北陸先端科学技術大学院大学研究室教育指針
Laboratory Education Guideline

研究室教育指針は、学則第３０条の３に基づき、研究指導の方法及び内容並びに修了までの研究指導の計画をあらかじめ明示するものです。
Based on the Article 30-3 of the general academic rules, the Laboratory Education Guideline is intended to clearly outline the methods and content of research guidance, as well as the plan for research guidance until completion.

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1. 研究テーマ / Research Theme

In this laboratory, we aim to establish novel approaches for materials discovery and property design by integrating Materials Informatics (MI) with materials science simulations, based on data science and computational science. The target materials systems cover a wide range, including organic, inorganic, and biomaterials, and span multiple length scales from atoms and molecules to clusters and bulk solids.

Our research methodologies are based on hierarchical materials simulations such as first-principles electronic structure calculations, molecular dynamics simulations, and computational thermodynamics. These approaches are combined with data-driven methods using machine learning and artificial intelligence, including deep learning, Bayesian optimization, evolutionary algorithms, annealing methods, and quantum annealing. These studies are conducted using the university's supercomputing facilities and laboratory-owned servers, supported by research infrastructures established through competitive research funding.

2. 修得が期待される能力 / Competencies expected to be acquired

研究室教育は必修 A 科目（先端）又は研究支援科目（融合）の一部として単位化されており、この欄はそれら科目のシラバス上の達成目標の一部となります。
Laboratory Education is accredited as a part of the Required courses A (Division of Advanced Science and Technology) or Research Support Courses (Division of Transdisciplinary Sciences), and this section constitutes a part of the course goals stated in the syllabus for such subjects.

(1) Master's Program

In the master's program, the primary goal is to systematically acquire the fundamental practices of research required for researchers and advanced engineers. Students are expected to develop the ability to independently and progressively carry out the entire research process under supervision, including acquiring specialized knowledge, conducting literature surveys, defining research problems, designing research methodologies, formulating research plans, performing research, and summarizing outcomes through a master's thesis and academic presentations.

In the first year of the master's program, students actively utilize coursework to consolidate their specialized knowledge while deepening their understanding of research backgrounds through literature surveys. They are expected to define research topics, examine appropriate research methods, and ultimately formulate their own research plans. Emphasis is placed on breaking down research plans into manageable tasks and steadily achieving small goals. This approach is grounded in mathematical problem-solving principles and aims to cultivate logical and quantitative thinking skills for structurally decomposing and solving complex research problems.

To ensure smooth progress in research, students are also required to acquire sufficient computational skills and proficiency in operating research-related computing environments at this stage. Even at the master's level, a passive, instruction-dependent attitude is not acceptable. Students are expected to gradually develop the ability to independently organize their research progress and challenges, and to appropriately report, communicate, and consult with supervisors in a timely manner.

In the second year of the master's program, students conduct research independently

based on their established research plans and develop the ability to systematically summarize their results. While the ultimate goal is the completion of a master's thesis, target outcomes are flexibly adjusted according to the student's career path. Students seeking employment after the master's program are encouraged to acquire the ability to clearly communicate their research to audiences from different fields or without scientific backgrounds. Students aspiring to enter the doctoral program are expected to compile their research findings into original research papers and, if possible, publish at least one first-author journal article during the master's program.

For students who decide at an early stage to pursue doctoral studies, the laboratory provides an environment that allows these goals to be advanced earlier, including early engagement in international conference presentations and original research publications.

(2) Doctoral Program

In the doctoral program, students aim to acquire the ability to independently define new research topics and lead research projects as autonomous researchers, building upon the research skills developed during the master's program. Beyond extending their master's research themes, students are expected to identify new research challenges based on trends in the broader research field and to manage multiple research projects in parallel.

Doctoral students are positioned not merely as supervised students but as collaborative researchers working on an equal footing with faculty members. Faculty members serve simultaneously as supervisors and research collaborators. Doctoral students are therefore expected to clearly organize their research objectives and challenges, proactively arrange discussions, and engage in constructive exchanges of ideas within limited time frames.

Students are required to decompose research plans into concrete tasks and independently manage research progress. This process fosters advanced quantitative and logical thinking skills necessary for overseeing complex research projects. Doctoral students are also expected to serve as mentors to master's students by providing guidance and research support within the laboratory.

