Welcome

Dear Participants,

As the Scientific Organising Committee it is a great pleasure to welcome you all to the University of Bath's fourth HPC Symposium. You have helped us put together an exciting and wide-ranging programme which includes a keynote lecture from Mark Chapman from the Bloodhound SSC who will give an overview of the project to drive a car at 1000mph and how HPC is enabling them to do so.

This year has seen the installation of the university's new HPC facility Balena, which will eventually provide almost twice the number of nodes as its predecessor Aquila, each of which have twice the number of cores. The machine consists of different components having GPU and Xeon Phi accelerators, high memory as well as dedicated nodes for development and visualisation. It represents a significant investment to support the variety of current and futures users as well as developers working at the university.

The programme for the day includes varied talks from across the university from an introduction to quantum chemistry calculations on the new HPC to applications in nuclear fuel, improving the scheduling of ambulance crews to statistical approaches in reconstructing the historical temperature record. There are also talks introducing new methodologies for solving partial differential equations and turbulence in flow as well as a talk from Allinea to explain how their software can help to debug and optimise code more efficiently on the different resources now available.

We hope that the material and different research and developments will be of interest to all HPC users and hope that the day will provide the opportunity to initiate new collaborations to maximise the benefit of HPC expertise across the university.

Yours faithfully,

The Scientific Organising Committee,

Dr Steven Chapman, Computing Services
Dr Stefano Angioni, Dept. of Mechanical Engineering
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

09:30 **Registration and refreshments**

10:00 **Welcome and introduction**
Prof David Bird, Dean of the Faculty of Science, Chair of the HPC Advisory Group

10:15 **Session 1**
Chair: **Prof David Bird**, Chair of the HPC Advisory Group, Faculty of Science

10:15 **High-Throughput Computing on Balena: Application to Ab Initio Lattice Dynamics for Material Characterisation**
Dr Jonathan Skelton, Dept of Chemistry

10:45 **Invited Talk**
Simplify software development on Balena
Avtar Cheema, Allinea

11:00 **Delegation photograph in atrium**

11:05 **Tea Break**

11:30 **Session 2 (in CB1.10)**
Chair: **Prof Richie Gill**, Dept of Mechanical Engineering

11:30 **Keynote**
***Mark Chapman**, Chief Engineer of the Bloodhound SSC Project*

12:30 **Lunch in the atrium**

14:00 **Session 3**
Chair: **Dr Michael Carley**, Dept of Mechanical Engineering

14:00 **Performance portable solvers for finite element discretisations of PDEs in Fluid Dynamics**
Dr Eike Mueller, Dept of Mathematical Sciences

14:30 **Vortex method modelling of flows using OpenMP**
Dr Stefano Angioni, Dept of Mechanical Engineering

14:50 **Hydrogen Defects in Stoichiometric UO_2**
Joseph Flitcroft, Dept of Chemistry

15:10 **Information-Theoretic Measurements of Coupling between Structure and Dynamics in Glass Formers**
Dr Rob Jack, Dept of Physics

15:30 **Tea Break**

16:00 **Session 4**
Chair: **Prof Steve Parker**, Dept of Chemistry

16:00 **Large scale spatial statistics for daily temperature reconstruction**
Dr Finn Lindgren, Dept of Mathematical Sciences

16:20 **Scheduling Ambulance Crews for Maximum Coverage**
Dr Gunes Erdogan, School of Management

16:40 **Highly Publicised Computing: HPC in the public eye**
Christopher Hendon, Dept of Chemistry

17:00 **Presentation of prizes**

17:10 **Wine and Cheese reception in the atrium**

18:00 **Close of meeting**

Posters

1. **Phase Stability of the Halide Perovskite $CsSnI_3$**
   E. Lora da Silva, Dept of Chemistry

2. **Simulating the vibrational properties of UO_3**
   Richard J. P. Driscoll, Dept of Chemistry

3. **$NaFePO_4$ Cathodes for Sodium Batteries: Why is Olivine More Promising Than Maricite?**
   Jenny Heath, Dept of Chemistry

4. **A performance-portable framework for atomistic simulations on parallel computers**
   William Saunders, Dept of Mathematical Sciences

5. **Isotope Effect Calculations in the Supramolecular Age**
   Philippe B. Wilson, Dept of Chemistry

