Master thesis project for Håkon Vikør Treider: Multiscale physics

The aim of a program on multiscale physics is to develop a first principle approach to systems of relevance for a variety of fields, from materials science to nano-technology and biological systems and even atomic nuclei and stars. Common to all these systems is that they entail a truly multiscale physics program that involves a proper understanding of the links between the various scales, starting from quantum-mechanical first principle studies of atoms, molecules and eventually other spatially confined systems to Density functional theories and finally microscopically derived potentials to be used in molecular dynamics calculations.

The computations required for accurate modeling and simulation of large-scale systems with atomistic resolution involve a hierarchy of levels of theory: quantum mechanics (QM) to determine the electronic states; force fields to average the electronics states and to obtain atom based forces (FF), molecular dynamics (MD) based on such an FF; mesoscale or coarse grain descriptions that average or homogenize atomic motions; and finally continuum level descriptions. By basing computations on first principles QM it is possible to overcome the lack of experimental data to carry out accurate predictions with atomistic resolu- tion, which would otherwise be impossible. Furthermore, QM provides the funda- mental information required to describe quantum effects, electronically excited states, as well as reaction paths and barrier heights involved in chemical reactions processes. However, the practical scale for accurate QM today is ¡1,000 atoms per molecule or periodic cell (a length scale of a few nanometers) whereas the length scale for modeling supramolecular systems in biology may be in the tens of nano- meters, while elucidating the interfacial effects between grains in composite materials may require hundreds of nanometers, and modeling turbulent fluid flows or shock- induced instabilities in multilayered materials may require micrometers. Thus, simulations of engineered materials and systems may require millions to billions of atoms, rendering QM methods impractical. Nonetheless, QM methods are essential for accurately describing atomic-level composition, structure and energy states of materials, considering the influence of electronic degrees of freedom. By incorporating time-dependent information, the dynamics of a system under varying conditions may be explored from QM-derived forces, albeit within a limited timescale (¡1 ps). The prominent challenge for theory and computation involves efficiently bridging, from QM first-principles, into larger length scales with predominantly heterogeneous spatial and density distributions, and longer timescales of simulation enough to connect into engineering-level design variables while retaining the appropriate accuracy and certainty. Equally challenging remains the inverse top-down engineering design problem, by which macroscopic material/process properties would be tunable from optimizing its atomic-level composition and structure. The aim of this large project is to to develop breakthrough methods to staple and extend hierarchically over existing to develop the necessary

tools to enable continuous lateral (multi-paradigm) and hierarchical (multiscale) couplings, between the different theories and models as a function of their length- and timescale range a strategy often referred to as First-Principles-Based Multiscale-Multiparadigm Simulation. The enclosed figure here displays some of these ideas. The ultimate goal is a reversible bottom-up, top-down

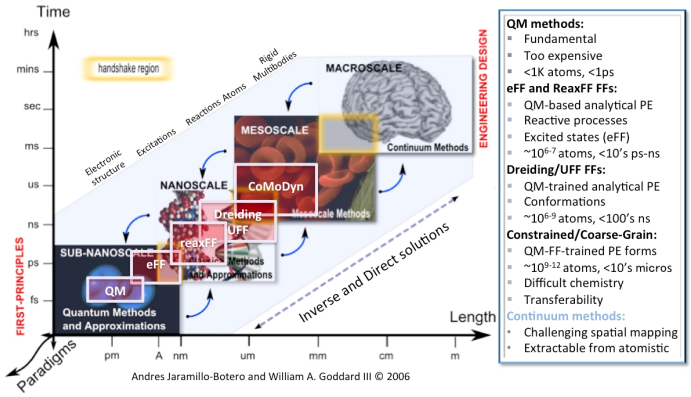

Figure 1: Example of multiscale hierarchy.

approach, based on first principles QM, to characterize properties of materials and processes at a hierarchy of length and timescales. This will improve our ability to design, analyze, and interpret experimental results, perform model-based prediction of phenomena, and to control precisely the multi-scale nature of material systems for multiple applications.

To achieve these goals, several theses projects are shortly defined below. These projects open also up for several fruitful collaborations between the involved MSc students. The group in Computational Physics has long-standing experience in defining projects where several students may find a common a ground, either from a formalism point of view or (and possibly and as well) phenomenological point of view.

The systems we have in mind are mainly molecules like SiO_2, H_2O, $CaCO_3$ and other more complicated molecules. To model the interaction between such molecules and eventually derive microscopic interactions can be done via several MSc projects. The aim of this thesis is to perform quantum-mechanical first principle calculations of selected molecules compounds and compare these results with parametrized potential model like the so-called ReaxFF potential.

Progress plan and milestones

The aims and progress plan of this thesis are as follows

- Spring 2016 and partly fall 2016: The first step is to set up a Hartree-Fock program for the H_2 molecule and parametrize an effective potential

for molecular dynamics calculations. These results will be compared to exisiting potential models.

- Fall 2016: The next step is to include a proper treatment of quantum mechanical effects by performing Coupled-cluster theory theory calculations to determine better correlations.
- Spring 2017: The final step is to obtained parametrized potentials for more complex molecules and use these in molecular dynamics calculations.

The thesis is expected to be handed in May/June 2017.