

## Memorable experiences as a visiting student at MIT

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I studied at Massachusetts Institute of Technology (MIT) for three months from June to September in 2015. In this report, I would like to introduce my daily life during the visit at MIT and the atmosphere that I felt in the laboratory.

The daily life in the Rutledge laboratory was slightly different from my home laboratory in Japan in that most of the members were international and about half of the members were doctor course students or post doctors. Since



Fig 1. A group photo of Rutledge group at Essex river tour

encountering doctor course students or post doctors in Japan was a rare event, this should be noted in this report. As one can imagine, the discussions tend to be insightful as well as practical because of their experience and helpful suggestions. I was lucky that one of the laboratory members, called Peter, sitting next to me was a specialist on molecular dynamics (MD) simulation and he became interested in the details of my research through the daily conversations. In MD simulation, there are numerous force field parameters that need to be set correctly for conducting simulation. The force field that I employed in my research was especially twisted and complicated since two types of force fields were combined and one of which borrowed its parameters from another force field, which literally requires one to be familiar with three different force fields to understand the true nature of the force field. Thus, finding errors in the parameter must be honestly difficult task. However, when I introduced the force field to him by showing a reference paper, he revealed the origin of the force fields and found a typo in one of the parameters in that paper. Once he started to check the values on the paper, he referenced his software, called EMC, developed by himself and comparing the values between those in paper and his software. He seemed to have learned the actual value of those force fields by heart through

developing the software and the research experiences. This is one of the most impressive incidents during the visit and I believe I would have spent days or weeks for debugging without his help.

Weekly meetings for sharing knowhow on research tools were also one of the most attractive activities in the laboratory. The concept of this weekly meeting was to share the useful tools that each laboratory members expertized in and that might be useful to others. Since there were experts on simulations, theories and experiments, variety of different tools and ideas were shared. One of the most impressive tools from the experimentalist side is JMP. Although JMP is a data analysis tool, it was introduced as a tool to compose the experimental design for minimizing the number of data points while achieving the sufficient accuracies to reveal the relationship underneath the data. In other words, utilizing this functionality, each experimental step and data points were selected to maximize the information in the parameter space in their experiments. Another interesting topic from the simulation side is the introduction to Julia language. Julia is a computer programming language designed for scientists aiming for writing their programs in MATLAB-like syntax while achieving numerical computing performance of C language. This language possibly enables one to write practical and fast scripts without concerning about the complicated ideas such as pointers in low-level languages. After this presentation, some of the group members including me started to play with Julia on their cluster to speed up programs for data analysis and discussed about the performance. Those active interactions including discussions and testing those tools via hands-on after the lunch meetings were also welcomed in the laboratory.

The "Infinite corridor" was an interesting place to stop-by and visit on the way back to home. There are numerous numbers of small advertising posters on events ranging from small in-house events to public conferences. There were also several emerging on-going topics that were still minor to discuss with

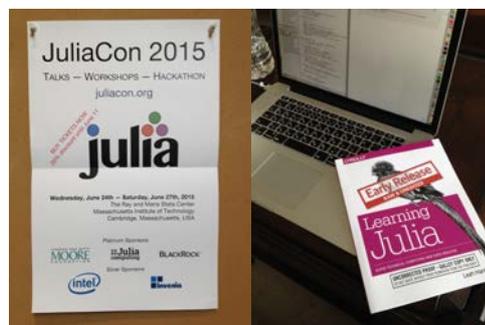


Fig 2. A poster on the infinite corridor for JuliaCon 2015 (left) and a pre-release copy on Julia language at the conference (right)

majority of people but potentially overcome the death valley of the technology. There was also a conference on Julia language that had been introduced in the weekly meeting during the period of my visit. The participants were joining from various fields, however they all seemed to be sharing the similar problems such as unreadable legacy programs for simulation and analysis and awkward integrity. Discussing about how to traverse from one language to Julia language (e.g. Python to Julia) for pursuing simplicity and performance of programs without sacrificing the productivity of research was enjoyable for me as a researcher.

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