Welcome

Dear Participants,

As the Scientific Organising Committee it is a great pleasure to welcome you all to the University of Bath's second HPC Symposium. The large number of participants, speakers and poster presenters demonstrates how successful the University's HPC service has been over the last years in driving research in many disciplines and across a wide range of scales - from Quantum Chemistry simulations of molecular structures via studying airflow in gas turbines to improving forecasts for global weather systems.

Aquila's 800 cores have been busy over the last year with an average utilisation of more than 80 percent. Looking forward, we hope that one the outcomes of this meeting will be a clearer vision of the future of the HPC service in Bath. Although currently the machine is mainly used for traditional MPI and OpenMP parallel programming, in the last six months two GPU nodes have been installed and the first users are already working with this new technology.

As you will see on the following pages we put together an exciting program for the day which includes a keynote lecture by Prof Mike Giles, one of the leading experts on using GPUs for Scientific Computing in the UK, a discussion session on the future of the HPC service in Bath and a very diverse selection of talks and posters from a wide range of departments within the University. Most importantly we hope that the meeting will be an opportunity for you as the users to exchange ideas on your research, network across all disciplines and have your say in the discussion session.

We would like to wish you both a successful and enjoyable day.

Yours sincerely,

the Scientific Organising Committee,

Dr Davide Tiana, Dept of Chemistry
Dr Steven Chapman, Computing Services
Dr Eike Mueller, Dept of Mathematical Sciences

PS: Don't forget that you can follow us during the meeting and afterwards on Twitter under **@BathHPC** and **#BathHPC2013**.

Programme

09:00 **Registration**

09:20 **Welcome and introduction**
Prof James Davenport, Dept of Computer Science

09:30 **Session 1**
Chair: **Prof James Davenport**, Dept of Computer Science

09:30 **Mr Chris Fullerton**, Dept of Physics
Exploring a dynamic transition in supercooled liquids using transition path sampling and point-to-set correlations

09:45 **Mr Alfonso Ramallo González**, Dept of Architecture and Civil Engineering
Using HPC to create an intelligent entity capable of recognising building energy performance by capturing basic thermal information

10:00 **Keynote**
Prof Mike Giles, Professor of Scientific Computing, University of Oxford
Future of HPC - trends, opportunities and challenges

11:00 **Symposium delegation photograph in atrium**

11:05 **Tea Break**

11:30 **Session 2**
Chair: **Dr Robert Watson**, Dept of Electronic and Electrical Engineering

11:30 **Dr David Roper**, Ansys Inc
What's new in Ansys

11:45 **Mr Christopher Hendon**, Dept Chemistry
Solving real life chemical problems with HPC: Removal of cork taint from wine

12:00 **Dr Keith Butler**, Dept of Chemistry
Bridging the gap; communication between theory and experiment using high performance computing

12:15 **Mr Chuan Li Yang**, Dept of Electronic and Electrical Engineering
Parallel CGLS technique for solving large scale EIT inverse problem

12:30 **Ms Li Chen**, Dept of Architecture and Civil Engineering
Modelling of marine renewable energy using OpenFOAM

12:45 **Dr Eike Mueller**, Dept of Mathematical Sciences
GPU implementation of elliptic solvers in numerical weather and climate prediction

13:00 **Lunch in the atrium**

14:00 **Session 3**
Chair: **Prof Steve Parker**, Dept of Chemistry

14:00 **Ms Jessica Bristow**, Dept of Chemistry
*Optical engineering of metal oxides: 3*d *impurities in Al_2O_3 and ZnO*

14:15 **Mr Lee Burton**, Dept of Chemistry
Computational analysis of Tin Sulfide for low-cost solar cells

14:30 **Dr Chris Eames**, Dept of Chemistry
Atomistic simulation studies of new materials for lithium ion batteries

14:45 **Dr Liang Sun**, Dept of Architecture and Civil Engineering
OpenMP implementation for FORTRAN on HPC

15:00 **Mr Ian Thompson**, Dept of Physics
Dynamic transitions for nearly-hard spheres

15:15 **Prof Robert Scheichl**, Dept of Mathematical Sciences
Teaching on Aquila – Introduction of parallel computing with MPI

15:30 **Tea Break**

16:00 **Presentation of talk and poster prizes**

16:05 **HPC Discussion**
Chair: **Prof David Bird**, Chair of the HPC Management Committee, Dean of Faculty of Science

17:00 **Wine and Cheese reception in the atrium**

17:30 **Close of meeting**

Poster Presentations

1. **Mr Nick Brincat and Mr Nick Williams**, Dept of Chemistry
   Defect chemistry and transport properties of Uranium Oxides

2. **Mr Yogesh Lalwani**, Dept of Mechanical Engineering
   3-D steady-state computations of ingestion through gas turbine rim seals

3. **Mr Clement Law**, Dept of Physics
   Simulations of lock and key colloids

4. **Dr Daniel Wolverson**, Dept of Physics
   Modelling a 2D semiconductor: MoS_2

