

Welcome

Dear Participants,

We, the Scientific Organising Committee, are delighted to welcome you to the University of Bath's 6th Annual HPC Symposium.

This year, we have two outstanding keynote speakers, Prof Simon McIntosh-Smith (University of Bristol) and Prof David Britton (University of Glasgow). Prof McIntosh-Smith will discuss how to deal with the increasingly diverse range of competing architectures that software developers are faced with, many of which are available on Bath's own Balena HPC facility. Prof Britton is a member of the ATLAS project at the Large Hadron Collider at CERN, and leads the GridPP project providing grid computing for particle Physics research. He will be talking about the evolution of the worldwide LHC computing grid, which is a key part of the research infrastructure that is pushing the boundaries of our understanding of the universe.

We also have a host of contributions from Bath University researchers, delivered as talks and "flash" poster presentations. The line up includes contributions from Physics, Maths, Chemistry, Architecture and Engineering, and covers topics ranging from method and software development to applications of quantum-chemical simulations and high-level finite-element methods to solve topical and challenging research problems.

The University's second-generation HPC cluster, Balena, has been in service for over two years now, and is seeing a consistently high utilisation from across the University and a growing number of users and research group, as well as being used to further the University's teaching and outreach activities. With 3,072 Intel Ivybridge CPU cores, which can deliver a peak CPU LINPACK performance of 57.5 TFLOPS, and the high-performance BeeGFS parallel filesystem, which is capable of an aggregate bandwidth performance of over 12GBytes per second, Balena has both the capacity and the capability to take on ambitious computational projects. In addition to the traditional x86-64 compute nodes and high-performance interconnect, Balena also provides Bath's researchers with access to a full complement of accelerator hardware, including GPUs from NVIDIA and AMD and the Intel Xeon Phi coprocessor, along with a remote visualisation service for graphically-intensive applications. Balena's Interactive Test and Development zone (ITDs) provides a dedicated environment for real-time access to results and for development of research software.

The Annual HPC Symposium showcases the breadth of research being carried out by the University's HPC community, and has evolved over its last five iterations into a forum for discussion and new collaborations.

We look forward to joining you for what promises to be an interesting and enjoyable event.

Yours faithfully,

The Scientific Organising Committee

Dr Steven Chapman, HPC Manager, Computing Services
Dr David Miranda, Department of Architecture and Civil Engineering
Dr Jonathan Skelton, Department of Chemistry

Programme

The Symposium will take place in Chancellors' Building, Room CB2.6 on Monday 12th June 2017

- 09:30 **Registration and refreshments**
- 10:00 **Welcome and introduction**
Prof David Bird, Chair of the HPC Management Group
- 10:15 **Keynote one**
Chair: Dr Steven Chapman, Computing Services
- 10:15 **"Xeon and Pascal and POWER, oh Phi!": how to cope in a world of increasingly diverse architectures**
Prof Simon McIntosh-Smith, University of Bristol
- 11:15 **Delegation photograph in atrium outside CB2.6**
- 11:20 **Break and poster viewing – Chancellors' Building level 2 atrium**
- 11:45 **Session one**
Chair: Dr Eike Müller, Dept of Mathematical Sciences
- 11:45 **Efficient Simulation of Rare Events**
Tobias Brewer, Dept of Physics and Dept Computing Science
- 12:00 **Multiscale Modelling of Aerospace Composites**
Dr Anne Reinarz, Dept of Mathematical Sciences and Dept Mechanical Engineering
- 12:15 **The role of HPC in building design: tackling global challenges**
Daniel Fosas, Dept of Architecture and Civil Engineering
- 12:30 **Session two**
Chair: Dr Rob Watson, Dept of Electronic and Electrical Engineering
- 12:30 **Quick fire 3-minute poster talks (see page 4)**
- 13:00 **Lunch – Chancellors' Building level 2 atrium**
- 14:00 **Keynote two**
Chair: Prof David Bird, Dept of Physics
- 14:00 **Evolution of the Worldwide LHC Computing Grid**
Prof David Britton, University of Glasgow

