WARWICK
THE UNIVERSITY OF WARWICK

Reliable Knowledge: How far can we trust electronic structure simulations?

Keith Refson

Department of Physics
Royal Holloway

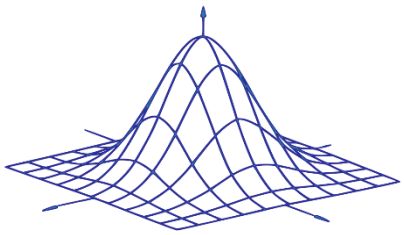
Tuesday, 3rd Nov, 4 p.m.
D202 Seminar room, School of Engineering, 2nd Floor

Abstract: In the last decade computer simulation based on density-functional theory or related electronic structure methods has risen to become one of the most heavily-used methods in the study of the structure and properties of solid-state materials. Research projects depend on off-the shelf computer programs to perform the computations, and it is taken on trust that the output of the calculations is a correct and faithful consequence of the equations of density-functional theory with the user-specified boundary conditions.

This dependence raises serious practical questions. Are the results a unique consequence of the physical theory, or do they depend on explicit or hidden numerical approximations? How reproducible are they by other groups using other programs? Are they trustworthy enough to be admitted as proven consequences of the theory? How is it possible to quantify the precision achieved when testing a hypothesis requiring sensitive numerical discrimination? And how can we be confident that the results are not merely the result of bugs in the computer code?

I will address these questions from the perspective of the CASTEP project, in particular how software engineering processes can reduce risk and promote robustness. I will discuss the improvements in pseudopotential technology and accuracy over the years, as one of the major uncontrolled approximations. And I will present the Delta project, a community-wide effort by code developers to systematically benchmark the precision of 15 solid-state DFT codes. The outlook is optimistic, and the results of simulations can now justifiably be regarded as a true consequence of the theory.

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



WCPM

Warwick Centre for Predictive Modelling