List of attendees

First Name	Surname	Department / Organisation
Stefano	Angioni	Dept of Mechanical Engineering
David	Bird	Faculty of Science
Jessica	Bristow	Dept of Chemistry
Keith	Butler	Dept of Chemistry
Clovis	Caetano	Dept of Chemistry
Michael	Carley	Dept of Mechanical Engineering
Steven	Chapman	Computing Services
Mark	Chapman	Bloodhound SSC
Avtar	Cheema	Allinea Software Ltd
Qiang	Chen	Dept of Architecture and Civil Engineering
E. Lora	da Silva	Dept of Chemistry
James	Davenport	Dept of Computer Science
Richard	Driscoll	Dept of Chemistry
Tina	Düren	Dept of Chemical Engineering
Gunes	Erdogan	School of Management
Joseph	Flitcroft	Dept of Chemistry
Chris	Fullerton	Dept of Physics
Feng	Gao	Dept of Architecture and Civil Engineering
Richie	Gill	Dept of Mechanical Engineering
James	Grant	Dept of Chemistry
Lewis	Hart	Dept of Physics
Jennifer	Heath	Dept of Chemistry
Christopher	Hendon	Dept of Chemistry
Christopher	Huggins	ClusterVision
Rob	Jack	Dept of Physics
Roger	Jardine	Computing Services
Surendra	Kaushik	Dept of Electronic and Electrical Engineering
Yuanpeng	Li	Dept of Mathematical Sciences
Finn	Lindgren	Dept of Mathematical Sciences
Vincent	Lister	Dept of Chemical Engineering
Roshan	Mathew	Computing Services
James	McClung	ClusterVision
Marco	Molinari	Dept of Chemistry
Chris	Molloy	Dept of Chemistry
Eike	Mueller	Dept of Mathematical Sciences
Steve	Parker	Dept of Chemistry
Michael	Proulx	Dept of Psychology
Andrew	Rhead	Dept of Mechanical Engineering

First Name	Surname	Department / Organisation
William	Saunders	Dept of Mathematical Sciences
Robert	Scheichl	Dept of Mathematical Sciences
Jonathan	Skelton	Dept of Chemistry
Liang	Sun	Dept of Architecture and Civil Engineering
Aron	Walsh	Dept of Chemistry
Yifei	Wang	Dept of Computer Science
Robert	Watson	Dept of Electronic and Electrical Engineering
Philippe	Wilson	Dept of Chemistry
Daniel	Wolverson	Dept of Physics
Ruoxi	Yang	Dept of Chemistry

Abstracts

Session 1

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

1.1 High-Throughput Computing on Balena: Application to *Ab Initio* Lattice Dynamics for Material Characterisation

Presented by: **Dr Jonathan M. Skelton**, Dept of Chemistry
Co-authors: *E. L. da Silva, A. J. Jackson, F. Brivio, J. M. Frost, J. K. Bristow, K. L. Svane, R. Yang, K. T. Butler, S. C. Parker and A. Walsh*

Lattice dynamics is a theoretical framework for modelling the phonons in periodic systems. When used with an *ab initio* force calculator such as density-functional theory (DFT), it is a powerful technique for first-principles computational materials characterisation. Applications include modelling the temperature dependence of material structure, studying thermodynamics and phase transitions, calculating lattice thermal conductivity, and simulating vibrational (e.g. IR and Raman) spectra. This talk will briefly introduce the core lattice-dynamics methodology, and will discuss the computational requirements of representative calculations. Results obtained with the University of Bath's new Balena HPC system will be presented, along with some benchmark data comparing her performance to other facilities (e.g. Archer).

Keywords – *computational chemistry, high-throughput computing, ab initio lattice dynamics, density-functional theory*

1.2 Invited talk: Simplify software development on Balena

Presented by: **Avtar Cheema**, Allinea

An overview of the software development tools from Allinea available on the Balena HPC system.