- 15:00 **Session three**
Chair: Prof Nigel Wilding, Dept of Physics
- 15:00 **Global Estimation of Air Quality**
Matthew Thomas, Dept of Mathematical Sciences
- 15:15 **Delivering a DLMONTE Workshop on Balena**
Dr James Grant, Dept of Chemistry
- 15:30 **Break and poster viewing – Chancellors’ Building level 2 atrium**
- 16:00 **Session four**
Chair: Dr Benjamin Morgan, Dept of Chemistry
- 16:00 **Hydrogen Defects in Hyperstoichiometric Uranium Dioxide**
Joseph Flitcroft, Dept of Chemistry
- 16:15 **Migration of Interstitial ions in Inorganic Perovskites**
Dibya Ghosh, Dept of Physics
- 16:30 **Higher-order DG discretisations on modern architectures with applications in NWP**
Jack Betteridge, Dept of Mathematical Sciences
- 16:45 **Matrix-free block smoothers for higher-order DG methods**
Dr Eike Müller, Dept of Mathematical Sciences
- 17:00 **Presentation of prizes**
- 17:10 **Pizza reception in Chancellors’ Building level 2 atrium**
- 18:00 **Close of meeting**

Posters

Dedicated session for presenting posters, they will give a three-minute flash presentation to introduce themselves and their work.

1. **Framework Rigidity Optimised Dynamic Algorithm (FRODA)**
Thomas McManus, Dept of Physics
2. **Performance Portable Molecular Dynamics**
William Saunders, Dept of Mathematical Sciences
3. **Synthetic Aperture Sonar Simulation using MATLAB with GPU Acceleration**
Ben Thomas, Dept of Mechanical Engineering
4. **Adsorption of Contaminants on Clay Mineral Surfaces**
Leyorla Ohene-Yeboah, Dept of Chemistry
5. **Parallelising tensor network algorithms with MPI**
Paul Secular, Dept of Physics
6. **Low-cost High-throughput Screening of All Inorganic Compounds**
Dr Keith Butler, Dept of Chemistry
7. **Imaging the Low Frequency Radio Sky**
Dr Martin Fullekrug, Dept of Electronic and Electrical Engineering
8. **Lattice dynamics of the Sn_xS_y system**
Dr Jonathan Skelton, Dept of Chemistry
9. **Particle Methods and Parallel Computing Algorithms for Simulation of Quasi-brittle Structures**
Dr David Miranda, Dept of Architecture and Civil Engineering

List of attendees

First Name	Surname	Department / Organisation
Jack	Betteridge	Dept of Mathematical Sciences
David	Bird	Dept of Physics
Russell	Bradford	Dept of Computer Science
Tobias	Brewer	Dept of Physics
David	Britton	University of Glasgow
Keith	Butler	Dept of Chemistry
Mark	Cahill	Dept of Computer Science
Steven	Chapman	Computing Services
Antony	Cleave	ClusterVision
Tadeo	Corradi	Dept of Mechanical Engineering
Rob	Deeth	Dept of Chemistry
Jessica	Dillon	Dept of Chemistry
Tina	Düren	Dept of Chemical Engineering
Joseph	Flitcroft	Dept of Chemistry
Daniel	Fosas de Pando	Dept of Architecture and Civil Engineering
Daniel	Fritsch	Dept of Chemistry
Martin	Fullekrug	Dept of Electronic and Electrical Engineering
Dibyajyoti	Ghosh	Dept of Physics
James	Grant	Dept of Chemistry
Surani	Gunasekera	Dept of Physics
Carmelo	Herdes	Dept of Chemical Engineering
Alan	Hunter	Dept of Mechanical Engineering
Robert	Jack	Dept of Physics
Roger	Jardine	Computing Services
Vera	Krewald	Dept of Chemistry
Eszter	Makkos	Dept of Chemistry
Ellie	Marsh	Dept of Architecture and Civil Engineering
Roshan	Mathew	Computing Services
Nick	McCullen	Dept of Architecture and Civil Engineering
Simon	McIntosh-Smith	University of Bristol
Thomas	McManus	Dept of Physics
Andrew	McRae	Dept of Mathematical Sciences
David	Miranda	Dept of Architecture and Civil Engineering
Benjamin	Morgan	Dept of Chemistry
Eike	Mueller	Dept of Mathematical Sciences

