The Computational Materials Design Facility (CMDF) for multi-paradigm Multi-scale simulations of complex materials, chemical, and biological systems

It has long been the dream of scientists and engineers to predict the properties of new materials from first principles (no empirical data) since this would allow new materials to be designed and optimized computationally prior to the difficult tasks of synthesizing and charactering them experimentally. Despite enormous improvements in the speed of accuracy first principles methods (quantum mechanics, QM) and the enormous growth in the computing power available for such applications, a QM calculation on the dynamics and properties of the $10^{10}$ atoms in a cubic micron of matter will likely not be practical our lifetimes. And certainly using QM to characterize the growth of cracks as a camshaft undergoes fatigue failure may have to await the days of Star Trek and Star Wars. This has motivated development of the hierarchical multi-paradigm multiscale Computational Materials Design Facility (CMDF) in which the materials properties of macrosystems are predicted from first principles through the hierarchy illustrated in the figure. We start at the electronic (quantum) level that requires no input of experimental data but is limited to 100’s of atoms. These results are fed to the atomic scale (ReaxFF and MD) via parameters in the force field (FF) that allow simulations on millions of atoms. The results of the atomistic MD calculations are used to derive lumped or coarse grain models that can be used for systems having billions of atoms to obtain constitutive equations and physical constants that are is fed into continuum and design scales. The CMDF allows independent software developed for various paradigms to be combined into one mixed-paradigm simulation for multiscale applications. The concepts developed within the CMDF framework make first principles materials modelling a reality. The CMDF was created to provide an environment for combining disparate computational tools (QM, FF, MD, mesoscale, and continuum dynamics) under one framework for first principles multi-scale multi-paradigm simulations within a scale-agnostic philosophy. The combination of these simulation tools in the CMDF framework allows detailed predictions of the mechanical, reactive, and electronic properties of complex systems. The CMDF is suitable for many classes of molecules and solids in a variety of environments and is now being used for simulations ranging from crack propagation in ceramics and shock induced chemical reactions, to contact resistance and conductance of nanoscale switches and performance of thermoelectric systems.

The availability of these new computational tools should allow us to start solving the inverse problem of identifying new structural combinations of materials capable of providing desired properties. Our recently developed Computational Materials Design Facility (CMDF) can seamlessly couple complex material simulations across multiple length- and time-scales. CMDF is a framework to study materials properties and processes using a hierarchy of methods based on distinct paradigms suitable for various overlapping scales, where the parameters at each level are based on a more fundamental theory (see the schematic shown in Figure 1). In the CMDF framework, different simulation tools and engines are called from a PYTHON scripting language level that allows scale agnostic combinations of various modelling approaches in addition to straightforward usage of the software on different platforms. In CMDF, complex calculation engines are “hidden” behind the PYTHON scripting layer and act as a black box for uncomplicated usage. To make such approaches of immediate relevance in analysis and experiment design, we will collaborate closely with experimentalists.

CMDF relies on the concept of using a hierarchy of overlapping modelling methods where the parameters at each level are based on a more fundamental theory. This provides an immediate interface to the modeling tasks associated with substrate-sensor interactions. CMDF allows on-the-fly interchange of computational engines, for instance allowing refitting of empirical force fields. In particular, for applications in high-time resolution chemical dynamics modeling, the concept of runtime refitting of empirical potentials and parameters in homogenized continuum theories is expected to be highly beneficial. On-the-fly detection of refitting needs or switch to low-level quantum methods can be achieved by performing the concept of virtual dynamics of systems or energy state evaluations.