DL_POLY's 25th Anniversary Special Meeting

Venue: Chicheley Hall, Chicheley Road, Newport Pagnell MK16 9JJ.
Date: 3rd November 2017

PROGRAMME

08.30-09.00 Registration with Tea/Coffee

09.00-09.05 Official opening (Ilian Todorov)

Chair: Ilian Todorov

09.05-09.35 Prof. Martin Dove (QMUL) - *Molecular dynamics simulations of carbon capture by porous hybrid materials*

09.40-10.10 Dr. Patrice Bordat (University of Pau) - *Solvation and free energy module implemented in DL_POLY: Study for a preferential CO2/CH4 adsorption in silica monoliths*

10.15-10.35 *Tea/Coffee Break*

Chair: Tim Forester

10.40-11.10 Prof. John Harding (University of Sheffield) - *Understanding biomineralisation: what has DL_POLY ever done for us?*

11.15-11.45 Dr. Simone Melchionna (ISC-CNR) - *Proteins and multiscale biology: the long time legacy of DL_POLY*

11.50-12.20 Prof. Richard Catlow (UCL/University of Cardiff) - *Molecular dynamics in Catalytic systems*

12.25-13.25 *Lunch*

Chair: Maurice Leslie

13.30-14.00 Dr. Kostya Trachenko (QMUL) - *Using DL_POLY to understand radiation damage effects and soft matter (glasses, liquids, supercritical fluids)*

14.05-14.35 Dr. P.-L. Chau (Institut Pasteur) - *General Anaestheics and Membrane Interactions*

14.40-15.10 Dr. David Quigley (University of Warwick) - *The Hackademic Approach to Simulations with DL_POLY*

15.10-15.30 *Tea/Coffee Break*

Chair: Neil Allan

15.35-16.05 Prof. Steve Parker (University of Bath) - *Atomistic Simulations of Oxide and Mineral Interfaces*

16.10-16.40 Prof. Martyn Guest (University of Cardiff) - *DL_POLY - A Performance Overview; Analysing, Understanding and Exploiting available HPC Technology*

16.45-17.25 Closing Remarks by Prof. William Smith -*A Short History of DL_POLY*

17.30-19.00 Free time to explore the site

19.00 Official Dinner

Prof. Martin Dove - *General Anaesthetics and Membrane Interactions*

Abstract: We have been investigating the process of absorption of CO_2 into porous materials, specifically zinc imidazole metal-organic framework materials. Our aim has been to look at the way in which molecules enter the material from the gas phase and then move through the channels, and for a study of dynamic mechanisms molecular dynamics is the ideal tool. The basic approach has been to begin with a gas above a slab of material, and through addition of a small pressure physically push the molecules into the porous materials as would happen in experiments. This is not quite as simple as it sounds. In my talk I will discuss how we developed the model, and give a number of representative results.

1. Molecular dynamics simulation study of various zeolitic imidazolate framework structures. M Gao, AJ Misquitta, LHN. Rimmer and MT Dove. *Dalton Transactions* **45**, 4289–4302, 2016
2. Molecular dynamics study of CO_2 absorption and desorption in zinc imidazolate frameworks. M Gao, AJ Misquitta, C Yang, IT Todorov, A Mutter and MT Dove. *Molecular Systems Design & Engineering* **2**, 457–469, 2017

Dr. Patrice Bordat - *Solvation and free energy module implemented in DL_POLY: Study for a preferential CO_2/CH_4 adsorption in silica monoliths*

Abstract: The presentation will first focus on the developments implemented in DL_POLY which are composed as follows:
-the species-species energy decomposition: it allows to know whether each molecular species is well thermally equilibrated and to determine the solvation energy of a solute in its environment,
-the solvatochromism using both a real molecule and a ghost molecule to define the ground state and the excited state of the solute surrounded by a solvent,
-the free energy calculation based on the thermodynamic integration where the mixing parameter is replaced by a mixing function in order to avoid singularities at the extremities.
Then, the presentation will concentrate on a recent research project dealing with the limitation of the emission of greenhouse gas. To achieve this strong constraint, we have studied the storage of CO_2 in silica monoliths with respect to the adsorption of CH_4. This strategy allows to use solid adsorbants, easy to synthetize and easy to manipulate while most of the studies deal with commercial powders. We will show that a high storage of CO_2 is in competition with a high selectivity of CO_2 vs CH_4, whatever the types of surface being either fully hydroxilated or partially methylated.

Prof. John Harding - *Understanding biomineralisation: what has DL_POLY ever done for us?*

Abstract: Both biomineralisation and bioattachment involve an interface between minerals (hard) and organic molecules, arrays and scaffolds (soft). Such an interface can exercise control in two directions. First, the binding of large molecules on surfaces can induce conformational folding and consequent effects on molecular function. On the other hand, soft matter in the form of molecules, arrays or scaffolds can control the nucleation and growth of crystals. The resulting materials have complex structures, often with distinctive features at different length-scales. This talk discusses three questions where large-scale molecular dynamics simulations using the DL_POLY suite of codes has helped us to understand the processes that are going on. We start with the solution chemistry and nucleation. What effect does the presence of organic molecules have on the species observed and in particular on the growth of clusters? Second we consider the issue of growth. How can organic molecules and arrays control the growth of a mineral? Is a flexible substrate an advantage or a disadvantage? Finally, if a surface is already present, what effect does it have on the conformation and stability of the molecules that are bound to them? And what has this got to do with the dating of fossils?

