Welcome

Dear Participants,

As the Scientific Organising Committee it is a great pleasure to welcome you all to the University of Bath's third HPC Symposium. As you will see in the following pages, you have helped us to put together an exciting program for the day which includes a keynote lecture from Prof. Martyn Guest, one of the leading experts on using HPC for scientific computing in the UK.

The day presents an opportunity to celebrate the diverse work that utilizes HPC at the University: from nanoparticles to global weather forecasting via DNA and gas turbines. While a number of projects use HPC to improve our understanding of renewable energy generation and storage, other researchers are developing algorithms and code for new technologies that increase the efficiency of programs reducing the time and resources required to obtain results.

In order to support research using HPC the university recently awarded funding in excess of £1million for a new resource to replace the aging Aquila, as well as increasing support for users. The first phase of Aquila came on-line in 2007 and the main machine has been in operation since 2009, while GPU nodes were introduced in 2012. The replacement will increase the capacity of HPC at the University, including more new technologies and features. To mark this investment, after a few words of welcome from the Deputy Vice Chancellor, Prof. Kevin Edge we will begin with an announcement on the replacement for Aquila, including the results of the naming competition.

We hope that the meeting will be an opportunity for you the users to exchange ideas on your research and build collaborations across disciplines while discovering the breadth of research that goes on in a dark room somewhere in the bowels of the university.

Yours sincerely,
the Scientific Organising Committee,

Dr Steven Chapman, Computing Services
Dr Eike Mueller, Dept of Mathematical Sciences
Dr James Grant, Dept of Chemistry

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

Programme

09:00   **Registration**

09:30   **Welcome and introduction**
Prof Kevin Edge, Deputy Vice-Chancellor

09:45   **Session 1**
Chair: **Prof David Bird**, Chair of the HPC Advisory Group, Faculty of Science

09:45   **Prof James Davenport**, Dept of Computing Science
Dr Steven Chapman and Dr Roger Jardine, Computing Services
Aquila2 Update

10:00   **Invited Talk:**
Dr Araxi Urrutia, Dept of Biology and Biochemistry
Uncovering the genomic basis of complexity through the analyses of 30million RNA sequences

10:30   **Mr Richard Driscoll**, Dept of Chemistry
An investigation into the vibrational properties of uranium minerals

10:45   **Mr Christopher Hendon**, Dept of Chemistry
Coffee

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

11:05   **Tea Break**

11:25   **Session 2**
Chair: **Prof Robert Scheichl**, Dept of Mathematical Sciences

11:25   **Invited Talk:**
Jeremy Purches, Director, High Performance Computing UK&I, NVIDIA Limited
GPU Accelerated Computing

11:45   **Dr James Grant**, Dept of Chemistry
Coarse-grained simulations: making simple work

12:00   **Mr Ian Thompson**, Dept of Physics
Moving data processing to GPUs, a day to a tea break

12:15   **Mr Will Saunders**, Dept of Architecture and Civil Engineering
A multi-GPU solver for the non-linear shallow water equations

12:30   **Dr Eike Mueller**, Dept of Mathematical Sciences
Massively Parallel Scalability of Elliptic Solvers on Thousands of GPUs

12:45   **Dr David Acreman**, University of Exeter
GW4

13:00   **Lunch in the atrium**

14:00   **Session 3**
Chair: **Prof James Davenport**, Dept of Computer Science

14:00   **Keynote**
Prof Martyn F. Guest, Cardiff University
Application Performance in Materials Science, Chemistry and Nanoscience –
Perspective, Performance and Challenges

15:00   **Dr Christopher Eames**, Dept of Chemistry
Combinatorial Search for High Capacity MXenes as New Energy Storage Materials

15:15   **Mr Adam Jackson**, Dept of Chemistry
Earth-abundant photovoltaics "from the beginning"

15:30   **Tea Break**

16:00   **Session 4**
Chair: **Prof Aron Walsh**, Dept of Chemistry

16:00   **Dr Douglas Ashton**, Dept of Physics
Effective interactions in highly size asymmetric mixtures

16:15   **Mr Jon Chesterfield**, Dept of Mechanical Engineering
Thoughts on robust distributed computation

16:30   **Dr Michael Carley**, Dept of Mechanical Engineering
Fast Multipole Methods for shellfish and aeroplanes

16:45   **Prof Robert Scheichl**, Dept of Mathematical Sciences
Multilevel Monte Carlo – Monte Carlo methods that are not embarrassingly parallel