First Name	Surname	Department / Organisation
Leyorla	Ohene-Yeboah	Dept of Chemistry
Remy	Overkempe	ClusterVision
Anuradha	Pallipurath	Dept of Chemistry
Steve	Parker	Dept of Chemistry
Loizos	Pelecanos	Dept of Architecture and Civil Engineering
Tom	Pennington	Dept of Mathematical Sciences
Benedek	Plosz	Dept of Chemical Engineering
Laura	Redfern	ClusterVision
Anne	Reinarz	Dept of Mathematical Sciences
Andrew	Rhead	Dept of Mechanical Engineering
William	Saunders	Dept of Mathematical Sciences
Paul	Secular	Dept of Physics
Jonathan	Skelton	Dept of Chemistry
Joel	Statham	Dept of Chemistry
Katrine	Svane	Dept of Chemistry
Ben	Thomas	Dept of Mechanical Engineering
Ian	Thompson	Dept of Physics
Sophie	Tournier	Dept of Chemistry
Joshua	Tse	Dept of Chemistry
Tom	Underwood	Dept of Physics
Edward	Wastell	Dept of Physics
Robert	Watson	Dept of Electronic and Electrical Engineering
Nigel	Wilding	Dept of Physics
James	Williams	Dept of Mathematical Sciences
Ian	Williams	Dept of Chemistry
Wenkai	Zhang	Dept of Chemistry

Abstracts

Keynotes

K.1 “Xeon and Pascal and POWER, oh Phi!”: how to cope in a world of increasingly diverse architectures

Presented by: **Prof Simon McIntosh-Smith**, University of Bristol

Chair: **Dr Steven Chapman**, Computing Services

The next wave of large scale supercomputers, termed “pre-Exascale machines”, will employ a more diverse range of computer architectures than we have seen since the 1990s. Designs will include Intel multi-core CPUs, many-core Xeon Phi, IBM POWER, NVIDIA GPUs, and even ARMv8-based CPUs. This diversity presents an enormous challenge to the scientific programmer, since we want our codes not just to work on these different machines, but to perform well. In this talk we will outline the growing problem, and discuss recent work in parallel programming languages and programming techniques to increase the performance portability of scientific software.

K.2 Evolution of the Worldwide LHC Computing Grid

Presented by: **Prof David Britton**, University of Glasgow

Chair:

The LHC Computing Strategy

In this talk I will describe the development of the Worldwide LHC Computing Grid, a global infrastructure of compute and storage that was pivotal in the discovery of the Higgs Boson in 2012. The current infrastructure moves over 100 Petabytes each month; stores data on the exabyte-scale; and is running of the order of half-a-million jobs simultaneously as we speak. However, these numbers are dwarfed by the requirements of the High Luminosity LHC that will start producing data in the middle of the next decade. I will discuss the current ideas on how we evolve our infrastructure to this new level within the constraints of maintaining a production-quality infrastructure and flat-cash budgets.

Session one

Chair: Dr Eike Müller, Dept of Mathematical Sciences

1.1 Efficient Simulation of Rare Events

Presented by: **Tobias Brewer**, Dept of Physics and Dept Computing Science

Co-authors: *Robert Jack, Russell Bradford*

We discuss a computational method to analyse rare events in physical systems. In particular, we consider a model of particles diffusing on a lattice (the symmetric simple exclusion process) and investigate the probabilities of rare events in which the particles move less than expected over a long period of time. The rare events are described by large deviation theory and the computational method used to calculate their probabilities is a cloning algorithm. The algorithm evolves a large number of systems simultaneously each of which is copied or deleted in a cloning process. We implement the algorithm using a C++ code which we have made faster using OpenMP and MPI parallelisation. The MPI communications required for the cloning process invoke large inefficiencies and we have sought to reduce these using HPC methods such as message packing, OpenMP-MPI hybridisation and non-blocking communication. We have utilised Allinea to profile our implementations and have investigated how they scale across multiple processors.