5. **Mr Stephen Yeandel**, Dept of Chemistry
   Computer modelling of oxide thermoelectric materials

6. **Mr Adam Jackson**, Dept of Chemistry
   Ab initio thermodynamics for energy materials

7. **Prof Ian Williams**, Dept of Chemistry
   The right answer for the right reason: Ensemble-averaged kinetic isotope effects

8. **Mr Federico Brivio**, Dept of Chemistry
   New hybrid materials for DSSC

9. **Dr Davide Tiana and Ms Jessica Bristow**, Dept of Chemistry
   Quantum Espresso, keep your life fast

List of attendees

First Name	Surname	Department
David	Bird	Faculty of Science
Thomas	Bradley	Dept of Physics
Nick	Brincat	Dept of Chemistry
Jess	Bristow	Dept of Chemistry
Federico	Brivio	Dept of Chemistry
Antoine	Buchard	Dept of Chemistry
Lee	Burton	Dept of Chemistry
Keith	Butler	Dept of Chemistry
Mark	Cahill	Dept of Computer Science
Michael	Carley	Dept of Mechanical Engineering
Steven	Chapman	Computing Services
Lifen	Chen	Dept of Architecture and Civil Engineering
John	Clark	Dept of Chemistry
Jez	Cope	Dept of Chemistry
Jonathan	Cox	Dept of Chemistry
Jenny	Crabtree	Dept of Chemistry
Simon	Crampin	Dept of Physics
James	Davenport	Dept of Computer Science
Dennis	Davis	Computing Services
Richard	Driscoll	Dept of Chemistry
Chris	Eames	Dept of Chemistry
Naomi	Eastman	Computing Services
Matteo	Fasiolo	Dept of Mathematical Sciences
Chris	Fullerton	Dept of Physics
Mike	Giles	University of Oxford
Han	Gong	Dept of Computer Science
James	Grant	Dept of Chemistry
Luisa	Gumina	Dept of Mechanical Engineering
Christopher	Hendon	Dept of Chemistry
Rob	Jack	Dept of Physics
Adam	Jackson	Dept of Chemistry
Roger	Jardine	Computing Services
Peter	Kubiak	Dept of Chemistry
Yogesh	Lalwani	Dept of Mechanical Engineering
Timothy	Lanfear	NVIDIA
Clement	Law	Dept of Physics
Chuan	Li Yang	Dept of Electronic and Electrical Engineering
Martin	Maclaren	Computing Services
Marco	Molinari	Dept of Chemistry

First Name	Surname	Department
Eike	Mueller	Dept of Mathematical Sciences
Steve	Parker	Dept of Chemistry
Simon	Pickering	Dept of Mechanical Engineering
Catherine	Pink	UKOLN
Chris	Pudney	Dept of Biology and Biochemistry
Jeremy	Purches	NVIDIA
Natalya	Pya	Dept of Mathematical Sciences
Alfonso	Ramallo-González	Dept of Architecture and Civil Engineering
David	Roper	Ansys Inc
William	Saunders	Dept of Mathematical Sciences
Robert	Scheichl	Dept of Mathematical Sciences
Robert	Stringer	Dept of Architecture and Civil Engineering
Liang	Sun	Dept of Architecture and Civil Engineering
Ian	Thompson	Dept of Physics
Davide	Tiana	Dept of Chemistry
David	Tompsett	Dept of Chemistry
Marianne	Vagle	Computing Services
Aron	Walsh	Dept of Chemistry
Yifei	Wang	Dept of Computer Science
Robert	Watson	Dept of Electronic and Electrical Engineering
Alexander	Whiteside	Dept of Chemistry
Ian	Williams	Dept of Chemistry
Nick	Williams	Dept of Chemistry
Stephen	Wood	Dept of Chemistry
Daniel	Wolverson	Dept of Physics
Ed	Wright	Dept of Physics
Stephen	Yeandel	Dept of Chemistry
Jun	Zang	Dept of Architecture and Civil Engineering
Henry	Zhao	School of Management
Qing	Zhou	Dept of Chemistry

Abstracts of talks and posters

Session 1

Chair: **Prof James Davenport**, Dept of Computer Science

1.1 Exploring a dynamic transition in supercooled liquids using transition path sampling and point-to-set correlations

Presented by: ***Mr Chris Fullerton**, Dept of Physics*

As a liquid is cooled towards its (experimental) glass transition it becomes extremely slow moving. It might be expected that this behaviour is accompanied by a dramatic change in structure, but this is not the case.

Considering an ensemble of trajectories of a glassy system, a novel phase transition is found between a state with high dynamical activity (fast moving) and one with low dynamical activity (slow moving).

This dynamic transition is linked to the slowing down that occurs in the liquid as it is cooled. We discuss simulating trajectories that are biased towards this low-activity state using transition path sampling and how we can use point-to-set correlations to try and identify why the inactive state is slow moving.

