先端研究拠点事業―国際戦略型―
「ソフトマターと情報に関する非平衡ダイナミクス」

研究者交流プログラム　派遣報告書

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派遣先

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共同研究

研究課題名	和文	
	英文	
場所（国名・都市）		ドイツ・ユーリッヒ
派遣期間		平成 25 年 9 月 7 日～平成 25 年 9 月 22 日

実際に行った研究活動、成果などを１－２ページ程度で記述してください。スペース不足の場合は、用紙を追加してください。

Centre européen de calcul atomique et moléculaire (CECAM) is a widely known European association whose mission Is to promote cooperation among researchers working on computationally intensive problems, and also to provide training to them on the latest techniques and methods. They do this by arranging several workshops, seminars, summer schools, and conferences every year. My visit to Germany was to two workshops arranged by CECAM, the topics of which are of great interest not only to me personally, but to our laboratory in general.

The first of these was called “Fast Methods for Long Range Interactions in Complex Particle Systems,” and detailed the latest developments in algorithm design and freely availalble software libraries for massively parallel computing. Improvements in parallel fast fourier transforms, in particular, is a topic that I was interested in hearing about, and indeed the explanation about the recently published libraries ScaFaCoS and PFFT was very useful and interesting, and something that I might use in my own research in the near future. In the hands-on sessions of this workshop, we practiced, among many other things, using MPI libraries. As the in-house programs in our lab are moving towards these techniques, the hands-on sessions proved to be quite topical and interesting.

The second workshop, “Multiscale modelling methods for applications in materials science”, concentrated on applications of the methods discussed during the first workshop. I personally got to meet and to have extensive discussions with one of the lecturers, Prof. Roland Faller, who is an expert in the field of membrane biophysics, and has recently done a lot of simulation work on systems called supported bilayers. This is indeed exactly the types of systems that I am currently focusing on in my research, and thus these discussions were indeed very useful. I also met and had long discussions with Dr. Vitalii Starchenko, one of the developers of a widely used simulation software, ESPResSo++. I have also kept in contact with him after the workshop. To analyze systems in my research I use something called local pressure profiles, but this method of analysis has not been implemented in its full form to most simulation suites. Luckily Dr. Starchenko has recently added this tool to ESPResSo++, making it a viable alternative to the tools that I am currently using.

I also enjoyed bonding with the younger generation of researchers, as many of the participants, like me, were PhD students. With them we got to see the most powerful computers in Europe, housed in the research center of the small town of Julich, the very same place where the conferences were held.