Keywords – *Rare Events, Large Deviation Theory, MPI, OpenMP, Hybrid Code, Non-blocking MPI, Allinea*

1.2 Multiscale Modelling of Aerospace Composites

Presented by: **Dr Anne Reinarz**, Dept of Mathematical Science and Dept Mechanical Engineering

Due to their very good strength to weight ratio, composite materials make up over 50% of recent aircraft constructions. The materials are manufactured from very thin fibrous layers ($\sim 10^{-4}$ m) and even thinner resin interfaces ($\sim 10^{-5}$ m). Finite element modeling of such materials is extremely challenging due to the huge aspect ratio between layer thickness and the size of the modeled structures (~ 10 m), as well as due to the varying anisotropic material properties and the large contrast between fibrous and resin layers.

I will describe how we implemented the two-level overlapping Schwarz preconditioner GENE0 in the high-performance numeric environment DUNE. This preconditioner leads to almost optimal scaling with respect to problem size and number of cores, allowing us to successfully tackle the difficult problems mentioned above. For the coarse space construction, GENE0 computes generalised eigenvectors of the local stiffness matrices on the overlapping subdomains and builds an approximate coarse space by combining the smallest energy eigenvectors on each subdomain via a partition of unity. This preconditioner has been proven to be robust for isotropic problems. I will show that it gives good results also for anisotropic problems and that it scales well over thousands of cores.

Keywords – *Composites, GENE0, DUNE*

1.3 Efficient Simulation of Rare Events

Presented by: Daniel Fosas, Dept of Architecture and Civil Engineering

Buildings represent the largest energy-consuming sector with a 30% share of the world's total. As such, they constitute one of the key contributors to the greenhouse emissions responsible for climate change, reason why the construction industry has been under pressure to deliver energy-efficient buildings. At the same time, a changing climate raises the concern that buildings designed under historical weather data might not be fit for purpose. The implications of a warmer weather with severer, longer and more frequent heat waves threaten both the well-being of occupants and the impact of energy saving policies. Furthermore, it has been suggested that the measures imposed by such policies can, in turn, exacerbate these health risks. Can we design healthy and resilient buildings that address current needs? HPC allows for unprecedented large-scale studies on overheating in buildings. This furthers the understanding of risk factors and helps quantifying the potential impact of hot weather events on occupants and the corresponding mitigation measures.

Keywords - *building physics, thermal comfort, overheating, health risks*

Session two

Chair: Dr Rob Watson, Dept of Electronic and Electrical Engineering

2.1 Framework Rigidity Optimised Dynamic Algorithm (FRODA)

Presented by: Thomas McManus, Dept of Physics

Co-author: *Stephen Wells, Alison Walker*

We report protein structural flexibility modelled by a heuristic method, using a simplified physics model to explore motion in all-atom steric detail while taking into account the highly important non-covalent interactions that are known to govern protein conformation. FRODA models large scale motions in constrained systems using heuristic, minimally demanding, computational methods. FRODA's validity has been widely demonstrated as a reliable companion to other, more rigorous, methods such as coarse-grained Molecular Dynamics. Constraints are applied to systems through structural analysis, which rigidifies less mobile sections. This permits larger relative motions of conjugated segments to one another through dihedral rotation of key 'hinge' like bonds. The driving forces behind these structural pathways are taken from normal mode analysis, constructing a Hessian around the assumption that changes to an equilibrated structure in a constrained system, be it lattice or protein, are derived in harmonic deviations around a starting location on the energy landscape. This work aims to carry these methods over to Fab and CDR examination and prediction in immunoglobins, whilst also improving its application in other protein structures by devising a more robust set of tools for analysing the extremely important non-covalent interactions.

