Research area in Strategic Objective *"Research innovation through autonomous-driven research systems"*

R&D Process Innovation by AI and Robotics:
Technical Foundations and Practical Applications

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Overview

With the remarkable progress that has been made in artificial intelligence (AI) and robotics technologies, autonomous approaches for research and development (R&D) that accelerate the process of scientific research and technology development are becoming a global trend. By introducing AI and robotics, in addition to freeing researchers and engineers from simple tasks at R&D sites, it also becomes possible to take on complex subjects that go beyond cognitive and physical functions of the researchers and engineers. As researchers and engineers advance in R&D in collaboration with AI and robotics, the nature of R&D will be revolutionized, enabling previously impossible scientific discoveries and technological innovations.

In this research area, our aim is to establish an autonomously driven R&D approach to create fundamental technologies that will lead to innovation in R&D processes utilizing AI and robotics, and to develop science and engineering through practical application utilizing AI and robotics. Specifically, we will develop AI and machine learning methodologies and build robotics systems as fundamental technologies for innovation in R&D process. We will be also worked on specific R&D subjects utilizing AI and robotics in scientific fields such as life science and materials science, and engineering fields such as measurement engineering, mechanical engineering. By closely linking the development of fundamental technologies and their application of scientific and technological research to practical subjects, our aim is to create new scientific discoveries and technological innovations while building a general-purpose framework for autonomously driven R&D.

This research area participates in the Ministry of Education, Culture, Sports, Science and Technology (MEXT)'s Advanced Integrated Intelligence Platform Project on Artificial Intelligence/Big Data/IoT/Cybersecurity (AIP Project).

Research Supervisor's Policy on Call for Application, Selection, and Management of the Research Area

1. Background

Conventional scientific research and technology development have been based on the intuition, experience, and inspiration of researchers and engineers. Therefore, the progress is made within the limits of humans' cognitive and physical abilities. In recent years, R&D subjects have become more complex. In order to address complex subjects via traditional approaches, it has been necessary to split complex targets into simpler elements. However, due to this splitting into elements, we are faced with the problem of misunderstanding the properties of the whole and a loss of overall optimality..

With the rapid development of AI and robotics in recent years, autonomous approaches that accelerate the R&D process are becoming a global trend. Utilizing the autonomous nature of AI and robotics will enable R&D that transcends the cognitive and physical functions of researchers and engineers, leading to scientific discoveries and technological innovations in unexplored areas. Additionally, the introduction of AI and robotics has the potential to fundamentally transform the R&D process.

2. Aim of this Research Area

Based on the above background, in this research area we will develop basic technologies for AI and robotics to innovate the R&D process, and then apply them to practical subjects in scientific research and technology development. In addition to *automation* (Note 1), which frees researchers and engineers from simple tasks by introducing AI and robotics, we will particularly promote research into *autonomy* (Note 2) based on the autonomous functions of AI and robotics. Through interactions with researchers and engineers, we aim to build a framework that enables systemic scientific discoveries and technological innovations. This will be achieved by having AI and robotics autonomously iterate *R&D process loops* (Note 3) such as hypothesis generation, prediction and analysis, experimental validation, and knowledge acquisition.

In the development of basic AI technologies, we are conducting research on machine learning theories and algorithms that can be used in scientific research and technology development. Additionally, we are developing methods to utilize them for hypothesis generation, performance prediction, experiment planning, and knowledge acquisition. Instead of a technology that is specialized to a specific R&D task, our aim is to develop AI technologies that have a certain level of generality and that can be applied to a wide range of R&D subjects.

In the development of basic robotics technologies, we are researching new robotics systems (including hardware and software research) that can be used in scientific research and technology development. Additionally, we are also building mechanisms to utilize them in the R&D process.

We are particularly developing autonomous robots equipped with AI that facilitate interactions with researchers and engineers. Instead of a technology that is specialized to a specific R&D task, we aim to develop robotics technologies that have a certain level of generality and that can be used for a wide range of R&D subjects.

In terms of practical applications to specific R&D subjects, our aim is to utilize AI and robotics to achieve scientific discoveries and technological innovations that could not be realized via conventional approaches. This applies to both scientific research (including science in general and not limited to specific fields such as life science or materials science) and technology development (including engineering in general and not limited to specific fields such as measurement engineering and mechanical engineering). Based on proposals from various scientific and engineering fields that are addressing challenging R&D issues, we are collaborating with researchers developing AI and robotics technologies and aiming for scientific discoveries and technological innovations.

