Collaborative Education for Next-Generation INnovators & Exploration of knowledge intersections

C-ENGINE

# C-ENGINE
## Case studies of Research Internships

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## Materials informatics, molecular search algorithm

## Kyushu University × DAICEL Corporation

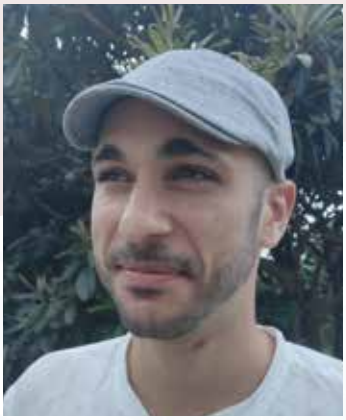
### Challenge Yourself with Research Internship
### Create the Seeds to Cultivate the Future

Research internships have been said to be beneficial for students and companies, but it has been very difficult to spread and establish them. We are tackling this problem by forming a consortium of several universities and several companies to create, disseminate and promote a new and unprecedented internship format.

University co-ordinators act as liaisons between students, university teaching staff and companies, and coordinate each case individually, thus improving the quality of research internships and expanding their volume. We are also accumulating know-how on the implementation of internships, and some good practices are already being developed. We are convinced that building on these examples and continuing the collaboration and communication will lead to the creation of innovations.

Collaborative Education for Next-Generation INnovators
& Exploration of knowledge intersections

# Crossing research innovation and cultural boundaries with mathematics



Edoardo FABBRINI
Kyushu University Graduate school of Mathematics
D2 Student (at the time of internship)

## Internship overview

Period : 2/Oct.2023 - 31/Oct.2023 (1 month)
Hosts: DAICEL Corporation
Production Engineering Center, Production Division
Title: Materials informatics, molecular search algorithm

### ■ What motivated you to come to Japan? Can you tell us about your background?

My main reason for coming to Japan is to having the opportunity to work with my supervisor, who works at Kyushu University. Undoubtedly, the prospect of immersing myself in the unique culture of Japan, a country that many Italians, including myself, admire for its rich history and vibrant pop culture, such as animation, was a thrilling part of my decision. I am originally from Italy and have a bachelor's degree in mechanical engineering and a master's in aeronautical engineering. I am currently enrolled in a PhD program in applied mathematics, where I work with my supervisor on mathematical modeling of mechanical and chemical systems. The topic I'm currently working on is not closely related to my undergraduate studies. However, I am grateful for the opportunity and value the experience I gained from the chemical informatics internship, despite the differences in my academic background.

### ■ What motivated you to participate in this internship despite being in a different field?

During this internship, I applied numerical calculations to solve chemistry problems. While some knowledge of chemistry was necessary, the primary focus was on utilizing mathematical methods. Mathematics is versatile and adaptable, and its methods can be applied across various fields. I have enjoyed applying mathematical modeling in diverse areas, so I found this challenge enjoyable. Working with quantum chemical calculations was challenging but also an excellent opportunity to apply my skills in a new field.

### ■ How do you think Japanese companies compare with Italian companies?

Before coming to Japan, I worked for a year in an Italian company. There is a common stereotype that Japanese people are always working; however, I found the working environment here to be very friendly. We often went out for meals and social gatherings, and I felt welcomed by the people around me. One cultural difference that surprised me was the practice of everyone cleaning the lab together after work. It doesn't matter what your position is, and everyone participates in the cleaning. This stands in stark contrasts to Italy, and I found it valuable in promoting mutual collaboration.

### ■ How has your work experience in Italy helped you in this internship?

During my year in Italy, I worked mainly in software development in the aerospace industry. This experience was particularly relevant for my internship in chemical informatics, as it involved a significant amount of coding. The skills I acquired in software development were beneficial, although the fields were different.

### ■ Were there any significant differences in how a Japanese company conducts research projects compared to Italy?

This internship was in DAICEL's research and development department, which is very different from the typical corporate environment in Italy. The way the research department operates is also different, so it is difficult to make direct comparisons. However, I would say that the success of the projects you work on often depends on how well you manage your team leaders and workflow.

### ■ How long and what was your role in the research project with DAICEL at Kyushu Univ you jointed prior to this internship?

I worked on a project at Kyushu University for about six months, where my supervisor had already started joint research with DAICEL. My role was to support the other team members in building a materials search engine to explore and discover new materials. I contributed by creating a framework to handle the functions and routines used in the system.

### ■ Did you have to do any preparation before starting your research internship?

In my case, I didn't have to do any preparation as I was already working on the same project before starting my internship. I think DAICEL selected me because I had already been involved in a joint research project with Kyushu University, so I did not need any special guidance or preparation. I didn't want to spend time merely "learning" during the 1-month internship; as it only lasted for one month, but thanks to my prior knowledge, I was able to dive right into the project.