17:00   **Presentation of talk and poster prizes**

17:15   **Wine and Cheese reception in the atrium**

18:00   **Close of meeting**

Posters

1. **Ms Jessica Bristow**, Dept of Chemistry
   An accurate and transferable interatomic potential for modelling metal-organic frameworks: BTW-FF

2. **Dr Steven Chapman**, Computing Services
   Aquila by Numbers

3. **Mr Joseph Flitcroft**, Dept of Chemistry
   Hydrogen Species in UO_2 – Defect Formation and Diffusion Paths

4. **Mr Christopher Fullerton**, Dept of Physics
   Investigating Amorphous Order in Stable Glasses Through Random Pinning

5. **Mr Chunde Liu**, Dept of Architecture and Civil Engineering
   The creation of current and future test reference weather years at a high spatial resolution for the built environment

6. **Mr Marco Molinari**, Dept of Chemistry
   Computational Solid State Chemistry @ Bath

7. **Mr Jonathan Skelton**, Dept of Chemistry
   M4: A Programme in Metastable Materials

8. **Mr Timo Peltola**, Dept of Physics
   Drift-diffusion Modelling of Hybrid Perovskite Solar Cells

9. **Prof Ian Williams**, Dept of Chemistry
   Solvent effects on organic reaction mechanisms

10. **Mr Philippe Wilson**, Dept of Chemistry
    Solvent effects on isotope effects: methyl cation as a model system

List of attendees

First Name	Surname	Department / University
David	Acreman	University of Exeter
Stefano	Angioni	Dept of Mechanical Engineering
Douglas	Ashton	Dept of Physics
Jakub	Baran	Dept of Chemistry
David	Bird	Faculty of Science
Nick	Brincat	Dept of Chemistry
Jessica	Bristow	Dept of Chemistry
Federico	Brivio	Dept of Chemistry
Lee	Burton	Dept of Chemistry
Keith	Butler	Dept of Chemistry
Michael	Carley	Dept of Mechanical Engineering
Steven	Chapman	Computing Services
Jon	Chesterfield	Dept of Mechanical Engineering
Jez	Cope	Dept of Chemistry
Rachel	Crespo-Otero	Dept of Chemistry
James	Davenport	Dept of Computer Science
Richard	Driscoll	Dept of Chemistry
Joao	Duro	Dept of Computer Science
Chris	Eames	Dept of Chemistry
Kevin	Edge	Vice Chancellor's Office
Paul	Evans	University of Exeter
Joseph	Flitcroft	Dept of Chemistry
Chris	Fullerton	Dept of Physics
Feng	Gao	Dept of Architecture and Civil Engineering
James	Grant	Dept of Chemistry
Martyn	Guest	Cardiff University
Christopher	Hendon	Dept of Chemistry
Nick	Hockings	Dept of Mechanical Engineering
Robert	Jack	Dept of Physics
Adam	Jackson	Dept of Chemistry
Roger	Jardine	Computing Services
Chunde	Liu	Dept of Architecture and Civil Engineering
Estelina	Lora Da Silva	Dept of Chemistry
Marco	Molinari	Dept of Chemistry
Eike	Mueller	Dept of Mathematical Sciences
Steve	Parker	Dept of Chemistry
Timo	Peltola	Dept of Physics
Simon	Pickering	Dept of Mechanical Engineering

First Name	Surname	Department / University
Jeremy	Purches	NVIDIA Limited
Andrew	Rees	Dept of Mechanical Engineering
Will	Saunders	Dept of Architecture and Civil Engineering
Robert	Scheichl	Dept of Mathematical Sciences
Tony	Shardlow	Dept of Mathematical Sciences
Jonathan	Skelton	Dept of Chemistry
Ian	Stewart	University of Bristol
Tatiana	Subkhankulova	Dept of Biology and Biochemistry
Ian	Thompson	Dept of Physics
Tural	Tunay	Dept of Mechanical Engineering
Araxi	Urrutia	Dept of Biology and Biochemistry
Alison	Walker	Dept of Physics
Aron	Walsh	Dept of Chemistry
Yifei	Wang	Dept of Computer Science
Robert	Watson	Dept of Electronic and Electrical Engineering
Rhys	Wheater	Dept of Physics
Nigel	Wilding	Dept of Physics
Ian	Williams	Dept of Chemistry
Philippe	Wilson	Dept of Chemistry
Stephen	Yeandel	Dept of Chemistry