Fore more information visit: http://www.allinea.com

Session 2

Chair: **Prof Richie**, Dept of Mechanical Engineering

2.1 Keynote:

Presented by: **Mark Chapman**, Chief Engineer of the Bloodhound SSC Project

Session 3

Chair: **Prof Michael Carley**, Dept of Mechanical Engineering

3.1 Performance portable solvers for finite element discretisations of PDEs in Fluid Dynamics

Presented by: **Dr Eike Mueller**, Dept of Mathematical Sciences
Co-author: *Colin Cotter, David Ham, Lawrence Mitchell (Imperial College), Robert Scheichl (Bath)*

Many problems in science and engineering require the fast solution of partial dif- ferential equations (PDEs). Finite element discretisations of the Navier Stokes equations are popular in atmospheric modelling since they allow the conservation of physical quantities on unstructured grids. However, this leads to significantly more sophisticated systems of equations than simple finite difference schemes and implementing the solver poses a significant challenge. The firedrake/PyOP2 toolchain allows the expression of grid-based algorithms at a high abstraction level in Python. Automatic code generation is used to generate optimised C-kernels for the computationally expensive iterations over the grid. This makes the implemen- tation of higher-order mixed finite element methods feasible while achieving the same performance as an implementation in a lower-level language such as Fortran.

We developed a bespoke solver with a geometric multigrid preconditioner for the pressure correction equation in atmospheric modelling; vertical line relaxation is used to handle the vertical anisotropy in flat domains and a Python abstraction was developed for dealing with the resulting column-wise algebra. We tested the performance of the solver for a linearised gravity wave system in a thin 2+1 dimensional spherical shell. Results are reported for the algorithmic- and parallel scalability both for lowest-order- and higher-order finite element discretisations.

Keywords – *Fluid Dynamics, PDEs, Finite Elements, Code generation, Python*

3.2 Vortex method modelling of flows using OpenMP

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

Vorticity is the fundamental property of any interesting flow, most easily seen in smoke rings, aircraft wakes, in geophysical flows such as hurricanes and torna- does, and as a stable structure in the atmosphere of Jupiter. In this work a parallel three dimensional (3-D) computational fluid dynamics (CFD) method has been developed for the modelling of unsteady flows via a vorticity distribution. The volume solver is based on the Kernel-Independent Fast Multipole Method, where

continuous distributions of vorticity are adaptively decomposed in a hierarchi- cal octtree. The code supports Eulerian and Lagrangian particle fluid flows and is inherently adaptive. The evolution equations are solved using multi-step ex- plicit methods. The software has been validated using analytical solutions, such as Hill's Spherical vortex and Gaussian cored vortex rings. The software has re- cently been parallelized using the OpenMP multi-threading library and run on a 6 core (12 threads) Intel processor.

Keywords – *Computational Fluid Dynamics, Fast Multi-pole Method, OpenMP*

3.3 Hydrogen Defects in Stoichiometric UO_2

Presented by: **Joseph Flitcroft**, Dept of Chemistry
Co-authors: *S.C. Parker[1], M. Storr[2], M. Molinari[1], N. Brincat[2]*
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As the most commonly used nuclear fuel UO_2 has received a large amount of research focus, predominantly on the oxidation to higher oxides such as U_4O_9, U_3O_7, U_3O_8, U_2O_5 and UO_3. However, despite the ubiquitous nature of hydrogen and its use in the fuel sintering process there is limited research on hydrogen species in UO_2. This means that the defect chemistry and the effect of hydrogen on the fuel stability is poorly understood.

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, Hydride, Hydroxyl, UO_2*

3.4 Information-Theoretic Measurements of Coupling between Structure and Dynamics in Glass Formers

Presented by: **Dr Rob Jack**, Dept of Physics

We analyze connections between structure and dynamics in two model glass formers, using the mutual information between an initial configuration and the ensuing dynamics to compare the predictive value of different structural observables. We consider the predictive power of normal modes, locally favored structures, and coarse-grained measurements of local energy and density. The mutual information allows the influence of the liquid structure on the dynamics to be analyzed quantitatively as a function of time, showing that normal modes give the most useful predictions on short time scales while local energy and density are most strongly predictive at long times.

Session 4

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

4.1 Large scale spatial statistics for daily temperature reconstruction

Presented by: **Dr Finn Lindgren**, Dept of Mathematical Sciences

The EUSTACE project will give publicly available daily estimates of surface air temperature since 1850 across the globe for the first time by combining surface and satellite data using novel statistical techniques. Designing and estimating a realistic stochastic model that can realistically capture the statistical behaviour of air temperature across a wide range of time-scales is not only a modelling challenge, but also a computational challenge. Existing methods for spatial statistics need to be scaled up to handle a large quantity of data, as well as to properly quantify the uncertainty of the temperature reconstructions in regions and time periods with small quantities of data.