### ■ Which part of this research internship project was the most challenging?

The most challenging part was time management. We already had a clear plan of what had to be done, but midway through the internship, we began running out of time as we worked on building modules that needed to integrate seamlessly with other sub-modules. The interlocking process was simple, but we had to rush a lot towards the end.

### ■ What did you gain from working at the DAICEL's research facility this time, and did it meet your expectations?

I had the opportunity to learn various new techniques, including Molecular Dynamics and Quantum Chemistry Computations, as well as structural dynamics methods like the Difference Element Method. This experience broadened my understanding of research methodologies. I checked "Deeper discussion with specialists of different research fields" because I engaged in numerous discussions with experts from various fields, including experimental chemists and organic chemistry specialists. These interactions allowed me to delve into discussions with specialists from diverse research areas. One of the most surprising discoveries during my time at DAICEL was the extensive use of advanced mathematics by the employees in their daily tasks, a practice I had not anticipated. This realization gave me a clearer perspective on the societal impact that university research can have. Also, working in the DAICEL computational cluster was a valuable experience. It offered a unique opportunity to engage with a sophisticated and costly system of interconnected machines. The knowledge of chemistry I gained has proven to be very beneficial and useful for my research in chemical informatics.

### ■ Did you encounter difficulties conducting research in Japan as a foreign researcher?

I am in a unique situation because most of my supervisors and the professors I work with are foreigners. The only surprise for me was the level of English proficiency among the students. While the professors speak fluent English, I had anticipated that more students would be equally fluent in conversational English. However, everyone made a genuine effort to communicate actively, and the overall environment was excellent.

### ■ How was life during the research internship?

During the internship, I stayed at a hotel provided by the company, about an hour away from DAICEL. The location was beautiful, especially the iconic white castle of Himeji. The local food was a delightful surprise, and we made it a point to explore as many local restaurants as possible. My colleagues were friendly and often took me to places like Kobe for some fun outings.

### ■ What are your future goals as a researcher?

As a researcher, my long-term goal is to consistently act as a bridge between scientists from different fields. I aim to build a network of collaborators from other scientific areas, such as chemistry, engineering, and biology, to transfer in these fields ideas, tools, and methodologies developed in mathematics. In this sense, being Japan home to some of the most developed industries in the world, it provides an ideal environment for pursuing this goal, and my internship at DAICEL is a clear example of that. My focus is not only on research; teaching is equally important to me, and I believe the two are deeply interconnected. Being a good mentor enhances my abilities as a researcher, and vice versa.

### ■ Do you have any advice for other students who want to do a research internship in Japan?

I encourage them to give it a try it. It's a unique experience. Don't hesitate to try!

# Students should carefully verify that the internship is truly research-oriented

Pierluigi CESANA
Kyushu University Graduate school of Mathematics
Institute of Mathematics for Industry
Associate Professor

### ■ What is your opinion about taking postgraduate students on internships while they are busy with their PhD research and thesis writing?

Students need to do research, develop their own academic background, and attend lectures. This was one of my biggest concerns, especially for a PhD student like Edoardo, who had just finished his first year. The actual research begins in the second year, and we were initially concerned that the research internship might delay this process.

However, this internship was well organized, and I was happy with the outcome. Internships are very important, especially in an applied mathematics program like that at Kyushu University.

Our University offers a PhD program in functional mathematics through the Institute of Industrial Mathematics (IMI). Thanks to our cooperation with industry, the internship provided not just a theoretical exercise, but also a practical experience that prepared Edoardo for the real-world challenges of his field. The one-month duration was reasonable and aligned well with the PhD program. We discussed the participation in the research internship in detail beforehand, which benefited both parties.

### ■ How do you think students can manage both their internship and doctoral studies?

Balance is essential, and in Edoardo's case, it made a lot of sense, both in terms of duration and subject matter.

Personally, I found it very beneficial through my own research internship experience as a student in the USA. I have also seen similar internships taking place at national research institutes there, where students have many options.

Kyushu University's internship program is effective because it is structured and well-planned. We spent a lot of time talking to companies to ensure that Edoardo was the right candidate and to clarify what he would be doing in his internship so that it was never makeshift.

### ■ Did you notice any changes in Edoardo after his one-month internship?

Yes, this internship was very beneficial for him, as it gave him the opportunity to explore similar topics from a different perspective through industrial research and coding on high-performance computers.

It also allowed him to work on a cluster server, which was instrumental in developing his technical skills and expanding his knowledge.These experiences will be advantageous for any future career he pursues. Furthermore, he would have developed a sense of discipline separate from his university studies by regularly reporting his progress to his supervisor and adhering to a schedule. Although it lasted only a month, it was an essential part of his education.