Keywords: *Statistical Mechanics, Monte Carlo Simulations, Glassy and Disordered Systems, Dynamic Phase Transitions*

1.2 Using HPC to create an intelligent entity capable of recognising building energy performance by capturing basic thermal information

Presented by: ***Mr Alfonso Ramallo González**, Dept of Architecture and Civil Engineering*
Co-authors: *M. Brown, D. A. Coley*

ENLITEN is research project with the objective of reducing carbon emissions from energy use within buildings by understanding, incentivising and influencing changes in the habitual behaviours of the buildings' occupants.

In ENLITEN we will capture data from 200 buildings, and that data will be sent to a central server that will estimate on-line the characteristics of the building. With this we will not only be able to know basic characteristics of the dwellings (such as the U-Value of the walls), but also, instantaneous actions such as an occupant opening a window despite the heating is one.

The large amount of data gathered from the buildings, will need to be stored in a central server, but also, the fact that hundreds of houses have to be analysed in real time, makes parallel computing ideal for our research.

Although the characterisation algorithm is not computationally expensive, performing such a large number of simulations instantaneously for all the buildings can only be possible using High Performance Computing in a centralised manner.

Keywords: *Computational Building Physics, elastic computing, artificial intelligence*

Session 2

Chair: **Dr Robert Watson**, Dept of Electronic and Electrical Engineering

2.1 What's new in Ansys

Presented by: **Dr David Roper**, Ansys Inc

2.2 Solving real life chemical problems with HPC: Removal of cork taint from wine

Presented by: ***Mr Christopher Hendon**, Dept Chemistry*
Co-authors: *A. Walsh*

Cork taint is the wet-dog smelling, mouldy and offensive tasting flavour of wine with impurities. The taint is attributed to 8 impurities; simple organic molecules that were either in the cork itself or from the bottling process. Sometimes a bottle of wine is corked from the day of bottling, whilst more frequently the impurities amplify over time. The result: your 1988 ChÃćteauneuf-du-Pape has turned rancid, undrinkable by even the most undeveloped palate.

There is currently no successful method for the removal of cork taint from wine. One of the more frequently experimented methods for this impurity removal is through the adsorption to a polymer, low-density polyethylene; cling film. Whilst this works for most impurities, it does not extract the 2 major organics responsible for taint, trichloro and tribromo-anisole (TCA and TBA). So how does HPC help solve this problem? Through the application of quantum mechanics we can precisely elucidate the physical properties of small organic molecules. Through investigations of TCA and TBA we can propose novel materials and methods for the extraction of taint from wine.

Keywords: *Computational Chemistry, Cork Taint, Wine, Polymers*

2.3 Bridging the gap; communication between theory and experiment using high performance computing

Presented by: ***Dr Keith Butler**, Dept of Chemistry*
Co-authors: *A. J. Jackson*

The gap between empirical observation and fundamental theory lies at the heart of many of the most fundamental debates in science. With the advent of high performance computing we have a valuable new tool in the attempt to reconcile fundamental theoretical models with measurable quantities. Using the example of the application of quantum mechanics for the design of photovoltaic devices we propose a scheme which examines the different routes through which we routinely address this divide. We explain the role of numerical experiments, made possible by high performance computing, in conjunction with intuitive heuristic models to facilitate the application of Schrödinger's equation to design fully functional photovoltaic devices.

Keywords: *Fundamental theory, numerical experiments, photovoltaics*

2.4 Parallel CGLS technique for solving large scale EIT inverse problem

Presented by: ***Mr Chuan Li Yang**, Dept of Electronic and Electrical Engineering*
Co-authors: *M. Soleimani*

Electrical impedance tomography (EIT) is a fast and cost-effective technique to provide tomographic conductivity image of a subject from boundary current-voltage data. EIT has potential applications in medical imaging as well as industrial processes and geophysics. 3D EIT imaging is gaining popularity as it allows volumetric tomography imaging. A time and memory efficient method for solving large scale 3D EIT inverse problem using a parallel conjugate gradient (CG) algorithm will be presented. To solve the inverse EIT problem Jacobian matrices are used. 3D EIT system with large number of measurement data can produce large size of Jacobian matrix; this could cause difficulties in the computer storage and the inversion process. One of challenges in 3D EIT is to decrease the reconstruction time and memory usage at the same time retaining the image quality. Firstly, a sparse matrix reduction technique is proposed using thresholding to set very small values of the Jacobian matrix to zero. By adjusting the Jacobian matrix into a sparse format, the element with zeros would be eliminated, which result in a saving of memory requirement. Secondly, a block-wise CG method for parallel reconstruction has been developed. By making use of multiple CPUs, computational speed has been increased dramatically. The proposed method has been tested using simulated data as well as experimental test samples. It enables large scale EIT problem to be solved efficiently. Image quality measures are presented to quantify the effect of sparse matrix reduction in reconstruction results. The author believes further computational benefits can be made by using HPC facilities.