Abstracts

Session 1

Chair: **Prof David Bird**, Faculty of Science

1.1 Invited talk: Uncovering the genomic basis of complexity through the analyses of 30million RNA sequences

Presented by: ***Dr Araxi Urrutia***, *Dept of Biology and Biochemistry*

Most of us will agree that a worm is a simpler organism compared to fish or a dog. These differences in complexity can also be understood as differences in the amount information required to build an organism of each species with more information being needed to encode the makings of more complex organisms. Ultimately, all these information needs to be encoded in the genome of each individual species. Surprisingly, however, the number of genes, considered the basic functional units in the genome has only a weak correlation with complexity measured as the number of different cell types in the body (such as skin and liver cells). By systematically analysing over 30 million RNA fragments (the molecules produced by gene activity) we obtained the first evidence for a strong association between organismal complexity and alternative splicing (a process by which one single gene can produce more than one distinct product). We further found that alternative splicing is a better predictor of complexity when compared to any other gene parameter previously associated with complexity. The results we have obtained are consistent in principle with a scenario where the diversification of the genes' products has allowed the increase in the number of nodes in the gene network promoting the appearance of additional stable states from which novel cell types can evolve. The results may also be of relevance to our understanding of how genomes store functional information.

1.2 An investigation into the vibrational properties of uranium minerals

Presented by: ***Mr Richard Driscoll***, *Dept of Chemistry*
Co-authors: *G C Allen, S C Parker, D Wolverson, M Molinari, I Khan, D Geeson*

Our research focuses on developing a strategy for rapidly identifying unknown uranium minerals and their origin. This is of particular importance in the field of nuclear forensics, which was established to prevent illegal trafficking of radioactive material. Of interest are uranium oxides, as these are used as fuel in nuclear rectors. A wide variety of secondary uranium minerals are also known, formed from the weathering of uranium oxides and containing the UO_2^{2+} (uranyl) cation. The mineral structures are layered, with uranyl groups and poly-anions (e.g. phosphate, silicate and sulphate groups) within the sheet and cations (e.g. magnesium, copper and calcium) and water molecules located in the inter- layer space.

Raman spectroscopy is a useful technique in discriminating between a range of uranyl minerals. It is a rapid, sensitive and non-destructive technique; portable devices are already available in the pharmaceutical industry and could be readily transferred to this area of nuclear forensics. We find a characteristic and strong peak is seen at a Raman shift of 750-900cm-1 for each mineral, corresponding to the uranyl symmetric stretching mode. Atomistic simulation methods provide insight into the local coordination of the uranium ion and ligands, highlighting the factors that contribute to the variation of vibrational properties among different minerals.

Keywords: *Computational Chemistry, Uranyl Minerals, DFT*

1.3 Coffee

Presented by: ***Mr Christopher H. Hendon**, Dept of Chemistry*
Co-authors: *Lesley Colonna-Dashwood, Maxwell Colonna-Dashwood*

In the apparently pretentious world of speciality coffee where focus is on flavour, brewers and consumers can be weighed down by pseudo-scientific concepts which dictate the extraction of coffee. The industry has focussed on minimising variables in the grind-size, the temperature of extraction and mass of coffee used. However, an often overlooked aspect of food chemistry is the role that water plays in the ex- traction, and resulting flavour. This talks aims to introduce the processes involved in coffee brewing and with the aid of quantum mechanics, explore how dissolved species in water dictate the flavour of our drink.[1] The concepts explored here apply to *all* extraction processes involving water

[1] C. H. Hendon, L. Colonna-Dashwood, M Colonna-Dashwood, *J. Agric. Food Chem.*, 2014, DOI: 10.1021/JF501687C

Keywords: *Computational Chemistry, GPUs, MPI*

Session 2
Chair: **Prof Robert Scheichl**, Dept of Mathematical Sciences

2.1 Invited talk: GPU Accelerated Computing

Presented by: *Jeremy Purches, Director, High Performance Computing UK&I, NVIDIA Limited*

2.2 Coarse-grained simulations: making simple work

Presented by: **Dr James Grant**, *Dept of Chemistry*
Co-authors: *S.C. Parker, M. Molinari*

We have developed a coarse-grained model of aggregating nano-particles demonstrating that simple models of the interactions between particles can reproduce behavior believed to occur within experiment. The general model has potential application in a number of areas of research but this will need investment.

In the first instance, addressing inefficiencies in the current code will likely yield significant benefits to compute time. Also to be of more general use inputs/outputs need to be standardized to, preferably existing, user-friendly formats. Of more technical interest however is the potential to make use of novel technologies with existing algorithms, one of the main parts of the program is a standard of computer games, and the implementation/development of (ideally, parallelisable) dynamic schemes.

