarding who owns the rights and interests concerning an invention, if the invention was autonomously made by AI. Since the process of invention using AI is often a black box, it can be difficult to explain in detail how the invention was made when filing an application for a patent.

The relationship between generative AI and copyright was mentioned as one of the issues in the "Tentative Summary of AI Issues" compiled by the AI Strategic Council in May 2023. From July of the same year, the Legal Subcommittee under the Copyright Subdivision of the Cultural Council, organized the issues from the perspective of eliminating the concerns of creators and other rights holders, and minimizing the risk of copyright infringement for businesses that have developed and provided AI services and for AI users. In March 2024, the "General Understanding on AI and Copyright in Japan" was compiled. This document organizes and clarifies the concept under the current Japanese Copyright Act. For example, with regard to the "AI development and training stage," it clarifies the scope to which Article 30-4 of the Copyright Act — which allows the exploitation of a work without the permission of the copyright holder as long as it is not for enjoyment of the thoughts or sentiments expressed in the copyrighted work, in principle— will be applied (what cases constitute "in cases that would unreasonably prejudice the interests of the copyright holder" in the proviso to that Article, etc.). With regard to the "generation and utilization stage," the report clarifies how dependence should be considered in the relationship between AI-generated material and existing copyrighted work used in the development of generative AI, in respect to similarity [1] and dependence, [2] which are the requirements for copyright infringement. In the future, the government will inform and raise awareness of the people in an easy-to-understand manner and will continue to hold discussions while taking into account the accumulation of specific cases, including judicial precedents and court precedents related to copyright infringement, the development of AI and related technologies, and the progress of discussions in other countries.

Regarding the patent system, most national or regional intellectual property offices in the world, including the United States Patent and Trademark Office and the European Patent Office, hold the position that an inventor should be a natural person. The Japan Patent Office has also announced that the indication of the inventor is interpreted to be limited to a natural person, and that it shall not be permitted to indicate in the column for the inventor of the application, etc. an entry that is not a natural person (e.g., machines including AI, etc.).[3]

1 The fact that a later work is the same or similar to an existing copyrighted work.
2 The fact that the reproduction, etc. was made in reliance on an existing copyrighted work.
3 Japan Patent Office, "Regarding indication of thee inventor, etc.." https://www.jpo.go.jp/system/process/shutugan/hatsumei.html