Dr. Simone Melchionna - *Proteins and multiscale biology: the long time legacy of DLPOLY*

Abstract: The simulation of biological matter has today reached a high level of sophistication, in particular as regarding to the study of systems ranging from macromolecules to cells, in motion or confined in a physiological environment. To tackle formidable biological problems, our root dates back to the early adoption of DLPOLY followed by the development of the DLPROTEIN software. Ever since, a multiscale approach has been developed based on representing macromolecules and cells in suspension via a hybrid Lagrangian/Eulerian framework. The framework has been utilized in a number of different projects. Next, I will illustrate examples of biosystems in crowded conditions, mimicking the cell interior, and the aggregation process of peptides at the onset of Alzheimer disease, a phenomenon greatly accelerated by solvent-mediated interactions. We will then look into the flow of blood cells in physiological vessels, and applications to cardiovascular medicine.
The example will allow us evaluating the potential of multiscale computing.

Prof. Richard Catlow - *Molecular dynamics in Catalytic systems*

Abstract: Optimising the performance of nano-particulate based materials requires a detailed understanding of their structures, dynamics and reactivities at the atomic and molecular level. The methods of contemporary computational chemistry and physics are proving exceptionally powerful in this quest for an atomic level understanding in nano-science.

Dr. Kostya Trachenko - *Using DL_POLY to understand radiation damage effects and soft matter (glasses, liquids, supercritical fluids)*

Abstract: Since I started my PhD in 1997, large parts of my research relied on using DL_POLY to understand physics of different disordered systems. This understanding was used to verify, predict or correct theoretical models and experiments. I review how I used DL_POLY over the last 20 years to understand high-energy radiation damage effects including our more recent work involving simulations of very large systems with up to 1 billion atoms in the simulation box. These simulations called for re-defining the way we run molecular dynamics (MD) simulations and for developing the code to calculate the properties of interest on the fly. I review what on-the-fly properties we were able to implement in DL_POLY and our current plans to complete these developments. I will also discuss how DL_POLY helped us understand thermodynamics of liquids and supercritical fluids, the theoretical problem deemed impossible. Recent MD simulations ascertain a new effect: emergence and evolution of the unusual gap in the phonon spectrum in k-space. In addition to understanding liquid dynamical properties, this result enables us to develop a solid-like approach to liquid thermodynamics based on phonons. This approach correctly predicts basic thermodynamic properties of liquids including their energy and heat capacity.

Dr. Pak-Lee Chau - *General Anaesthetics and Membrane Interactions*

Abstract: The interaction of general anaesthetics with membranes are studied using molecular dynamics simulations with DL_POLY. The simulation pressure is increased, and some general anaesthetics are found to aggregate inside the membrane.

Dr. David Quigley - *The Hackademic Approach to Simulations with DL_POLY*

Abstract: I will discuss experiences with hacking together an approach to accelerate simulations of crystallisation on top of DL_POLY, including some thoughts on how the current generation of "hackademic" programmers can benefit from access to this and other mature simulation packages. Using the crystallisation of ice as an example system, I will demonstrate how these and other accelerated simulations motivated new studies into the structure and representation of ice in molecular simulations, linking to presentation of some more recent Monte Carlo work on the stability of ice polytypes.

Prof. Steve Parker - *Atomistic Simulations of Oxide and Mineral Interfaces*

Abstract: Molecular Dynamics and DL_POLY in particular has proven to be a powerful and valuable tool for studying oxide and mineral interfaces. Furthermore, it is clear that interfaces control many important material properties and by developing a detailed atom-level understanding we can begin to predict ways for improving and controlling material behaviour. In the first part of this presentation I will briefly summarise the impact that DL_POLY has had on our research at Bath by considering two examples where historically, it demonstrates its value, both in terms of being able to handle polarizability via the shell model and giving valuable insights into the structure and dynamics at the mineral-water interface. In the second part I will describe some of our current work on modelling oxides and minerals, where we applying the approaches to energy materials and pollutant separation. In each case our focus is to improve our understanding of their behaviour, particularly the impact of additives and interfaces. The energy materials range from thermoelectric, solid oxide fuel cell and battery materials to nuclear fuels. The work on pollutant separation and remediation includes identifying the factors controlling the transport and reactivity at surfaces, of particularly silicate minerals, often in aqueous conditions. Thus the aim is to show that DL_POLY is useful for giving insights and can be applied to a wide range of complex interfaces.

Prof. Martyn Guest - *DL_POLY - A Performance Overview Analysing, Understanding and Exploiting available*

Abstract: This talk considers the performance attributes of DL_POLY, as measured and analysed over the past two decades. Following a brief overview of HPC technology, and the direction of travel over that period, we define the benchmark cases – for both DL_POLY Classic and DL_POLY 3 & 4 – used in generating a helicopter view of performance across well over 100 HPC systems – from the Cray T3E/1200E to today's Intel Skylake clusters. Consideration is given to the tools that have proved helpful in analysing the code's performance. With a more rigorous analysis of performance on recent systems, we discuss the optimum choice of processor and interconnect, and present power measurements when running the code, comparing these to measurements for other community codes.

Prof. Bill Smith - *A Short History of DL_POLY*

Abstract: DL_POLY project overview and recent work on stochastic thermostats.