Keywords**:** *Electrical impedance tomography, large scale 3D EIT problem, parallel reconstruction, sparse Jacobian*

2.5 Modelling of marine renewable energy using OpenFOAM

Presented by: ***Ms Lifen Chen**, Dept of Architecture and Civil Engineering*
Co-authors: *J. Zang, A. Hillis*

Following the issue of climate change and energy demand, the development of marine renewable energy is attracting increasing attention. A rigorous approach is required leading to the better design of wave energy converters with increased efficiency. Very few WECs can currently be simulated by theoretical analysis due to the complicated nature of wave-structure interactions. The use of CFD codes is becoming increasing important in engineering design work. OpenFOAM, a free, open-source library, has been applied in coastal engineering successfully in my research group. Following the success, the proposed research focuses on developing a numerical model based on OpenFOAM to predicting wave-WEC interactions.

In CFD simulations, the solution domain and time domain are discretised into a number of cells and time steps, respectively. The numerical solutions are broadly affected by mesh resolution and type. High resolution mesh is required to obtain more accurate results, which means high computational costs. Running in parallel is the best way to address this problem. Satisfactory results, which will be presented at the symposium, have been obtained by running OpenFOAM in parallel on distributed processers, including a local multiprocessor machine and the central HPC system, *Aquila*.

Keywords: *offshore engineering, OpenFOAM, MPI, multi-cores*

2.6 GPU implementation of elliptic solvers in numerical weather and climate prediction

Presented by: ***Dr Eike Mueller**, Dept of Mathematical Sciences*
Co-authors: *R. Scheichl*

Many Numerical Weather and Climate Prediction models require the fast solution of an elliptic partial differential equation (PDE) at every model timestep and equations with a very similar structure are encountered in many other applications in geophysical modelling in ``flat'' geometries. With increasing grid resolution these elliptic PDEs can only be solved on operational timescales if highly efficient algorithms are used and their performance and scalability to large problem sizes can be guaranteed on novel computer architectures. Recently Graphics Processing Units (GPUs) have been shown to give significant speedups for many applications in Scientific Computing. We ported a Preconditioned Conjugate Gradient Solver for a typical meteorological model equation to a GPU in the cuda programming model and demonstrated both the relative and absolute performance of the solver on the recently acquired nVidia M2090 GPU node of aquila. As the algorithm is memory bound, it is important to minimise global memory transfers. We achieved this by exploiting the tensor structure of the underlying grid and elliptic operator, which allows the recalculation of local matrix stencils instead of loading them from memory, and by fusing different kernels in the main loop. In total we were able to achieve a speedup of around $50\times$ relative to the sequential

code on a Sandybridge CPU and can utilise 25-50% of the theoretical peak global memory bandwidth. The optimised code is about four times faster than a matrix-explicit GPU implementation based on the existing CUBLAS and CUSPARSE libraries.

Keywords: *Numerical Weather and Climate Prediction, Geophysical Modelling, Elliptic PDEs, Iterative Solvers, GPUs*

Session 3

Chair: **Prof Steve Parker**, Dept of Chemistry

3.1 Optical engineering of metal oxides: 3d impurities in Al_2O_3 and ZnO

Presented by: ***Ms Jessica Bristow**, Dept of Chemistry*
Co-authors: *A. Walsh*

We have performed a systematic investigation of the chemical processes due to the presence of transition metal impurities in the structure of corundum (Al_2O_3) and zincite (ZnO), in particular those that give rise to colour.

One major result concerns the blue colour of sapphire ($\alpha - Al_2O_3$ with Fe and Ti impurities), the origin of which is at the centre of a long-standing debate. The mechanism has been analysed at different levels of theory (Born ionic potentials, Hartree-Fock, and Density Functional Theory). We identify that nearest neighbour Ti and Fe pairs exist in a Ti^{III}/Fe^{III} ground-state configuration. The charge transfer from Ti to Al (i.e. from Ti^{III}/Fe^{III} to Ti^{IV}/Fe^{II}) is responsible for the blue colour of sapphire. In contrast to the general assumption, the Ti^{IV}/Fe^{II} configuration is a metastable state that occurs due to optical excitation. A spin relaxation calculation confirms the lowest energy system to contain a spin down electron on the titanium, confirming the instability in the aliovalent pair and suggesting this is due to Coulomb hole interaction.

We have also considered more complex defect configurations involving three species. We propose that a tri-cluster between $Ti^{III} - (Ti^{IV}/Fe^{II})$ in which the titanium cations are edge-sharing and the Ti^{IV}/Fe^{II} pairs are face-sharing, could exist. This defect aggregate leaves the charge transfer energies unchanged, potentially increasing the stability of the Ti^{IV}/Fe^{II} pairs. Intra-valence d-d transitions and intervalence Fe to Fe charge transfer cannot occur at the appropriate wavelengths for colouration. All predictions are consistent with available spectroscopic measurements.