4.2 Scheduling Ambulance Crews for Maximum Coverage

Presented by: **Dr Gunes Erdogan**, School of Management
Co-authors: *Prof Erhan Erkut, Prof Armann Ingolfsson and Prof Gilbert Laporte*

This paper addresses the problem of scheduling ambulance crews in order to maximize the coverage throughout a planning horizon. The problem includes the subproblem of locating ambulances to maximize expected coverage with probabilistic response times, for which a tabu search algorithm is developed. The proposed tabu search algorithm is empirically shown to outperform previous approaches for this subproblem. Two integer programming models that use the output of the tabu search algorithm are constructed for the main problem. Computational experiments with real data are conducted on an HPC cluster, which were completed within 2 weeks of real time and uses about 3 years of CPU time. A comparison of the results of the models is presented.

Keywords – *Ambulance location, scheduling, metaheuristics, integer programming*

4.3 Highly Publicised Computing: HPC in the public eye

Presented by: **Christopher Hendon**, Dept of Chemistry

From the prediction of tomorrow's weather and carreling disease epidemics to ultra-high throughput trading on stock markets, for better or worse HPC affects the lives of everybody. Yet its practitioners are often scene as 'boffins' far removed from the reality of every day life. HPC in the University of Bath is undoubtedly at the forefront of UK research, and this talk discusses the various levels of HPC which impact society. From the application of quantum chemistry in coffee extraction, to the prediction of new materials for batteries and solar energy, I explore not only how HPC is applied, but also how HPC is portrayed in the public's eye.

Keywords – *HPC, Perception, Application*

Posters

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

Presented by: **E. Lora da Silva**, Dept of Chemistry
Co-authors: *J. M. Skelton, Stephen C. Parker and Aron Walsh*

Materials modelling usually focuses on systems in thermodynamic equilibrium; however, interesting physics tend to occur for systems perturbed by external stimuli such as temperature, pressure or light. $CsSnI_3$ is an interesting halide-perovskite system, which exists in a number of phases, including two high-temperature forms and two ground-state phases. In order to bring new insight into the (meta)stability of these polymorphs, we model the effects of temperature using lattice dynamics within the quasi-harmonic approximation (QHA), where the temperature dependence of structure and properties can be obtained from a series of harmonic-phonon calculations at volumes about the 0 K equilibrium. Within this framework, we obtain the temperature dependence of a number of structural properties, i.e. cell volume, Bulk modulus and Grüneisen parameter. We also map out the relative Gibbs free energy of the phases, which is compared against the temperature-dependent Helmholtz energy obtained from the equilibrium structure within the purely harmonic approximation. We observe negative-frequency modes in the black cubic (Bα) and the black tetragonal (Bβ) phases, and we find that the Bβ phase is not stable at any temperature, with the phonon band dispersion displaying negative optic modes which pass through all the high-symmetry wavevectors in the Brillouin Zone. The main contributions to the negative modes are found to be motions of the Cs atom inside the perovskite cage. The cubic Bα structure shows a zone-boundary instability at the equilibrium (0 K) lattice constant, while at finite temperature additional negative modes develop at the zone centre, indicating a ferroelectric instability.

Keywords – *Forcefields, MOFs*

P2 Simulating the vibrational properties of UO_3

Presented by: **Richard J. P. Driscoll**, Dept of Chemistry
Co-authors: S. C. Parker, M. Molinari, D. Wolverson (Physics), G. C. Allen (University of Bristol)

DFT has been used to simulate the vibrational properties of five polymorphs of UO_3, which demonstrated good agreement with existing Raman and IR spectra. This allows the modes seen experimentally to be indexed using the simulated data. Four phases of UO_3 contain uranyl bonding, but the uranyl stretches are seen to shift to lower wavenumbers in two phases, which results from a more constrained environment around the uranyl oxygen atoms. Contrary to the experimental spectrum presented in this work, the $Pm\bar{3}m$ structure of δ-UO_3 did not produce any Raman activity, however, a C2/c unit cell produced Raman peaks that agreed well. The structure of β -UO_3 is disordered, therefore the presence of uranyl bonding is not seen in experimental data, but is inferred from comparing the spectra.

Keywords – *DFT, Spectroscopy, Uranyl*

P3 $NaFePO_4$ Cathodes for Sodium Batteries: Why is Olivine More Promising Than Maricite?