"Automation" and "autonomy" in this research area are defined as follows. "R&D process loop" is also defined as follows, but it is not necessarily limited to this definition, and we expect that there will be more open-ended and challenging proposals.

[Note 1: Automation]
The process of improving work efficiency and productivity by having a machine or system perform human work within a programmable range by executing actions as instructed by the system based on pre-programmed procedures and decision criteria.

[Note 2: Autonomy]
Autonomous systems flexibly respond to their environment and act based on their own judgement. Even when information is limited or when conditions change, the system grasps and understands the surrounding situation, and then searches for and executes optimal solutions to achieve its goals.

[Note 3: R&D process loop]
A loop consisting of multiple R&D tasks in scientific research and technology development that aims to realize scientific discoveries and technological innovations. Although the specifics vary for each problem, most R&D involves an iterative process of the following tasks: 1) generate a promising hypothesis, 2) prediction and analysis the performance of the hypothesis, 3) verifying the performance of the hypothesis via experiments, and 4) organizing the experimental results and acquiring knowledge. In this research area, this series of R&D processes is referred to as the "R&D process loop." Note that the components of the loop are not limited to hypothesis generation, prediction and analysis, experimental verification, and knowledge acquisition; any process that is generic to a wide range of scientific research and technology development can be considered to be a component task of a loop.

3. Specific Research and Development Examples

In order to realize the above aims, we will work on the following research in particular, but will not necessarily be limited to these areas and expect that there will be more open-ended and challenging proposals.

(1) Research on AI and machine learning technologies for R&D process innovation

- Research on generative AI for generating hypothesis in R&D (examples: research on theories/algorithms for generative AI; molecular design via generative AI; automatic report generation via generative AI, etc.)
- Research on AI that performs experimental planning and process optimization for R&D (examples: research on theories/algorithms for AI-based experimental planning; research on algorithms for process optimization, etc.)
- Research on AI for analyzing multimodal data (examples: development of vision and language models; computer vision and natural language processing applications for R&D, etc.)
- Research on the fusion of AI and simulations (examples: simulations utilizing AI; construction of new simulation technologies by integrating data-driven and model-driven approaches, etc.)

(2) Research on robotics systems for R&D process innovation

- Research on autonomous robots that can flexibly respond to their environment and act on their own judgement (examples: research on robot motion generation, research on robots that recognize their environment through autonomous trial and error, etc.)
- Research on autonomous robots that can grasp and understand their surrounding situation and then execute plans to achieve their goals even with limited information or in changing conditions (examples: research on task planning and motion planning, etc.)
- Research on interactions between robots and researchers/engineers (examples: research on introducing the know-how of researchers/engineers into robots; research on how to provide feedback from the robots to the researchers' five senses, etc.)
- Development of robotics systems that perform experiments that cannot be realized by researchers and engineers due to their physical limitations (examples: robots that perform experimental operations on very tiny objects; robots that perform complex tasks based on diverse information, etc.)

(3) Research on scientific discovery and technological innovation utilizing AI and robotics

- Research topics that aim to make new scientific discoveries from large and diverse data sets that exceed the cognitive capabilities of researchers and engineers (targeting all scientific fields,

including life science and materials science)

- Research topics that aim to develop technologies for advanced experimental systems that exceed the physical abilities of researchers and engineers (targeting all engineering fields, including measurement engineering and mechanical engineering)
- Research topics that aim to make scientific discoveries made possible through the use of AI and/or robotics (targeting all scientific fields, including life science and materials science)
- Research topics that aim to develop technologies made possible through the use of AI and/or robotics (targeting all engineering fields, including measurement engineering and mechanical engineering)

[Keywords]

Machine learning, deep learning, generative AI, large language models, Bayesian inference, causal inference, human computation, multimodal measurement and analysis, extraction of tacit knowledge, integration of AI and simulation, autonomous robots, robust control, reinforcement learning, imitation learning, data-driven control, motion planning, human interface, laboratory automation, machine vision, bioinformatics, materials informatics and other field-specific informatics technologies, process optimization, life science, materials science and other scientific fields, measurement engineering, mechanical engineering and other engineering fields.