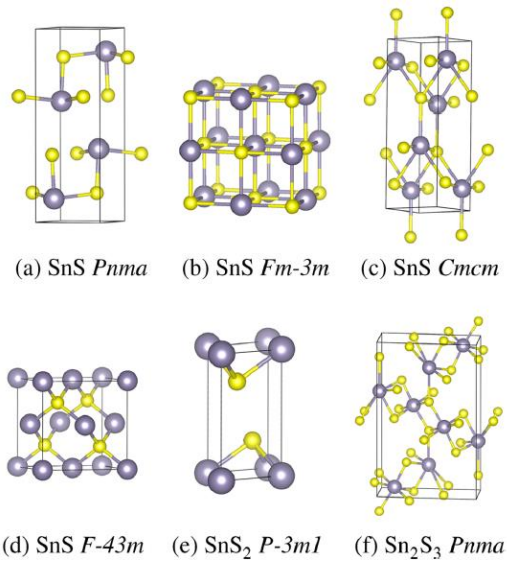
Also of interest we have plotted the spin density profiles between two titanium cations when neighbouring, which depict a sharing of electron density between the species. We propose this to be why the Ti^{III}/Ti^{IV} charge transfer remains unassigned in absorption spectroscopy.

3.2 Computational analysis of Tin Sulfide for low-cost solar cells

Presented by: ***Mr Lee Burton**, Dept of Chemistry*
Co-authors: *A. Walsh*

For photovoltaic (PV) technology to provide a significant fraction of society's energy supply, device components must be abundant, cheap and non-toxic. One exciting candidate that satisfies the above criteria as well as exhibiting almost ideal electronic properties is tin sulfide (SnS). For example, SnS is reported to have a higher optical absorption coefficient and a more suitable electronic structure for light absorption than current commercially available materials. However, the record device efficiency for tin sulfide PV cells is only 2.0 %, far below other candidate materials.

We employ first-principles calculations to study the multiphasic tin sulfide system (see figure), with the goal of identifying the limiting properties in PV devices. Our approach provides insight into thermodynamic stabilities, reaction pathways and electronic configurations, which allows us to ultimately comment on the applicability of a given phase. We are also able to predict the characteristic signatures of different structures and suggest methods to discern between them.


(a) SnS *Pnma* (b) SnS *Fm-3m* (c) SnS *Cmcm*

(d) SnS *F-43m* (e) SnS_2 *P-3m1* (f) Sn_2S_3 *Pnma*

One of our key results to date includes the prediction that a recently reported structure of SnS, which has been lauded as a potential solar material has been mis-assigned. This phase is unstable, with large negative phonon modes and spontaneous distortions upon introduction of moderate conditions (*e.g.* 300K). This represents, for the first time, atomistic simulations that contradict empirical observations, using a systematic and methodical approach that is able to probe directly where uncertainties in experiment overlap.

Keywords: *Computational Chemistry, Sustainable Energy, Semiconductor Physics*

3.3 Atomistic simulation studies of new materials for lithium ion batteries

Presented by: ***Dr Chris Eames**, Dept of Chemistry*
Co-authors: *M. S. Islam*

The lithium ion battery is one of the crowning achievements of materials science. Billions of cells are manufactured every year to power personal electronic devices such as mobile phones and laptop computers. The search is on for the next generation of materials for lithium batteries for use in electric vehicles. These must be low cost, safe and offer a high energy density and capacity as well as a long cycle life. In this talk the contribution of high performance computing to lithium battery research will be outlined. Using lithium iron silicate as an example material we will show how key

battery properties such as the voltage, capacity and charge rate can be computed using density functional theory and interatomic potentials based techniques in a parallel computing environment. These methods reveal atomic scale insights into the influence of the electronic and atomic structure upon the macroscopic properties of the battery.

Keywords: *Computational Chemistry, Energy Materials, Lithium Batteries*

3.4 OpenMP implementation for FORTRAN on HPC

Presented by: ***Dr Liang Sun**, Dept of Architecture and Civil Engineering*
Co-authors: *J. Zang*

OpenMP has been successfully implemented in a FORTRAN program for hydrodynamic analysis. Background of the numerical codes will be introduced at the beginning of the talk. In the following slides, the original sequential codes will be analyzed. Details of OpenMP implementation for the specific codes will be explained in the main part of presentation. Emphasis will be put on how to formulate the matrix equation in parallel and solve it using Intel Math Kernel Library (Intel MKL). The key issue of data race will be also highlighted. Some tests for the modified codes have been carried out on HPC. Computational time for small and large scale problems has been considered. Finally, some concluding remarks will be given based on the tests.

Keywords: *FORTRAN, OpenMP, Intel MKL, hydrodynamic analysis*

3.5 Dynamic transitions for nearly-hard spheres

Presented by: ***Mr Ian Thompson**, Dept of Physics*

We stochastically simulate the development of particle systems through time by generating trajectories, flipbook-stye animations of the system. We collect trajectories and measure how much particle motion there is within them, their dynamic activity. Entire trajectories are accepted or rejected with respect to their activity in a manner analogous to ordinary Monte Carlo moves. We have discovered a phase transition between a dynamically active and inactive phase consistent with the colloidal glass transition.