Opportunities are provided for participation in international collaborative research projects, depending on the student's research topic and aptitude. In addition, students are encouraged to gain firsthand experience in international research environments through short-term study abroad programs and visits to overseas research institutions, thereby developing a global perspective on their research activities.

The most important objective of the doctoral program is the continuous production of original research papers. Doctoral students are expected to actively participate in conferences, workshops, and research meetings, engage in discussions within the research community, and demonstrate the initiative and independence necessary to establish new collaborative research themes.

3. 研究指導方針 / Research Guiding Principle

Guided by the principle that "cutting-edge, world-level research provides the best possible education," this laboratory places strong emphasis on timely degree completion while fostering the ability to conduct independent research as researchers and advanced engineers. Research supervision is carried out in a stepwise, systematic, and well-planned manner, taking into account the entire process from research initiation to thesis preparation and degree examination.

Students learn the full research process—ranging from understanding research backgrounds and defining problems to planning, executing research, and producing research outcomes—through participation in ongoing research projects and collaborative studies. Special emphasis is placed on decomposing research plans into concrete tasks and steadily accumulating achievements, thereby cultivating problem-solving skills based on mathematical and logical reasoning.

Even in the emerging field of Materials Informatics, the laboratory emphasizes the importance of thoroughly understanding established materials science knowledge and theoretical foundations. Rather than focusing solely on novelty, we encourage students to

“stand on the shoulders of giants” and pursue research that balances fundamental understanding with advanced applications.

Master’s students are expected to move beyond a passive, instruction-dependent approach and develop an autonomous research attitude characterized by proactive reporting, communication, and consultation. Doctoral students are supported in their development as independent researchers who lead research projects as equal collaborators with faculty members and actively engage with the research community.

4. 研究室活動の内容及び方法 / Content and Methods of Laboratory Activities

□日次活動 / Daily Activities：

This laboratory emphasizes flexible research activities tailored to individual research topics and progress and does not impose fixed core hours in principle. At the same time, to foster professional research habits, students are encouraged to arrive at the laboratory by 10:00 a.m. on weekdays, except when there are legitimate reasons such as coursework and prior notification has been given.

□週次活動 / Weekly Activities：
□月次活動 / Monthly Activities：
□不定期活動 / Occasional Activities：

Research supervision is primarily conducted through individual meetings, typically held about once every two weeks depending on research progress. Additional meetings may be arranged as needed, including rehearsal sessions prior to conference presentations. Visits to collaborating universities, research institutes, and companies, as well as domestic and international travel for research discussions, are regarded as integral parts of laboratory activities.

Participation in workshops and area meetings (approximately two to three times per year), domestic conferences (spring and autumn), and international conferences (approximately once per year) is encouraged to promote dissemination of research achievements and interaction with the research community. Doctoral students are also encouraged to conduct sub-theme research at overseas institutions.

5. 年間スケジュール / Annual Schedule

本学の全学共通の年間スケジュールは「履修案内」の「学位取得に至るスケジュール」を参照してください。（本学HP 参照：ホーム＞教育＞履修関係＞履修案内）

Please refer to the “Degree conferment schedule for the master’s program/doctoral program” in the “Degree Completion Guide” for university-wide common schedule (JAIST website: Home >Education>Taking Courses>Degree Completion Guide)

For the master’s program, students primarily complete coursework during the first year (1-1 and 1-2 terms), and generally finish the required credits by the 2-1 term. In the latter half of the first year, students engage in preliminary research aimed at preparing a research proposal. By the end of the 2-2 term, they submit a research proposal that includes preliminary computational results. From the second year onward, students conduct full-scale research, complete their master’s thesis, submit it in early February, and undergo thesis examination in mid-February. Domestic academic conferences are typically held in March (spring) and September (autumn).

In the doctoral program, students finish coursework and acquire required credits during the first and second years and submit their research proposal at the end of the first year. In the third year, students apply for degree candidacy in September, undergo a preliminary dissertation review around December, and hold a public dissertation defense in January, aiming to complete the doctoral dissertation.

N.B. The above schedule applies to students enrolling in April, while for those enrolling in October, the same schedule applies, with all milestones shifted by approximately six months relative to the enrollment date.