### ■ You have previously carried out joint research with DAICEL. Is it common to send students on research internships as part of such joint research?

Yes, we have sent many students from Kyushu Universi-

ty on research internships, although I was not directly involved. Some of our students had the opportunity to intern at companies with close links to chemistry, including pharmaceutical companies, chemical manufacturers, and research institutions. Currently, we run industrial research groups with several companies. These companies play a crucial role in our research, as they bring real-world problems to our attention and work with our students to develop innovative solutions. It is an ongoing partnership, and we maintain strong relationships with many industries. Depending on the project, more students can participate in the internship.

### ■ If students face difficulties during their research internship, do you advise them on how to solve problems?

In my experience, internships provide a unique opportunity for students to apply their knowledge and skills to real-world problems. For instance, Edoardo began working on problems related to the DAICEL collaboration, which proved to be a valuable experience. Most students undertake internships alongside their research. Although these may not be directly related, they are still worthwhile. I did not intervene in Edoardo's internship, and he was able to solve the problems himself. The mentors from DAICEL actively monitored his progress, so Edoardo was able to learn how to interact with individuals in various roles. I believe this experience helped him expand his network and build valuable relationships for the future.

### ■ Were you concerned about intellectual property (IP) during his internship?

We are always aware of IP issues, especially in joint research projects. In Edoardo's case, we dealt with IP issues separately and made sure that all agreements were properly established from the start.

Through this case, we discovered that Japanese Universities, including Kyushu University, have a certain flexibility regarding IP. If you take the time to build trust with your industrial partners, you can discuss these issues openly and find a compromise that works for everyone. In this instance, there were no conflicts, as everything was made clear from the beginning.

### ■ If compromising too much on how intellectual property (IP) is handled, it could lead to IP leaks. Is there any concern that students might unintentionally share confidential information?

In this case, Edoardo's mentor in DAICEL was a highly experienced professional with a PhD in chemistry and a solid academic background, so he was well aware of these issues. Edoardo's mentor was always open to finding compromises, and we appreciated his positive and pleasant approach. This spirit of collaboration has made our ongoing partnership not only successful but also mutually beneficial.

### ■ Sometimes companies see research internships as an opportunity 'to teach and give to' students, but do you see research internships as a 'give and take' with specific benefits for the company?

Yes, exactly. Internships are beneficial for both students and companies. The company gets fresh ideas and valuable contributions from the student while the student learns and grows through the experience.

### ■ Based on your experience, what are your thoughts on research internships in general?

Research internships are a fantastic opportunity for students to expand their networks, acquire new skills, and gain valuable experience. However, in some cases, the internship may become part of the company's everyday routine work, and the objectives might not be fully achieved. Therefore, students should carefully verify that the internship is truly research-oriented.

At Kyushu University, we value internships across all types of companies. While students are often drawn to well-known firms, they can also make a significant impact at smaller or less well-known companies. I have seen several cases of small start-ups in Japan that offer great opportunities for students. This open-minded approach can lead to unexpected and rewarding opportunities. I hope that C-ENGINE will provide similar internship opportunities in the future.

# Challenges of a research internship successfully implemented in-house

Yu KANEKO
DAICEL Corporation
Production Engineering Center, Production Division
Senior engineer

## ■ What was your research internship like this time?

This time, the research was based on joint research, and the final output was to run the program that had been created jointly with Kyushu University and our company as well. However, within a week or so of Ed-san's arrival for his internship, we were able to run the program in-house, and he went on to conduct a material search for the wavelengths of chemical absorption using this technology, which was a step up from the main theme to actual research and development based on the joint research technology. This was a step up from the main theme. Although the schedule was relatively overcrowded, Ed-san was excellent and completed it without difficulty, leaving us with a successful outcome. He told us that he originally came from a different field, but we didn't get that impression at all, so we assume that he had studied enough at the university before starting his internship.

## ■ What impression did the intern students give you?

When I met Ed-san at Kyushu University before I started this internship, I had the impression that he spoke easy to understand English and were easy to talk to. That impression has not changed throughout the internship. On the other hand, at first I thought that simulation in a different field might be somewhat difficult, but my perception changed dramatically when I saw the way he reliably grasped our requests and produced output. I also felt that his attitude towards work was different from those of other students.

I felt very grateful that he was extremely diligent and had a work style of coming in laboratory firmly on time and leaving on time. He was always aware of the outputs of carrying out his research tasks, and were able to effectively follow the cycle of proposing his own project policies, formulating his own strategies to achieve them, and we were receiving weekly interim reports, which is used as the basis for further feedback. I believe that he was able to effectively follow the cycle of giving feedback to the next action based on this. Therefore, we were able to leave the work to him with peace of mind.