Keywords: *Computational Physics, Biased Monte Carlo Simulations, Dynamic Transitions, Statistical Mechanics*

3.6 Teaching on Aquila – Introduction of parallel computing with MPI

Presented by: ***Prof Robert Scheichl**, Dept of Mathematical Sciences*
Co-authors: *E. Mueller*

One of the biggest hurdles in getting more people to use modern supercomputing facilities such as aquila or HECToR is a lack of basic understanding what parallel computing is and how parallel programs work. In this talk I will briefly describe a course that we teach to the students on the MSc in Modern Applications of Mathematics and that is an optional unit on our MMath programme, where students get a basic introduction into Scientific Computing and into Parallel Computing with MPI. Apart from letting students try their hands at writing their first parallel code, the course also aims at giving students a better understanding of the effects of rounding errors and an efficient use of the memory hierarchies on modern processors. The course has been very successful and the feedback from students is extremely positive. The fundamental problem highlighted in the first sentence is likely to get even worse with the advent of novel multicore architectures, such as GPGPUs or the Intel MIC multiprocessor, and it will thus become even more important to include such a course in modern computational science and engineering degrees. The course is also open to PhD students.

Keywords: *Teaching, MPI, Introduction to Parallel Computing*

Posters

P1 Defect chemistry and transport properties of Uranium Oxides

Presented by: ***Mr Nick Brincat and Mr Nick Williams**, Dept of Chemistry*
Co-authors: *M. Molinari, S Parker*

There has been a resurgence of interest in the actinides and their oxides, particularly uranium, because of their role as nuclear fuels and increased awareness of problems such as CO2 emissions, energy security and dwindling fossil fuel reserves.

Uranium displays a number of oxidation states that give rise to a complex family of binary oxides in the UO_2-UO_3 range (U^{4+}-U^{6+}). UO_2 is particularly susceptible to oxidation and the formation of defects and defect clusters (e.g. 2:2:2 Willis and cuboctahedral clusters) is a well-documented phenomenon. Both defect chemistry and transport of matter (oxygen or uranium depending on the operating temperature) leads to variation of the sample composition and ultimately to phase changes.

Here we use DFT and potential based techniques to investigate these two topics. Computational methods have been used to complement experimental examination of these materials as they offer convenient and alternative means of investigating their properties.

DFT techniques are used to evaluate the fundamental properties and relative stabilities of UO_2, U_3O_8 and UO_3 phases and defects in UO_2 to provide insight in to the oxidation of U and its role in the transition between different oxides.

When studying the transport properties of UO_2 it is essential to go for bigger systems which include structural features that represent real samples. Molecular dynamics is then utilised to calculate the diffusion of oxygen within nuclear fuels. Whilst past studies have focused on diffusion in polycrystalline materials fundamental questions remain as to the effect individual defects such as grain boundaries have on the oxidation of the material. To this end both tilt and twist grain boundaries have been simulated. Depending on the temperature range the rates of diffusion were observed to be anisotropic and enhanced at both the grain boundary interface and in the region immediately surrounding it.

Keywords: *UO_2, DFT, Atomistic*

P2 3-D steady-state computations of ingestion through gas turbine rim seals

Presented by: ***Mr Yogesh Lalwani****, Dept of Mechanical Engineering*

The application of CFD in turbomachinery has long been used in industry; however the complex and transient nature of rotating flows in a rotor-stator interaction, has made these simulations time-consuming, taking up to several weeks or months of computational time. My research is focused in fast steady-state computations for the study of ingestion through gas turbine rim-seals, investigating the various approaches to solve the complicated 3D unsteady flow behaviour within the wheel-space of a gas turbine.

The minimum sealing air flow needed to prevent overheating of the rotor-stator wheel-spaces in gas turbines is a major concern today. Too much sealing air would reduce the overall engine efficiency, which is harmful for carbon dioxide emissions to the environment; too little air could lead to overheating and catastrophic failure. Therefore, it is important to understand the mechanisms of annulus hot gas ingestion (ingress) into the rotor-stator wheel-space to assist engine designers in determining the best seal geometry for the minimum use of sealing air.

The commercial computational fluid dynamics code CFX 13/14 has been employed to carry out simulations to investigate the fluid mechanics of general rim-seal geometries in a 3D model of a turbine stage. The mainstream annulus, seal and wheel-space geometries are based on an experimental test rig used at the University of Bath. The calculated peak-to-trough pressure difference in the annulus, which is the driving mechanism for ingestion, is in good agreement with experimental measurements. There is also good agreement between the computed and measured effectiveness and swirl ratios in the wheel-space.

Keywords: *ANSYS, MPI, Gas Turbines, Ingestion, Ingress, Steady-State Computations, CFD (Computational Fluid Dynamics)*

P3 Simulations of lock and key colloids

Presented by: **Mr Clement La**w, Dept of Physics
Co-authors: *R. Jack, N. Wilding*

Lock-and-key colloids are particles with complementary geometrical shapes [1]. The lock is a spherical particle with a spherical cavity on its surface into which a spherical key particle fits. When combined with, for example, a polymer they self-assemble [1] into 'snow man'-like assemblies, 'caterpillar'-like chains and potentially new states of matter [2]. To describe these processes, we consider a potential that quantify how the colloidal particles interact. The shapes of the colloids mean that the depletion potentials may have quite complicated forms. Nevertheless, we show how they can be measured, using a state-of-the-art Monte Carlo algorithm [2]. We use these measurements to develop a simplified potential that will enable rapid and accurate simulation of self-assembly in these systems.

