World Center of Education and Research for Trans-disciplinary Flow Dynamics
International Internship Program

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Research title: Modeling issues in Molecular Dynamics simulations of confined lubricant flow.
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The research I conducted during my GCOE international internship period aimed to better understand and improve the modeling of thermal and mechanical boundary conditions in molecular simulations of nano-scale lubricated contacts.

In the experimental context, the macroscopic boundary conditions of pressure, velocity, and temperature of rubbing surfaces in lubricated contacts are often well known and can be controlled within a satisfactory precision for experimental purposes. However, it remains technically impossible to accurately control or even measure the conditions in a small local region of the contact especially in the case of nanoscale confinement. Such confinements are observed in many modern applications such as optical disk drives, micro motors, heavy duty rolling-element bearings, etc.

While simulations aim to realistically replicate the experiments or applications, it is still impossible, due to computational limitations, to model any full contact explicitly as a molecular system. Thus, Molecular Dynamics simulations usually investigate only some local sub regions of a full real contact. Most molecular interactions can be modeled efficiently by existing force fields, however the choice of appropriate boundary conditions and the physically-acceptable methodology of their application remain the most challenging and crucial problematics in these types of simulations, and unfortunately the least accounted for factors in the tribological literature.

The research during my internship period allowed me to develop, under the guidance of IFS researchers Professor T. Ohara and Associate Professors T. Tokumasu and G. Kikugawa with whom I had very fruitful discussions that I am very grateful for, new algorithms for handling both mechanical conditions of normal load (pressure) and shearing as well as thermal conditions at the simulation boundaries. In the new model, instead of applying constant velocities to the substrates, the shear velocity is allowed to softly accommodate to the friction forces from the lubricant molecules in the same way as in experimental rigs which experience stick-slip motion of the tip in contact due to the lubricant friction rather than continuous smooth motion. The application of pressure was also improved by increasing significantly the equivalent mass of the surfaces as to replicate real surfaces. Finally, the advanced Phantom Molecules method which solves the generalized 3D Langevin equations at the substrate boundary was also used in order to simulate the realistic conductivity and heat capacity of substrates.

In addition to programming, testing, and validation of the newly introduced algorithms which themselves are impressive in the actual tribology context, I also performed comparison simulations with classical approaches for imposing boundary conditions. The results for the mechanical conditions showed that stick-slip motion can occur at nano-scale lubricated contacts and that it results in an attenuation of the lubricant velocity slip near the boundaries. It seems that the molecular system accommodates in a more realistic manner to the boundary conditions than seen with classical simulation approaches. The thermal boundary conditions, on the other hand, define the route and the molecular mechanisms of heat dissipation from the lubricated contact. The heat dissipation mechanisms have direct influence on friction in such systems especially at high levels of shearing.

I would like to express my gratitude to the IFS professors whom I mentioned previously as well as all of the members (students and staff) of the Tokumasu Laboratory who warmly welcomed me with outstanding kindness and very friendly environment. I was also very lucky to learn a lot from them about the Japanese culture and lifestyle and to be invited to several parties and seasonal activities. That's in addition to weekly seminars, and finally the ICFD conference which concluded my stay in Sendai. I also want to thank all of the staff of the GCOE office for the organization of this internship program and can only hope that the collaborative work continues between Tohoku University and INSA-Lyon and personally, that I get the chance to get back and visit Sendai and IFS in the near future.

“Time stops, and each photo tells a story”

Welcome party in a traditional restaurant

Celebrating the birthday of Yuko, lab’s secretary

Traditional Imoni barbeque at the river side with students and staff of the Tokumasu laboratory

Sendai City view from the site of Sendai Castle

ICFD 2009 conference with Prof. Vergne and Assoc. Prof. Tokumasu and Kikugawa (from right to left)

Last day photos with laboratory students and staff