Keywords: *Computational Chemistry, GPUs, Coarse-grained models*

2.3 Moving data processing to GPUs, a day to a tea break

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

Long data processing routines can make simple questions daunting to answer. Weighted histogram analysis method (WHAM) is an algorithm used in statistical mechanics to reduce the time taken for simulations by orders of magnitude. Statistically relevant data can be obtained in reasonable timescales and separate datasets combined into a single distribution during post-processing. At the core of the analysis is the requirement to calculate many exponentials and weight large datasets, a highly parallelisable task. By moving from serial code on CPUs to Aquila's GPUs the analysis time was reduced from a day to 5 minutes.

Keywords: *GPUs, Data processing*

2.4 A multi-GPU solver for the non-linear shallow water equations

Presented by: **Mr Will Saunders**, *Dept. of Mathematical Sciences*
Co-authors: *Robert Scheichl, Eike Mueller*

The Shallow Water Equations are used to describe the flow of fluids in multiple applications. Principally these flows consist of a small characteristic length in the vertical direction in comparison to the characteristic length in the horizontal direction, for example ripples on the surface of a pond. Here we are interested in their use for modeling the flow of pressure waves in the atmosphere. Fast efficient computation of a solution is essential for weather modeling due to the large data sets and limited time.

Current Graphics Processing Units (GPUs) provide much faster computation than Central Processing Units (CPUs) but require the problem to be structured in a highly parallel form. Presented is an implementation with Forward Euler as an explicit method, designed to efficiently run upon multiple GPUs.

Keywords: *Shallow water, GPUs, MPI*

2.5 Massively Parallel Scalability of Elliptic Solvers on Thousands of GPUs

Presented by: ***Dr Eike Mueller,*** *Dept of Mathematical Sciences*
Co-author: *Robert Scheichl*

In last year's HPC Symposium we presented first results for the GPU implementation of iterative solvers for elliptic problems in Numerical Weather and Climate Prediction. As the code is memory bound, minimising references to global GPU memory is important and was achieved by using a matrix-free implementation.

In the future high-resolution weather forecast models will have to solve equations with $O(10^9 \ 10^{12})$ unknowns. To solve problems of this size on operational time scales, it is crucial to develop efficient and highly scalable solvers which can run on novel processor architectures. We implemented a geometric multigrid solver and demonstrated that it can reduce the total solution time by an additional factor of four (compared to CG). We extended the implementation to work across multiple GPUs by using the Generic Communication Library (GCL) for inter-GPU halo exchanges.

We tested the scalability of our solvers on the EMERALD cluster and on up to 16384 GPUs of the Titan supercomputer (# 2 in www.top500.org, Nov 2013). On Titan we were able to solve an equation with $5.5 \cdot 10^{11}$ unknowns in about 1 second, achieving a performance of up to 0.78 PetaFLOPs/s. As the code is memory bound, the more relevant performance indicator is the achieved global memory bandwidth; our solvers could use between 25% 50% of the theoretical peak value. In a socket-to-socket comparison the multigrid solver is about a factor four faster than the equivalent CPU implementation on HECToR.

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

2.6 GW4
Presented by: Dr David Acreman, University of Exeter

Session 3

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

3.1 Application Performance in Materials Science, Chemistry and Nanoscience – Perspective, Performance and Challenges

Presented by: **Prof Martyn F. Guest**, *Advanced Research Computing (ARCCA), University of Cardiff*
Co-author: *Christine A. Kitchen*

The need for computational materials and chemistry codes to utilize effectively high-end computing platforms is often taken as read; however, there is little doubt that this presents a major challenge for the discipline. In 2012, leading scientists from Europe across all major user disciplines updated the Scientific case for HPC in a White Paper entitled "*The Scientific Case for High Performance Computing in Europe 2012-2020; from Petascale to Exascale*". This wide-ranging report captured the current and expected future needs of the scientific communities through the conclusions of five sector-based panels. We focus here on the needs in Materials Science; while Exaflop machines are essential and higher computational power will enable significantly increased accuracy, some important fields will be limited by throughput and data management.

Just as the drive to exascale platforms remains an elusive goal, so commodity-based clusters continue to provide a cost effective solution for the material scientist and computational chemist. Detailed cluster architecture – node and interconnect – determines the ability of such clusters to address the differing demands from the fields of capability and capacity computing. We consider the performance of a number of key codes – NWChem, GAMESS-UK, ONETEP, CASTEP, Quantum Espresso, CP2K, DLPOLY and GROMACS – on a variety of HPC systems. We identify the challenges in scaling to large processor counts and the associated bottlenecks.