## ■ What do you feel you gained from this research internship?

The programs used in the research are not always designed to run on Windows, so If the system configuration inside the computer does not match and does not work, tuning is required on a case-by-case basis. This time, the challenge was a complex program running on a computer server, but we were able to implement the algorithm developed at Kyushu University in-house, which was a great achievement. It was also a great benefit to have the effectiveness of the algorithm demonstrated in a research topic reduced to a simple task. As a result, he achieved the software and a manual for use and we are actually using the algorithm to conduct molecular searches in-house and are currently in the process of using it. This case resulted in an approach being completed with a high potential of applicability, so his advisor offered to do additional research after Ed-san returned to the university.

### ■ Intern students were impressed by the way your company makes use of advanced mathematics.

There are many situations in which mathematics can be utilized in chemical companies. Our department specializes in numerical analysis, and our work includes process analysis, fluid analysis, and computational science. I believe that we have a group of employees with strong mathematical backgrounds. Ed-san originally specialized in fluid mechanics and was often seen interacting with employees who were simulating fluids. I was also impressed that many employees in the company were positive about communicating in English and actively engaged in discussions with Ed-san.

### ■ Have there been any changes in your company's staff as a result of the internship?

Even employees who were somewhat uncomfortable with English felt that the threshold for communicating in English had been lowered. In addition, the group that conducts molecular exploration using machine learning seems to have been positively influenced afterwards through this discussion on machine learning with Ed-san.

### ■ What were your own difficulties and innovations as a mentor?

There were times when we had difficulty communicating in English, but it did not interfere with our work at all. Ed-san was able to anticipate our moves and respond to them. With his extensive social experience, he gave the impression of being a working doctor, and we could work in a relaxed atmosphere among adults.

I and other employees have worked hard to create an environment where Ed-san could fit in with his surroundings and create opportunities to communicate with various people. Thanks to this, Ed-san built good relationships with many employees while doing his job. Ed-san was also very open to dinner invitations, and we sometimes went to a ramen restaurant after work or sightseeing in Kobe or Himeji with other interns on weekends. Ed-san's preference for in-person collaboration was respected by the team. Even on days when I was working remotely, other team members were able to work effectively with Ed-san.

### ■ How did you handle IP in your research internship?

This time, as a part of this R&D assignment, we asked him to conduct color tuning from a different perspective than our in-house work. In addition, intellectual property was separated and examined beforehand. In addition, we chose content that would produce results in three weeks. Because of the research internship through joint research, we had a trusting relationship with the professors and students, and Ed-san was able to carry out his research activities while taking confidential information into consideration.

# Mentor's perspectives

### ■ Does your company accept many international students for research internships?

International students may come to us 2 or 3 times a year. Not only our own internships, but also at the request of organizations that support internships for international students, and at the request of universities with which we collaborate. Last year, two students, including Ed-san, did internships in our department and another student in other department. We often have internships for international students, for varying periods of time and from different countries, but I think the trend is towards students from Europe and the US.

### ■ What types and fields of study would you like to accept students from in the future?

During the period of the Covid-19, it was difficult to carry out internships in experimental fields, but now such restrictions are getting fewer and we would like to consider accepting students who wish to take part in experimental programs, mainly in chemistry, which is our business in the future,

### ■ Lastly, any comment to the intern students?

This time, based on joint research with Kyushu University, we were able to bring in Ed-san, who had been working with us, as an intern. We feel that it was a great achievement to have obtained in-house implementation of the new algorithm, which was the result of our joint research. I also think that Ed-san's working and work attitude was very impressive. It was a very good research internship that captured these ideas and we have given him a high rating in his assessment report. We hope that Ed-san will use his experience with us to develop his future life and career path.

## Take a challenge of C-ENGINE's research-internship and prove yourself!

C-ENGINE is a consortium of leading Japanese companies and major universities to promote research internships that are beneficial to both graduate students and companies.

C-ENGINE's research internships start with finding a point that matches your research and society. The program is customized and tailor-made for each case, based on a mutual understanding of others' situations and the areas in which you and the company can collaborate.

We look forward to your active use of this program as an excellent opportunity for you to join a company's research institute, get involved in R&D work as a company member, gain a deeper sense of your relationship with society, broaden your research horizons, and obtain guidelines for considering what career path you would like to pursue in the future.

The IDM (Internship Dynamic Matching) system is open to all the C-ENGINE member students! Once you register on the IDM system, you can browse and apply for the variable research internship themes. If you still need to register, please check it using the QR code/link below!

**Register your account for IDM system!**

https://www.c-engine.org/student/registration/

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**Collaborative Education for Next-Generation INnovators & Exploration of knowledge intersections**

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