Warwick Centre for Predictive Modelling Seminar Series

Uncertainties in classical effective potentials: sources and quantification strategies

Peter Brommer
School of Engineering
University of Warwick

Thursday, 14th May, 4 p.m.
R0.12, Ramphal Building, Ground Floor

Abstract: In atomistic simulations, classical effective potentials or force fields have become the accepted gold standard for large-scale molecular dynamics simulations. They treat all electronic degrees of freedom implicitly, and the energy of a system (and as its derivative the forces on the atoms) only depend on the position of the atoms. In this way, the computational cost of first-principles methods (like density functional theory) can be avoided to simulate many millions of atoms. Unfortunately, the approximations used to obtain such effective potentials are largely uncontrolled, and the uncertainty incurred on using them in simulations is unknown a priori.

In this talk I will describe how effective potentials are typically derived, for example using the force matching approach. This will then allow me to demonstrate the sources of uncertainty in this process, e.g. noisy/incorrect/insufficient input data or inaccurate models. I will then discuss potential strategies to propagate this uncertainty first to an effective potential and then further on to quantities of interest determined from molecular dynamics simulations. This would then allow predictive atomistic simulations that provide solid information about the validity and precision of the results.

More info: http://www2.warwick.ac.uk/fac/sci/wcpm/seminars