**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」**

# 共同研究プログラム　派遣報告書

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**共同研究**

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| 研究課題名 | 和文 | 生体組織の物理モデリングに関する研究 |
| | 英文 | Physical modeling of biological tissue |
| 派遣期間 | | 2015 年 2 月 12 日～2015 年 3 月 6 日 |

During my stay at Prof. Joanny's lab in the Curie Institute I worked mainly with Dr. Philippe Marcq. This is intended to be the start of a collaboration to develop agent-based computational models capable of describing tissue dynamics. The motivation for your work was a recent experiment performed by one of Dr. Marcq's colleagues, Benoit Ladoux, in which cells placed in a circular ring spontaneously start to rotate in one direction. I spent the first 3-4 days discussing with Dr. Marcq and reviewing the literature he had provided on the dynamics of migrating cells/tissues. After our first discussions, we realized that before looking at collective motion in tissues, we should ensure that our computational model can adequately describe the dynamics of single cells crawling on substrates. Fortunately, this is one of the first problems that experimentalists considered and many detailed works can be found in the literature. In particular, Dr. Marcq has pointed out that the nature of the traction forces plays a critical role in determining the motion of the cell. Up until now, no previous computational model has attempted to describe these interactions accurately. This is one of the main objectives of our work.

To start, we will build upon previous work that has shown that the shape of the cell can be directly correlated to the traction forces exerted on the substrate. This provides a clear recipe for determining the active forces that give rise to the motion of the cell. Identifying a suitable candidate for the cell/substrate interactions was the most difficult part. For the cellular model, we decided to use the SEM method developed by Newman, which is very simple yet powerful. In this method, cells are represented as a discrete collection of sub-elements which interact with specific inter and intra-celullar potentials. For the substrate we chose an elastic medium, modeled as a lattice of point particles tethered to their equilibrium position by an elastic spring. The benefit of the computational approach we have chosen is the fact that it can be easily implemented within a Molecular Dynamics framework. Indeed, the SEM model has already been incorporated into LAMMPS. LAMMPS is a very sophisticated MD code that is open source and can run in parallel and on GPUs.

Once we decided on the model and tool we wanted to use, I focused my efforts on learning how to use LAMMPS. It took me around a week to be able to compile LAMMPS and learn how to run the simulations. After this, I started to create the necessary input configurations needed for our simulations. I was able to setup the 2D lattice that will be used as a substrate and specify the substrate-substrate and cell-cell interactions. All this could be achieved with no coding on my part. However, to specify the cell/substrate interactions in the way we wish, we will need to modify the code. This is work in progress.

In addition to my work on the implementation of the model within LAMMPS, I was able to hold discussions with theoreticians and experimentalists collaborating with Dr. Marcq. In particular, I was able to visit Benoit Ladoux's laboratory and discuss with several of his PhD students and PostDocs on their experiments. Discussing their experiments I was able to gain invaluable insight into the dynamical behavior we are interested in modeling. I was also able to explain the computational model we would like to implement and listen to their feedback. They clarified many aspects on the biological nature of the system that I was not familiar with and gave me several ideas for how to test our model.