

## PhD - Computational Lubricant Modelling

**Research Topic** Determining Lubricant Properties for Quantitative EHL by Molecular Dynamics.

**Institute** Ghent University, Belgium

**Departments** EEMMECS - Dept. of Electrical Energy, Metals, Mechanical Construction, and Systems

CMM – Center for molecular modeling (prof. Toon Verstraeten)

**Research Group** Tribology @ Soete Laboratory

**Funding** 3 years – 100% occupancy rate

**Statute** PhD Student

**Min. Requirements** Master of Science in Mechanical, Chemical or Physics Engineering.

**Assets** Experience with MD / LAMMPS

Experience with Fluid Mechanics/ Lubrication

### Job description

Thermo-Elastohydrodynamic Lubrication (TEHL) is a specific lubrication regime which typically occurs in non-conformal contacts, such as ball bearings, roller bearing, gear teeth,... and is therefore very relevant in many machine applications. TEHL is characterized by thin lubricant films (50 nm-1  $\mu$ m) in which the hydrodynamic pressure can reach values up to GPa range (1-5 GPa), inducing elastic deformation of the opposing contact surfaces. At such high pressures, the lubricant becomes compressible, and behaves in a highly non-Newtonian way by local solidification and shear-thinning.

Accurate and quantitative computational simulation of TEHL (Reynolds, CFD) requires therefore an accurate description of the lubricant's compressibility and the rheology (i.e. piezo-viscosity and shear thinning) as well as the thermal properties (specific heat, conductivity), wall slip and cavitation. Today, however, mainly empirical constitutive models are applied, which typically involve curve fitting of experimental data, obtained for a particular common lubricant and under specific conditions. Hence, their range of applicability is rarely questioned when applying them to other lubricants, surface materials or operating conditions. Obviously such generalized empiricism does not contribute to the versatility, accuracy and reliability of continuum computational methodologies.

In the past decades **Molecular Dynamics (MD)** has emerged as a more sophisticated computational approach to study interfacial phenomena and thin film rheology. Such computational approach offers the advantage to obtain an accurate estimate of the lubricant's thermo-mechanical properties, by direct simulation of the lubricants molecular structure subject to different conditions of pressure, temperature, shear etc..

**Your job** will consist of developing a Multiscale Modelling framework, in which non-equilibrium Molecular Dynamics is exploited to derive appropriate constitutive relations that can be used in continuum simulation techniques i.e. local thermomechanical properties of lubricants, near-wall effects, molecular layering, mechanochemistry etc.

### Profile

1. You hold a Master degree in Mechanical, Physical or Chemical engineering.
2. You have a strong motivation for conducting scientific research at a high level.
3. You possess good analytical, and technical skills
4. You are interested in computational mathematics and Advanced Scientific Computing.
5. Experience with programming in C++, Matlab, Python or equivalent is an advantage.
6. You have knowledge and experience with Molecular Dynamics (LAMMPS)

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UGent - EEMMeCS - Soete Laboratory

7. Experience with Fluid Mechanics and/or Tribology is an asset.
8. You take responsibility for the development of your project in a well-structured, thorough way, and you're able to solve problems independently. You display creativity in solving problems, generating ideas or finding new ways of working.
9. You have an open personality and willing to contribute to the team and participate in didactic projects.
10. You have excellent communication skills in English, both orally and written. Knowledge of Dutch is certainly an asset.

### Contract

1. The PhD-project starts as soon as possible.
2. We offer today an 100% research position for 36 months (3 years), with intention to extend with 12 months. After probation period of 6 months, a fixed-term contract will be offered on condition of positive evaluation.
3. The salary and appointment terms are consistent with the current rules for PhD degree students. The net salary for a starting PhD student (unmarried) is about €2000,-.
4. The scholarships for the PhD degree are subject to academic approval. The successful candidate will be enrolled in the doctoral program of Ghent University (<http://www.ugent.be/doctoralschools/en> ).

### Application

For further information on the project and/or application, please contact Prof. Dieter Fauconnier ([dieter.fauconnier@ugent.be](mailto:dieter.fauconnier@ugent.be)) or Prof. Toon Verstraelen ([toon.verstraelen@ugent.be](mailto:toon.verstraelen@ugent.be) ).