4. Anticipated Research Approach

In this research area, in order to advance both technical foundations and practical application of autonomously driven R&D, we will conduct our research in close collaboration with researchers developing basic AI technologies (AI field), basic robotics technologies (robotics field), and researchers working on practical scientific research or technology development (practical R&D field). We expect researchers in each field to take the following initiatives.

- Researchers in the AI field are expected to work on collaborative research to promote autonomously driven R&D in collaboration with researchers in the robotics and practical R&D fields while also promoting cutting-edge AI theories and algorithms research.
- Researchers in the robotics field are expected to work on collaborative research on introducing AI to robotics and on applying robotics to practical R&D tasks while also advancing research on cutting-edge robotics technologies.
- Researchers in the practical R&D field are expected to collaborate with the AI and robotics fields, working on challenging research projects that can only be realized through the utilization of AI and robotics.

In this research area, through each collaboration, we expect to advance discussions on the nature of R&D activities, social acceptability, and science communication for when a highly autonomous R&D approach is established. Although PRESTO is individual-based research, we will actively encourage

the selected researchers to promote collaboration within the field, interact with industry, and utilize data through data infrastructure such as RIKEN. In order to maximize the results not only of this research area but also of the JST Strategic Basic Research Programs, we will collaborate with related CREST and PRESTO research areas and jointly hold workshops and symposiums as necessary. We will also promote efficient and effective research through technical collaborations and research exchanges with research areas such as the following, which are currently ongoing: the JST-Mirai Program's "Common Platform Technology, Facilities, and Equipment" mission area of "Accelerating Life Sciences by Robotic Biology"; the Moonshot Research & Development Program's Goal 3 of "Realization of AI robots that autonomously learn, adapt to their environment, evolve in intelligence and act alongside human beings"; the RIKEN Center for Advanced Intelligence Project (AIP) and TRIP-AGIS; and the Data generation and utilization materials R&D projects(DxMT).

5. Research Period and Budget

The research period is within three and a half years, and the budget at the time of application is 35 million yen (excluding indirect costs). During the research period, additional budget allocation may be made for collaboration activities to promote autonomously driven R&D approaches.

6. Points to Note for Application

In this PRESTO research, through truly impactful but difficult-to-achieve research we hope to produce incisive results that will help the next generation of leaders step up. Therefore, we will positively evaluate original and challenging proposals and approaches that have the potential to contribute to the goals of this research area and that are not afraid of failure.

This research area aims to establish an autonomously driven R&D, and is primarily looking for proposals in the AI, robotics, and practical R&D fields (general scientific fields including life science and materials science, as well as general engineering fields including measurement engineering and mechanical engineering) (however, proposals from different perspectives that promote R&D via an autonomous R&D approach are also welcome). Proposals in the AI field should not be tailored to specific issues in the field, but should be broadly applicable to autonomous R&D approaches. Additionally, please also describe your outlook regarding collaboration with the robotics and practical R&D fields. Proposals in the robotics fields should not be tailored to specific issues in the field, but should be able to broadly promote autonomous R&D approaches by giving robots autonomy. Additionally, please also describe your outlook regarding collaboration with the AI and practical R&D fields. Proposals in the practical R&D field should clearly state what kind of changes will be brought to the field if the target R&D issues are solved. Additionally, please also describe your outlook on how AI and robotics can be used to solve the target issues.

As mentioned above, this research area encourages research in collaboration with other fields after

a project has been selected, and as such we look forward to receiving research proposals that include not only proposals from your own specialization, but also potential collaborations with other fields (however, when collaborating with researchers outside of this PREST, they will not be eligible for additional budgetary allocations). If you plan to collaborate with other fields, please describe how your research will contribute to the development of autonomously driven R&D approaches through collaborations with other fields, and what benefits the collaboration will bring to both your and the researchers with whom you will collaborate. At the time of your application, it is not necessary to make a detailed research plan for the collaboration with other fields; it is sufficient to simply describe the outlook.

This research area, as a member of Advanced Integrated Intelligence Platform Network Laboratory (AIP Network Laboratory) that constitutes MEXT's AIP project (on Artificial Intelligence/Big Data/IoT/Cybersecurity), contributes to the research collaboration activities with the RIKEN Center for Advanced Intelligence Project and other related research institutions.