Keywords – *Protein Modelling, Computational Physics, Computational Biology, Efficient Modelling*

2.2 Performance Portable Molecular Dynamics

Presented by: William Saunders, Dept of Mathematical Sciences

Co-author: *Eike Müller, James Grant*

Molecular dynamics codes simulate the fundamental properties of matter by following the trajectories of a collection of model particles which interact via phenomenological potentials. We present a separation of concerns based approach to create portable high performance Molecular Dynamics and analysis codes within a high level framework. Such a framework allows the domain specialist to produce efficient code without knowledge of high performance computing. Furthermore through automatic runtime compilation, user codes can automatically target advanced hardware architectures such as Graphics Processing Units and distributed memory systems without user prompting.

Within the framework a user formulates 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 short 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, CPUs, Python*

2.3 Synthetic Aperture Sonar Simulation using MATLAB with GPU Acceleration

Presented by: Ben Thomas, Dept of Mechanical Engineering

Co-author: *Alan Hunter*

Synthetic aperture sonar (SAS) is a technique used for generating images of the sea-floor. The process involves the use of an Autonomous Underwater Vehicle (AUV) traversing a path, transmitting sonar pings and receiving their echoes. By coherent integration of the received echoes along the path, it is possible to focus the data into images with centimeter-order resolution. Moreover, by traversing a scene multiple times at different depths, it is possible to estimate the depth of the seafloor at each image pixel. This 3D data can be utilized to improve target detection and classification algorithms, and also enable the monitoring of sediment transport and man-made underwater structures such as wind or tidal turbines.

In order to develop and evaluate algorithms which perform sea-floor depth estimation, it is desirable to rapidly simulate the echo data generated from repeated passes past a known target. This is a computationally expensive process, since each target must be represented by a very high density point cloud. The interaction between the sonar ping and the target must be modelled for all AUV locations along multiple tracks, requiring trillions of Euclidian distance calculations to be performed.

For rapid algorithm development, MATLAB is the programming language of choice. Using the built-in Parallel Computing Toolbox™ allows acceleration of expensive calculations using parallel processing on both CPUs and GPUs. Balena's quad-GPU nodes are vital for allowing simulations to be run in a manageable amount of time, greatly increasing the rate of algorithm development.

Keywords – *Sonar, MATLAB, GPUs*

2.4 Adsorption of Contaminants on Clay Mineral Surfaces

Presented by: Leyorla Ohene-Yeboah, Dept of Chemistry

Co-author: *J.Grant, J.Skelton, S.C.Parker*

The accumulation and persistence of hazardous compounds (HCs) in surface and ground water as well as living organisms have emerged as an adverse effect of human anthropogenic behaviour. A variety of HCs, from emerging contaminants found in pharmaceutical residues and personal care products to household chemicals, biocides/pesticides and manufacturing wastes persist in the environment. Some of these compounds have been shown to cause adverse effects in aquatic organism as well as promote increased risk of developing thyroid disorders, tumours and diabetes. In this study, we aim to build on the foundations of our understanding of how HCs interact with the environment by applying atomistic simulation methods to determine the physicochemical factors controlling the distribution of pollutants and their metabolites in aqueous and terrestrial environments, and then apply this to identifying sustainable ways of control their transport. Clay minerals are ubiquitous in the environment, so they provide a good start for our study. Additionally, it has been suggested that clay minerals could act as geosorbants for the remediation of organic pollutant, so an evaluation of their adsorptive properties would be useful. Initial studies centred on HCs adsorption on two model clay surfaces; sodium montmorillonite and pyrophyllite. Simulations were performed using a combination of dispersion corrected DFT on HPC systems to calculate the adsorption energy and identify favourable sites for HC adsorption on clays in vacuum and water. Our initial investigation focused on 10 molecules including dibenzo-dioxins and two poly-chlorinated derivatives, chloro- and hexachloro-benzene, emerging contaminants amphetamine and two other derivatives and MDA and

its analogue MDMA. These compounds were chosen to detect the links between the chemical properties of these HCs and their possible fate and effects in the environment.