[1] Sacanna et al, Nature 464, 575 (2010)
[2] Ashton et al, arXiv:1304.3675 [cond-mat.soft]

Keywords: *Computational Chemistry, GPUs, MPI*

P4 Modelling a 2D semiconductor: MoS_2

Presented by: **Dr Daniel Wolverson**, Dept of Physics

Molybdenum sulphide is a layered crystalline material that can be produced down to a single layer thickness; that is, one sheet of Mo atoms with single sheets of S atoms above and below. Graphene, derived from graphite, is the most well-known material of this type since the award of the Nobel Prize in Physics in 2010 to Andre Geim and Konstantin Novoselov for its discovery. In preparing such 2D materials or tailoring them for applications, the measurement of the frequencies at which the atoms in the crystalline lattice vibrate has turned out to be a crucial diagnostic tool for answering questions such as the number of layers present, the degree of perfection of the crystalline layer, and the extent to which the layer is distorted by the forces acting on it that arise from its 3D environment.

Interpretation of the results of such measurements requires the simulation of the vibrational modes of perfect and distorted layers. Recently, we have carried out simulations of single-layer MoS_2 [1] on Aquila, using the Quantum Espresso code (open source and available under the GNU licence). This code is based on density functional theory, uses plane wave methods and pseudo potentials, and stands out from similar DFT codes due to its ability to calculate vibrational modes of crystals very efficiently via density functional perturbation theory. The QE code runs on anything from cell phones and playstations to BlueGene and is fully compatible with parallel architectures and MPI. As an advertisement for the availability of this code in Bath, we shall present some of our results onMoS_2, together with a summary of the computational resources we required.

[1] Physical Review B 87, 081307(R) (2013)

Keywords: *MoS_2, lattice dynamics, Raman, PWSCF, Quantum Espresso, MPI*

P5 Computer modelling of oxide thermoelectric materials

Presented by: ***Mr Stephen Yeandel***, *Dept of Chemistry*
Co-authors: *M. Molinari, S.C. Parker, D.C. Sayle and R. Freer*

Traditional power generation techniques are inefficient. Up to 66% of energy is lost as heat to the environment. Thermoelectric (TE) materials are built into simple solid-state devices to reduce this energy loss by converting heat directly into usable electricity. State of the art devices are currently based on the higher chalcogenides, lead, bismuth and other highly toxic elements. Basing TE devices on oxide based materials is a promising alternative due to their high thermal stability, low toxicity and large margin of improvement by employing nanostructuring (i.e. introducing grain boundaries or nanopores) and band engineering (i.e. doping).

Our research explores these two aspects and employs both potential based and DFT methods to investigate the role of nanostructuring in lowering the lattice thermal conductivity of oxides and band engineering to enhance electrical conductivity.

Oxides currently suffer from high thermal conductivity which substantially reduces their thermoelectric figure of merit (ZT). Careful nanostructuring may help reduce the thermal conductivity of the materials and hence boost ZT. Molecular dynamics can provide a tool to study different levels of nanostructuring, calculating the thermal conductivity of different nanostructured materials.

Work on nanostructured magnesium oxide has demonstrated an order of magnitude reduction in the thermal conductivity compared to the bulk material. Additionally, specific features of the nanostructure have been related to the thermal conductivity profile, offering qualitative guidance on future nanostructure engineering for thermal conductivity. The perovskite type material SrTiO3 has also been investigated and the thermal conductivity of different grain boundaries is currently being calculated.

Band engineering is addressed using a combination of plane wave pseudopotential and all-electron calculations to optimise the pure and doped structures of $CaMnO_3$. The semi classical coefficients are calculated using the Boltzmann theory as implemented in the BoltzTraP code.

Keywords: *Computational Chemistry, Thermoelectric, Thermal Conductivity, Molecular Dynamics, Band Engineering, Perovskite*

P6 Ab initio thermodynamics for energy materials

Presented by: **Mr Adam Jackson**, Dept of Chemistry
Co-authors: A. Walsh

Computational modelling allows materials to be studied in an idealised, directly-comparable way. In recent years it has become practical to model solid-state thermodynamic properties *ab initio* (i.e.

with no experimental input). This is especially helpful for working on energy materials, which often require very high purities, specialised equipment and expensive or toxic precursors. An approach is outlined for modelling chemical reaction free energies including temperature and pressure effects. In practice, local calculations in Python and MATLAB are used for data processing and generation of more demanding quantum chemistry calculations. These are carried out in batches on HPC clusters across hundreds or thousands of cores. The preferred code for this project is FHI-aims, which is modern and highly-scalable.

