Creating a reactive force field engine for materials physics simulations

Open: Now (Oct 2020)

Aim/Purpose: To develop a simulation engine for the CHAMPION codebase.

Background: The CHAMPION codebase [1], developed at the Division of Materials Physics (MaP) at Chalmers, as of today consists of a package for analysing and detecting dynamic structures in atomistic trajectories. Overall *ab initio* molecular dynamics (AIMD) simulations yield accurate descriptions of the atomic interactions, but are only capable of simulating behaviour on (very) small scales. In contrast, classical molecular dynamics (MD) simulations are able to simulate several thousands of atoms for several ns, but here the accuracy is limited by the accuracy of the force fields (FF) used. Unfortunately, widely used FFs fail to allow the MD simulations to accurately represent more complicated materials, such as predict transport properties in battery electrolytes – largely due to the extensive coulombic interactions present. The idea is to let CHAMPION tackle this through a machine learning software capable of finding system specific FFs from AIMD simulations.

Project: Write and develop a MD simulation engine within the CHAMPION framework able to run reactive FFs – which allows for bonds to form and break during the simulation. The simulation engine will leverage CHAMPION's ability to detect time-dependent groups of strongly interacting atoms, while using a well-established mathematical form of the FF, thus combining the simplicity and computational efficiency of current FFs with the flexibility of handling chemical reactions. The starting point is for example the GROMACS code base [2] – one of the best MD softwares to date. This thesis provides the opportunity to develop an understanding of computational materials physics and implementing it using high performance computing (HPC) methods in a modern C++ environment – thus knowledge and skills in C++/OOP is a clear advantage to bring.

Time-plan: Each MSc thesis is *ca.* 20 weeks. Week 1-5: Literature on current MD engines and CHAMPION. Week 3-10: Suggesting/trying out a solution on how to implement a reactive FF. Week 6-18: Development of a working MD engine compatible with CHAMPION and HPC. Week 15-20: Writing the MSc thesis and prepare for the presentation.

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[1] R. Andersson, F. Årén, A. A. Franco and P. Johansson "CHAMPION: Chalmers Hierarchical Atomic, Molecular, Polymeric & Ionic Analysis Toolkit." in manuscript (2020).
[2] H. J. C Berendsen, D. van der Spoel, and R. van Drunen. "GROMACS: a message-passing parallel molecular dynamics implementation." *Comp. Phys. Comm.* 91 (1995) 43-56.

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