ROLLAND DORIAN

RIKEN internship summer 2025

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COMPUTATIONAL MOLECULAR SCIENCE RESEARCH TEAM

Reasons for application

20th November 2024

Dear RIKEN Internship Program Committee,

I am writing to apply for a 12-week internship at RIKEN between June and mid-September 2025. This internship is a key component of my Master's studies in engineering at CY Tech and represents an important milestone in my academic and professional journey. I aspire to join the Computational Molecular Science Research Team (Nakajima TL) to further develop my knowledge of high-performance computing (HPC) and its applications in computational chemistry while contributing meaningfully to the team's innovative projects.

At CEA Grenoble, I gained hands-on experience in HPC workflows, including Bash scripting, software compilation, data transfer, job scheduling, and post-processing. I also conducted a comparative study on Rust and Fortran, analyzing their performance in parallelized environments. These experiences deepened my understanding of supercomputing workflows and sparked my interest in optimizing their various stages, from task submission to data analysis.
I am particularly motivated to explore RemoteManager, currently being developed at CEA, and its potential application to the Fugaku supercomputer for workflows involving NTChem and BigDFT. Additionally, the idea of using machine learning workflows or large language models (LLMs) to simplify supercomputing tasks, such as job submission or simulation setup, excites me. These tools could improve the accessibility and efficiency of computational chemistry systems for researchers worldwide. Collaborating with the Nakajima Team would provide a unique opportunity to refine my skills while contributing to pioneering research in computational molecular science. I am eager to learn how tools like NTChem are developed and deployed on state-of-the-art platforms like Fugaku, gaining valuable insights into HPC applications in chemistry and materials science.

Finally, I am inspired by Japan's culture of innovation and precision, which seamlessly blends technological advancement with tradition. Working at RIKEN would be an enriching experience, both professionally and personally, and would allow me to immerse myself in an environment that values collaboration, respect, and excellence.

Thank you for considering my application. I am excited about the opportunity to contribute to the Nakajima Team's research and to acquire invaluable skills in HPC workflows and computational molecular science.

Sincerely,

Rolland Dorian