Presented by: **Jenny Heath**, Dept of Chemistry

Sodium-ion batteries are currently an area of growing interest as alternatives to lithium-ion batteries, largely due to the relative abundance of sodium and their resultant cost advantages; there is potential for sodium-ion cells to become a preferable option for large-scale grid storage. Olivine $NaFePO_4$ is a candidate material to act as a suitable cathode for sodium-ion batteries. However, unlike $LiFePO_4$, $NaFePO_4$ does not crystallize in the olivine structure; its most thermodynamically stable form is the maricite polymorph, but this shows poor electrochemical behavior, which is not fully understood. Olivine sodium phosphates have previously been studied using atomistic simulation techniques, although there are no previous investigations into defect and Na conduction properties for maricite-structured materials. Here, our atomistic study of maricite $NaFePO_4$ indicates that anti-site Na/Fe defects are the most favourable type of defect, as found in the olivine counterparts. For the olivine material, the Na migration pathway with lowest energy (0.4 eV) runs along b-axis channels. In contrast, for the maricite compound the only possible Na-ion migration pathway was found to have a high-energy barrier (1.7 eV) due to the lack of open channels within the framework structure resulting in a low rate of sodium ion diffusion.

P4 A performance-portable framework for atomistic simulations on parallel computers

Presented by: **William Saunders**, **Dept of Mathematical Sciences**
Co-author: Dr Eike Mueller, Dr James Grant, Prof Robert Scheichl, Prof Stephen Parker

We present the idea of a novel technique to create portable high performance Molecular Dynamics codes within a high level framework. Such a framework enables the development of user defined simulations within a reasonable time frame by providing a high level development language. A successful framework should interpret this high level language to produce efficient and highly parallel machine code. This abstraction allows the domain specialist to produce efficient code without knowledge of high performance computing. Furthermore through automatic runtime compilation, user codes should automatically target advanced hardware architectures such as Graphics Processing Units and Intel Xeon Phi coprocessors without user prompting.

Within the framework a user could formulate a simulation using functions and classes predefined by a set of python modules without any deeper code development. An example of a more involved usage case is the investigation of a trial, newly developed, potential between particles. In this scenario the user writes a relatively small piece of python code to describe the potential alongside a C kernel implementing the interaction. The framework automatically loops over all pairs of atoms within the prescribed cut off distance and applies the C kernel to each atom pair. The framework automatically combines the C code for atom looping with the C kernel for the potential to produce an overall efficient operation.

Keywords – *Computational Chemistry, GPUs, MPI, Framework*

P5 Isotope Effect Calculations in the Supramolecular Age

Presented by: **Philippe B. Wilson**, Dept of Chemistry
Co-authors: Prof. Ian H. Williams

Until recently, KIE calculations have employed old theory for small molecules in a vacuum, whereas most problems of current interest involve very large condensed-phase supramolecular systems, either in solution or in enzyme active sites: the traditional methods are no longer appropriate. Huge advances in computational methodology for realistic simulations of large systems by means of QM/MM methods have taken place and, specifically, the use of subset Hessians and ensemble averaging has been demonstrated, showing that the widely-used Bigeleisen equation for KIE calculations is both incorrect and unnecessary in supramolecular applications with subset of atoms since it ignores environmental coupling. However, errors are minimised if the isotopic sensitivity of all subset degrees of freedom is included, providing that these include specific non-covalent interactions as well as covalent bonds, and that a correct Hessian is employed. Furthermore, the benefit of determining a KIE as the quotient of average isotopic partition function ratios taken over independent collections of thermally-accessible configurations of reactant structures and transition structures (TSs) has been shown. Evidently, these recent practices require significant testing and resource due to the range of system sizes and accuracy (QM region) considered. In QM/MM simulations, the size of the QM region, and the manner in which it is described dictate the resource required. In comparison, the MM calculation takes little time, resulting in a significantly QM-biased time and resource constraint.

Recent developments have addressed one half of the problem: how to treat the influence of kinetic-energy coupling on KIEs in subsets embedded in very large systems. Now we must address the other half which concerns potential energy. Although QM/MM methods have opened up supramolecular possibilities, most of the applications to KIEs have been wedded to a molecular outlook: selection of the QM region is usually made in a ‘molecular’ manner in order to avoid placing the QM/MM boundary through covalent bonds and, furthermore, the subset of atoms included in the Hessian determination has been the same as the QM region.

Keywords – Computational Chemistry, QM/MM, Gaussian, Isotope Effects, Biomolecules

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
James Grant
Stefano Angioni
Katie Williams
Roshan Mathew

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 day.

For more information about the University's HPC service visit: www.bath.ac.uk/hpc