Finally, just as performance is perhaps the key metric for experienced practitioners, so to the novice user ease-of-use is arguably of greater importance, with the availability of web-based scientific gateways providing an essential tool. We consider the availability of such resources as part of the High Performance Computing (HPC) Wales service in the UK. Funded to provide computational services to industry and SMEs in particular, we outline the services provided to the Advanced Materials and Manufacturing communities.

3.2 Combinatorial Search for High Capacity MXenes as New Energy Storage Materials

Presented by: **Dr Christopher Eames**, *Dept of Chemistry*
Co-author: *Prof. M. S. Islam*

MXenes are a newly discovered family of graphene compounds which exhibit unique properties useful for a number of applications. These two-dimensional materials are composed of alternating layers of graphene and early transition metals with a surface coating of functional groups. Recently, intercalation of ions onto the surface of MXenes was demonstrated with a high rate performance and a high energy storage capacity, which makes MXenes viable as electrode materials for batteries.

However, a large number of compositions are possible and the systematic synthesis and characterisation by experiment has proved slow.

In this study we perform a global search for MXenes with a high energy storage capacity using high performance computing. All combinations of intercalating ion (Li^+, Na^+, K^+ and Mg^{2+}), transition metal (Sc, Ti, V, Cr, Zr, Nb, Mo, Hf, Ta) and surface functional group (F, H, O, OH) have been screened using density functional theory based calculations. A number of promising compounds are identified which have a higher storage capacity than the current anode of choice graphite (capacity 372 mAh/g). In particular, Mg^{2+} intercalation into compounds such as Sc_2C and Ti_2C offers a theoretical capacity in excess of 700 mAh/g and should be the focus of future synthesis attempts.

3.3 Earth-abundant photovoltaics "from the beginning"

Presented by: **Mr Adam Jackson**, *Dept of Chemistry*
Co-authors: *Jonathan M. Skelton, Davide Tiana, Aron Walsh*

Thin-film photovoltaics have the potential to supply a significant proportion of global energy needs. However, the search for affordable, abundant materials has led to increasingly complex target materials. In particular, Cu_2ZnSnS_4 (CZTS) has the potential to be highly competitive, but is proving difficult to produce experimentally. *Ab initio* calculations including lattice dynamics have given insight into the chemical system around this material, providing guidelines for experimental programmes. Ongoing work includes the use of genetic algorithms and dynamic simulations to study the vapours of sulfur, a well-known but poorly-understood material.

Session 4
Chair: **Prof Aron Walsh**, Dept of Chemistry

4.1 Effective interactions in highly size asymmetric mixtures

Presented by: Dr Douglas Ashton, Dept of Physics
Co-author: Nigel Wilding

When large particles, such as colloids or large molecules, are mixed with small particles, the smaller species can induce an effective interaction between the larger species. In the case of colloids this is known as the depletion interaction, a purely entropic interaction that can drive self-assembly and phase transitions. Depletion can be highly directional if the colloids are non-spherical in shape, it can also be many-body in nature. Both of these cases make theoretical treatments difficult and simulations over such different length scales do not fare much better.

Over the last several years we have been developing computational methods, such as the geometric cluster algorithm (GCA) and staged insertion, to deal with large size-asymmetry. The result is a suite of algorithms and statistical methods that we can use to calculate effective interactions, quantify many-body effects and check the results against large scale explicit depletant simulations. This requires smart algorithms and big computers. As an example I will show how indented colloids can

form network-liquids with novel phase behaviour.

4.2 Thoughts on robust distributed computation

Presented by: **Mr Jon Chesterfield**, *Dept of Mechanical Engineering*

It is attractive to believe that software runs exactly as written, or even exactly as the author intended. In some senses this is the case - text editors and web browsers usually work as expected. Compilers are likely to be more reliable than the code they build. Nevertheless, software engineering is not applied mathematics! There are a wide range of failure modes available for a simple program and rather more for distributed computing.

This talk will introduce a collection of ways in which our programs can get the answer wrong. It will summarise some of the existing research on ameliorating these negative effects. Finally it will conclude with a discussion on how robust software engineering techniques from other fields may be applied to HPC.

Depending on how much progress has been made by the author between now and June, there may even be benchmarks.