This approach will allow us to bridge the gap between fundamental models and large-scale processing conditions, bringing theoretical insights to complex phase equilibria. The aim is to select viable routes for the sustainable production of next-generation photovoltaic materials under modest reaction conditions.

Keywords: *Quantum chemistry, task farming, Python, PyLab, MATLAB, FHIaims*

P7 The right answer for the right reason: Ensemble-averaged kinetic isotope effects

Presented by: ***Prof Ian Williams**, Dept of Chemistry*

Back in the late 90s, my group pioneered hybrid quantum/classical calculations of kinetic isotope effects for explicitly solvated chemical reactions using software developed in Bath and implemented on Unix workstations. In general these calculations were restricted to a single arrangement of the (classical) solvent molecules around the (quantum) solute as it transformed from its reactant configuration (an energy minimum) to its transition-state configuration (a first-order saddle point). Apparently, a “poor” (but quick) quantum method in the quantum/classical combination gave a “poor” result in comparison with experiment, whereas a “good” (but slow) quantum method gave a “good” result. However, consideration of a small number of alternative solvent configurations yielded a range of different results with the “poor” method alone that varied by as much as the difference between results of the “poor” and “good” methods for a single configuration. Recently we performed ensemble averaging for the same reaction (chloromethane hydrolysis in water) but with many different solvent configurations sampled from a molecular dynamics simulation. The average kinetic isotope effect $k(CH_3Cl)/k(CD_3Cl)$ calculated with the (“good”) B3LYP/6-31+G(d,p)/TIP3P method is in good agreement with experiment, whereas the (“poor”) AM1/TIP3P method is not. This comparison is meaningful because it includes consideration of uncertainties owing to sampling of a range of representative thermally-accessible solvent configurations: we get the right answer for the right reason. The calculation for each sampled configuration is performed serially with a combination of the Dynamo and Gaussian09 codes on a single Aquila CPU but with many configurations efficiently distributed over many CPUs.

Keywords: *Computational Chemistry, extremely coarse parallelism*

P8 New hybrid materials for DSSC

Presented by: ***Mr Federico Brivio**, Dept of Chemistry*

One alternative to silicon photovoltaics is given by dye-sensitized solar cells (DSSC). Such devices provide a good solution for cheap, flexible solar technology. However, one limitation is the limited spectral response of traditional dye molecules. We focus on a new class of dye with the perovskite structure, which can be derived from CsSnI3. In particular, the inorganic cations can be replaced by molecular cations (e.g. NH4+) to produce hybrid perovskite materials.

Firstly, we have performed a computational study to systematically characterize the inorganic derivatives of CsSnI3 that are obtained by changing the metals and the halide in the original composition. A route to engineering the electronic properties of this class of materials is identified. Furthermore, the preference for ferroelectric distortions is addressed through the relative stability of the cubic and tetragonal perovskite phases.

Secondly, we have investigated the orientational disorder of molecular cations within the perovskite lattice. In general, the barriers to rotation are small, but coherent ordering of molecular dipoles results in a spontaneous ferroelectric distortion to a series of low symmetry phases.

We are currently investigating the excited-state and optical properties of these systems.

P9 Quantum Espresso, keep your life fast

Presented by: ***Dr Davide Tiana**, Dept of Chemistry*
Co-authors: *J. Bristow*

Since the advent of the quantum mechanics, the biggest challenge that theoretical chemists had to deal with was the computational effort required to perform calculations. Following the Moore's law, computers capability has improved exponentially in the last decades, making the computational chemistry from a niche science to a common tool used to confirm and explain chemistry. On the other hand, the presence of bi-electronic integrals (6 dimension objects) during the solution of the Schrodinger equation still limits the size of the systems that can be calculated using not empirical methods. For these reasons theoreticians have been spending a lot of effort in improving the codes making them faster using numerical libraries and parallelisation - and "lighter", developing algorithms to reduce the computational cost of such integrals.

Quantum Espresso (QE) is an open source program to perform studies on solid state using either plane-wave or Car-Parrinello molecular dynamics. Originally written in Fortran 95 and C - the code is openMP-MPI parallelised - the program now exists also as a GPU version (CUDA).

In this work we show how, fully taking advantages of optimised algebraic libraries and exploiting the parallelisation on different levels, QE can linearly scale up to thousands cores.

Keywords: *Computational Chemistry , Quantum Espresso*

Acknowledgements

First and foremost, we would like to thank our speakers, poster presenters and session chairs for facilitating the insightful and thought-provoking discussions of the day.

Special thanks go to the members of the Scientific and Local Organising Committees for their invaluable input during the planning stages:

Steven Chapman
Eike Mueller
Davide Tiana
Naomi Eastman
Yogesh Lalwani
Rosemary Green
Steph Jewitt
Vicky Evans
Sarah Griffin

We appreciate our ground crew for their help and hard work on the day.

Finally, thanks to you, the attendees, for your participation and for truly making this a productive Forum.