Science and Technology Facilities Council

Scientific Computing

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Computational Science Centre for Research Communities

Simulation software fuels workflow efficiency in the nuclear industry

Nuclear powered energy has been a part of life in the UK since 1956 with the opening of the first nuclear power station, Calder Hall at Windscale in Cumbria. Although the aim of Calder Hall was to produce weapons grade plutonium, it became the first nuclear power station in the world to generate electricity in 'commercial quantities'.[1] During the 63 years since Calder Hall opened, it has become widely recognised that using nuclear fuel to generate electricity demands robust control and storage procedures to safely manage these challenging materials, and the responsibility for this lies with a number of businesses. One of these, the Atomic Weapons Establishment (AWE), is responsible for manufacturing, maintaining and developing warheads for the UK's nuclear deterrent.

Computational scientists from the Science and Technology Facilities Council (STFC) and Queen Mary University, London (QMUL) are developing new software that helps AWE and others in their work.

The DL_POLY software suite

STFC's Scientific Computing Department (SCD) manages a collaborative computational project known as CCP5. Under this project, SCD scientists led by Professor Ilian Todorov have developed a suite of software called DL_POLY, a molecular dynamics simulation package that provides scalable performance from a single processor workstation through to a high performance parallel computer.

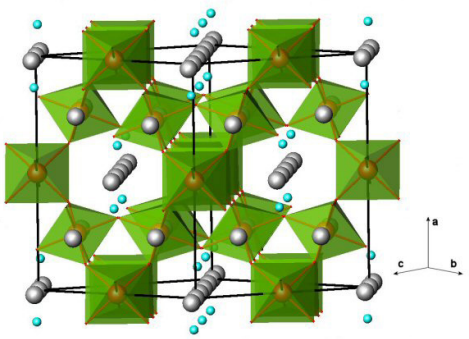
The scientists have teamed up with Professor Kostya Trachenko at QMUL to develop a new functional tool within the DL_Software suite that can simulate the effects of radiation damage in materials. This will be invaluable to the AWE, which carries out a range of experimental and theoretical research into the ageing of radioactive materials such as metals and oxides.

Using the DL_Software, it is possible to build a representative model of an actinide oxide system and simulate how that system ages through time, in different environments and temperature ranges.

Modelling complex boundaries

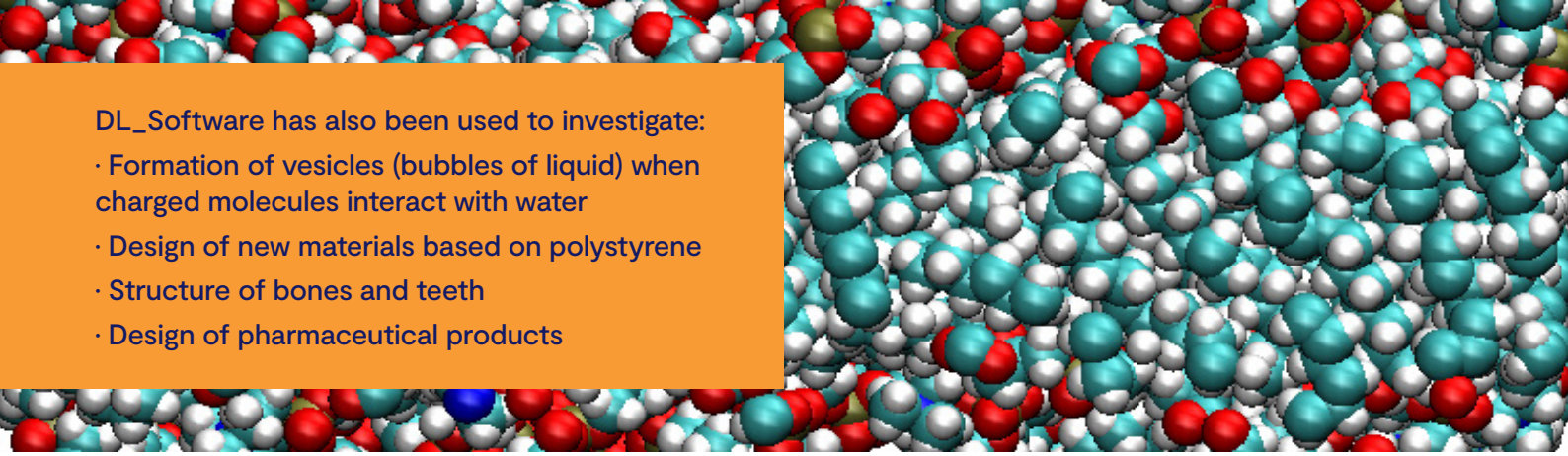
Over the last 10 years AWE, working in collaboration with the University of Bath, have used the DL_Software suite to develop ever more realistic models of actinide materials including the oxide overlayer and, for example, how grain boundaries[2] (the interface between crystals comprising the material) affect the transport of gaseous species through the material.

The new functional tool developed with QMUL is providing another vital element in understanding these processes.



Understanding the ageing process is vital to designing the optimum storage conditions and environment. This is where the DL_Software plays a key role.

Professor Mark Storr
Materials and Analytical Science, AWE



DL_Software has also been used to investigate:

· Formation of vesicles (bubbles of liquid) when charged molecules interact with water

· Design of new materials based on polystyrene

· Structure of bones and teeth

· Design of pharmaceutical products

Impact of DL_Software

Having confirmed that simulations reproduce experimental results it becomes possible to streamline workflows where computational predictions inform business decisions. This streamlining reduces the number of experiments needed, thereby reducing costs and speeding-up research.

The suite of DL_ Software plays a key role in this by providing a range of compatible software that unifies the input/output user experience, thereby removing the time-consuming process of converting models between different software codes. Consequently, DL_Software helps drive efficiency by making the workflow simpler.

How can you get DL_POLY?

First you need to register at:

· scd.stfc.ac.uk/Pages/DL_POLY-Registration.aspx

· Or, scan the QR code to the right.

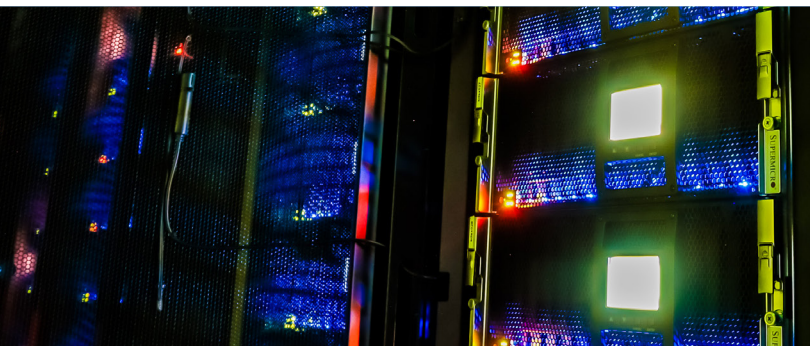
Then, follow the instructions that are emailed to you on successful registration.

The new functional tool developed as part of the DL_Software suite was funded by a grant from Queen Mary University, London, to Professors Todorov and Trachenko. CCP5 is supported by CoSeC (Computational Science Centre for Research Communities).

1. “Calder Hall Power Station”. The Engineer. 5 October 1956. Retrieved 30 March 2011.

2. N.R. Williams, M. Molinari, S. Parker, M. Storr. ‘Atomistic investigation of the structure and transport properties of tilt grain boundaries of UO_2’ Journal of Nuclear Materials 458 (2015) 45–55.

Queen Mary University of London



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