Keywords: *Software engineering, memory corruption, multi-threading, message passing*

4.3 Fast Multipole Methods for shellfish and aeroplanes

Presented by: **Dr Michael Carley,** *Dept of Mechanical Engineering*
Co-author: *Stefano Angioni*

The Fast Multipole Method (FMM) is the state of the art technique for the fast evaluation of field defined by integrals over general source distributions. We describe two current applications of this method, each presenting its own particular difficulties:

1. As part of a NERC-funded project studying the hydrodynamics of ammonoids, we are developing an implementation of the kernel-independent FMM to be used in a Lagrangian Vortex Method code for the computation of flows around these animals, based on evaluation of a Biot–Savart integral for fluid velocity. This is primarily an exercise in coding and integration with existing free software, to produce a general library which can be used in a variety of applications.

2. So far there appears to be no FMM for the fast evaluation of retarded potentials, such as arise in computing transient solutions of the wave equation. This is a bottleneck in solving large-scale scattering and radiation problems such as arise in computing noise around airports, or wind-turbine installations, where the acoustic field must be evaluated at $O(10^9)$ points in space, and $O(10^5)$ in time. In particular, there seems to be no approach which translates readily to the problem of computing noise from moving sources, such as aircraft

taking off or landing. We present some results from an initial study using a 'classical' multipole approach, based on spherical harmonics, achieving high data compression and orders of magnitude speed-up in field evaluation.

Keywords: *Fast Multipole Method, acoustics, hydrodynamics, Biot–Savart, spherical harmonics, retarded potential, wave equation*

4.4 Multilevel Monte Carlo – Monte Carlo methods that are not embarrassingly parallel

Presented by: ***Prof Robert Scheichl***, *Dept of Mathematical Sciences*

One of the most promising novel techniques for uncertainty quantification in large-scale engineering and physical systems is the multilevel Monte Carlo (MLMC) method. It uses a hierarchy of numerical models (e.g. different grid resolutions for discretisations of differential equations) to dramatically reduce the complexity of plain vanilla Monte Carlo methods. Typically, the number of levels in the model hierarchy and the number of samples (or ensemble size) on each level are adjusted adaptively (on the fly) in the MLMC algorithm. Therefore an optimal parallel implementation requires careful load balancing and highly non-trivial scheduling of the various tasks on the multiple levels.

This is joint work with Björn Gmeiner, Ulrich Rüde (both University of Erlangen-Nürnberg) and Barbara Wohlmuth (TU Munich).

Keywords: *parallel uncertainty quantification, large-scale engineering systems, multilevel Monte Carlo, load balancing*

Posters

P1 An accurate and transferable interatomic potential for modelling metal-organic frameworks: BTW-FF

Presented by: ***Ms Jessica Bristow***, *Dept of Chemistry*
Co-authors: *Davide Tiana and Aron Walsh*

Metal organic framework (MOFs) are versatile materials with suggested applications including gas storage and separation, semiconductor devices and drug delivery systems. Formed *via* the self-assembly of metal and organic linkers, the potential geometric structures and composition of MOFs is vast. Property prediction prior to synthesis is therefore essential in order to identify the most promising material systems. One method to rapid and accurate property prediction of MOFs is to develop an *ab-initio* derived forcefield that is transferable across the full range of MOF structure types. Our universal analytical interatomic potential BTW-FF (Bristow-Tiana-Walsh Force Field)[1] is in the initial stages of derivation and has the aim of accurately recreating MOF structures and properties regardless of metal or ligand identity.

Our presentation will summarise current progress and future aims of the BTW-FF. We have derived a transferable force-field for carboxylate ligands including BDC (benzene-1,4-dicarboxylate), BPDC (biphenyl-4,40-dicarboxylate), BTC (benzene-1,3, 5-tricarboxylate) and PDC (pyrene-2,7-dicarboxylate) and incorporated these with derived metal potentials to recreate the MOF structures: IRMOF-1, IRMOF-10, IMOF-14, UIO-66, UIO-67, HKUST-1 and MIL-125 all with < 3% error on the lattice constants. Properties such as bulk modulus, phonon frequencies and thermal expansion coefficients will also be reported for each structure in justification of the accuracy of the derived forcefields.

Keywords: *Forcefields, MOFs*

P2 Aquila by Numbers

Presented by: ***Dr Steven Chapman***, *Computing Services*

P3 Hydrogen Species in UO_2 – Defect Formation and Diffusion Paths

Presented by: ***Mr Joseph Flitcroft***, *Dept of Chemistry*
Co-authors: *S.C. Parker[1], M. Storr[2], M. Molinari[1], N. Brincat[1]*
  [1] *Department of Chemistry*
  [2] *AWE Aldermaston, Reading*

UO_2 has received a lot of interest as a nuclear fuel, due to concerns such as CO_2 emissions, energy security, energy cost and decreasing fossil fuel supplies. There is a gap in the knowledge of UO_2 of how H species dissolved in a UO_2 matrix behave. UO_2 comes into contact with H when it is sintered before being used as a fuel.

The aim of this project is to investigate the structure, stability and transport of hydrogen species in uranium matrixes, predominately UO_2 using *ab initio* modelling techniques. Computational techniques provided a safe route to explore the defect properties, such as diffusion pathway and formation of H interstitial species in UO_2.

DFT (GGA+U) has been used to investigate a range of hydrogen species in UO_2, with collinear magnetic ordering, at different interstitial sites and evaluate their formation energies. Interstitial hydrogen species include the hydrogen (proton), hydride and the hydrogen radical. These give the end members of feasible diffusion paths between interstitial sites. As hydrogen diffuses through the UO_2 matrix, there are electronic changes to the host matrix, with the uranium sites accepting or donating electrons; this results in the oxidation states of the uranium ions ranging from III to VI depending on the number of electrons involved in the process. The diffusion is further complicated by the possibility of hydrogen forming covalent species with the oxygen of the host matrix. Our results show the complexity of the energy landscape of hydrogen diffusion. This implies that there is a large feasible choice of diffusion paths for H species suggesting that there might not be a unique most stable diffusion mechanism.

Keywords**:** *Computational Chemistry, DFT, H, UO_2*

P4 Investigating Amorphous Order in Stable Glasses Through Random Pinning

Presented by: Mr Christopher Fullerton, Dept of Physics
Co-author: Robert L. Jack

We investigate the response to randomly pinning particles in equilibrium configurations of a supercooled liquid and configurations from stable glassy states associated with large deviations in the dynamical activity. The distribution of the overlap between configurations sharing pinned particles reveals the presence of amorphous order in the glassy states with an associated length scale that is of at least the system size. This helps to explain the origin of their stability.

Keywords: Statistical Mechanics, Disordered Systems, Large Deviations, Transition Path Sampling

P5 The creation of current and future test reference weather years at a high spatial resolution for the built environment

Presented by: **Chunde, Liu**, Dept of Architecture and Civil Engineering

The methodology for creating future weather files which play a key role in designing buildings able to be resilient to climate change has been developed in this research. The test reference weather years (TRYs) which have been widely used for building design are available for 14 locations only in UK. Also, these weather files cannot reflect climate changes in the future years because they were created from the 23 years of observed weather data (1983-2005) in past decades. Thus, the building energy performance assessments based on the current weather files are lack of confidence. This research aims to generate probabilistic TRYs based on the outputs of UKCP09 weather generator from now till 2080s under three different carbon emission scenarios reported by the Intergovernmental Panel on Climate Change (IPCC). The methodology has been turned into MATLAB codes and each run can produce 100 TRYs at one specific location, under one carbon emission scenario and for one future time period. Based on them, probabilistic TRYs with required percentile which could explain uncertainties of climate models can be produced. We are planned to create probabilistic TRYs in a certain format that can be applied to building energy simulation packages at 5 km resolution across UK so that building designers are able to make a more convincible building energy performance prediction than ever before. Therefore, High Performance Computing (HPC) computer is essential for doing such gigantic calculations and dealing with such huge weather data.

Keywords: *Probabilistic Test Reference Years, UKCP09 Weather Generator, MATLAB*

P6 Computational Solid State Chemistry @ Bath

Presented by: *Mr Marco Molinari, Dept of Chemistry*
Co-authors: *S.C. Parker (Chemistry), N.A. Brincat, J. C. Crabtree, R.J.P Driscoll, J.M. Flitcroft, T.V. Shapley, N.R. Williams, L.N. Woronycz, S.R. Yeandel, J.D. Baran, J. Grant*

The CSSC Group applies modelling tools to understand environmentally important materials and their properties, complementing and guiding experiment. We use techniques based on quantum force field and coarse-grained approaches using local and national HPC facilities. The aim of our research is to develop and apply novel simulation techniques to extend our understanding of structure, stability and reactivity of ceramics and mineral interfaces.

Keywords: *Computational Chemistry, DFT, Potential models, Coarse-grained models, Minerals, Interfaces*

P7 M4: A Programme in Metastable Materials

Presented by: *Mr Jonathan Skelton, Dept of Chemistry*
Co-authors: *Rachel Crespo-Otero, E. Lora DaSilva, Steve C. Parker and Aron Walsh*

"M4" is a new research programme at the University of Bath, which aims to develop functional materials whose properties can be tuned through the generation and control of long-lived metastable states. It is a broad and highly interdisciplinary collaboration between experimental and theoretical researchers, spanning expertise in synthesis, characterisation, modelling, and device fabrication.

Computational chemistry is a core component of the project - by providing a fundamental understanding of properties and switching behaviour across a range of systems, it can support and guide experimental work, and can ultimately help to enable the rational design of materials tailored to particular applications. Modelling the diverse range of materials being targeted requires an equally diverse set of computational tools, and in some cases also necessitates the development of new methodology to work with challenging systems and phenomena.

This poster will showcase a range of the systems currently being investigated under the M4 project, and will illustrate how HPC and experiment can work together to design and optimise new materials with interesting functionality.

Keywords: *Computational Chemistry, Density-Functional Theory, Materials Modelling*

P8 Drift-diffusion Modelling of Hybrid Perovskite Solar Cells

Presented by: *Mr Timo Peltola*, *Dept of Physics*
Co-author: *A.B. Walker*

We have modelled a hybrid organic-inorganic perovskite solar cell by assuming a planar N-I-P-heterojunction structure and charge carrier movement by drift and diffusion. Our results indicate that charge collection is improved by a large built-in field in the perovskite.

Keywords: *Perovskite, solar cell*

P9 Solvent effects on organic reaction mechanisms

Presented by: *Prof Ian Williams*, *Dept of Chemistry*
Co-authors: *George Ledward, Max Seccombe, Jose Recatala*

The GAUSSIAN09 and fDYNAMO programs on Aquila have been used to perform quantum-mechanical (QM) and hybrid quantum-mechanical/molecular-mechanical (QM/MM) calculations of geometries and energies for species along the reaction pathways for three different organic reactions, with either implicit or explicit solvation methods, each as an undergraduate research project.

(1) No ion-pair intermediate was found in the SNi rearrangement of alkyl chlorosulfite to chloroalkane and sulfur dioxide; the barrier to concerted reaction by means of a strongly dipolar transition structure was found to diminish with increasing solvent polarity treated by the polarized continuum model (PCM).

(2) Formation of 1-chloroethyl acetate from acetaldehyde and acetyl chloride in the presence of aluminium trichloride in dichloromethane solution (treated by PCM) appears to proceed more or less concertedly within a cyclic reaction complex.

(3) Energy minimizations of QM clusters of ethene bromonium surrounded by water molecules located within a 3.25 Å radius embedded within a frozen environment of ~1000 MM waters, initiated from 100 different starting configurations of the explicit solvent, generally preserved the cyclic structure of the bromonium cation as a discrete species with a local potential energy minimum. But free energy profiles obtained from QM/MM potentials of mean force at 300 K show either no barrier to formation of a ring- opened protonated bromohydrin or a barrier due (presumably) to the need to re-orient the nucleophilic water molecule within its hydrogen-bonded local environment.

Keywords: *Computational Chemistry, GAUSSIAN09, fDYNAMO*

P10 Solvent effects on isotope effects: methyl cation as a model system

Presented by: **Mr Philippe Wilson**, Dept of Chemistry
Co-author: Ian William

The isotopic sensitivity (CH_3^+ vs. CD_3^+) of the equilibrium between methyl cation in vacuum and in solution has been investigated. GAUSSIAN09 has been used on Aquila to perform quantum-mechanical calculations of geometries and vibrational frequencies with both implicit and explicit solvation methods. Two alternative options for describing the shape of the solute cavity within the widely-used polarised continuum model for implicit solvation were compared: the UFF method (the GAUSSIAN09 default) and the UA0 method (the older GAUSSIAN03 default) give equilibrium isotope effects which vary as a function of the relative permittivity of the dielectric continuum in opposite directions. To determine which trend is correct, the isotope effect was also obtained as the average over 41 structures from a hybrid quantum-mechanical/molecular-mechanical molecular dynamics (fDYNAMO) simulation for methyl cation explicitly solvated by many water molecules. Finally, GAUSSIAN09 calculations for methyl cation interacting with small numbers of explicit water molecules have shown that the equilibrium isotope effect varies as a function of decreasing intermolecular C···O distance in opposite directions, depending upon whether the water molecules are located "axially" (symmetrically above and below the CH_3 plane) or "equatorially" (symmetrically in-plane along the CH bond directions).

Keywords: *Computational Chemistry, GAUSSIAN09, fDYNAMO*

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