Keywords – *Computational Chemistry, GPUs, VASP*

2.5 Parallelising tensor network algorithms with MPI

Presented by: Paul Secular, Dept of Physics

Co-author: *Dr Stephen Clark*

My PhD involves working on the Tensor Network Theory (TNT) research software project (www.tensornetworktheory.org). During this first year, I hope to develop MPI parallel versions of the Time Evolving Block Decimation (TEBD) and Density Matrix Renormalisation Group (DMRG) algorithms for 1D tensor networks. These networks are known to quantum physicists as "matrix product states" (MPS) and to mathematicians as "tensor trains". I am interested in them as an efficient representation of certain 1D quantum lattice states, meaning their dynamics can be simulated classically using HPC. In this talk I will introduce these tensor networks and in my poster I will present the aforementioned parallel algorithms.

Keywords – *Tensor network theory, TEBD, MPI, tensor trains*

2.6 Low-cost High-throughput Screening of All Inorganic Compounds

Presented by: Dr Keith Butler, Dept of Chemistry

The discovery of functional materials is critical for technological advancements that will play a role in addressing global challenges, ranging from catalysis for sanitation, semiconductors for harvesting solar energy, and biomimetic materials for health. There is a concerted global effort to reduce the time it takes to realize new materials via databases, high-throughput screening, informatics, and mapping out the "materials genome."

Here, we show how the compositional space for stoichiometric, inorganic materials can be quantified by simple rules and how the vast space can be explored quickly and cheaply with the use of key chemical concepts and element properties in the search for candidate materials with target properties. We exemplify the application of this approach by identifying a chalcogenide material with potential for water-splitting applications and carrying out a comprehensive search for new compositions that could adopt the widely studied perovskite crystal structure.

Keywords – *Computational Chemistry*

2.7 Imaging the Low Frequency Radio Sky

Presented by: Dr Martin Fullekrug, Dept of Electronic and Electrical Engineering

2.8 Lattice dynamics of the Sn_xS_y system

Presented by: J. M. Skelton, Dept of Chemistry

Co-author: L. A. Burton, A. J. Jackson, F. Oba, S. C. Parker and A. Walsh

The tin sulphides Sn_xS_y are a family of sustainable energy materials with technological applications including photocatalysis and photovoltaics (PV). Despite being promising in theory, the efficiencies of current champion SnS-based solar cells are well below those of other flagship materials. A major barrier to progress is the rich phase chemistry of the sulphides: there are five known/proposed phases of SnS, as well as the S-rich SnS_2 and Sn_2S_3 compositions. This makes preparation and characterisation experimentally challenging, and, at the same time, phase impurities have been shown to negatively impact performance. By utilizing modern, high-throughput HPC systems, including Balena, we have been performed a comparative study of all seven Sn_xS_y compounds. We have applied state-of-the-art ab initio lattice-dynamics calculations to rank the phase stabilities, resolving two long-running controversies in the field, viz. the identity of the cubic phase of SnS, and the thermodynamic stability of Sn_2S_3 . We have also, for the first time on such complex systems, modelled a complete set of infrared and Raman spectroscopic data. This provides “fingerprints” for characterising the four bulk-stable materials, SnS₂, Pnma and π -cubic SnS and Sn_2S_3 , and for identifying them where they occur as impurities.

Keywords – *density-functional theory, lattice-dynamics calculations, energy materials, tin sulphides, thermodynamics, spectroscopy*

2.9 Particle Methods and Parallel Computing Algorithms for Simulation of Quasi-brittle Structures

Presented by: Dr David Miranda, Dept of Architecture and Civil Engineering

Co-author: Chris Williams, John Orr

Numerical models to predict the behaviour of structures play an important role in science and engineering. They enhance the optimization of structures and the development of new materials and their applications. In this work we present a parallelized algorithm based on systems of particles, to model quasi-brittle materials and structures. Despite the relatively high success of the standard continuum mechanics to predict the behaviour of certain classes of materials such as rubbers and metal alloys, it is generally accepted that an equivalent predictive capacity has not yet been achieved using continuum damage mechanics. When cracks become large enough, the hypothesis of material continuity becomes inappropriate. The proposed model avoids the continuity hypothesis, considering a finite set of material particles and interparticle bonds where cracks may develop by disruption of those bonds. The implementation proposed is based on the Message Passing Interface (MPI) framework, considering strategies for serialization, scattering, mapping and reduction of data. Furthermore, strategies for post-processing and visualization of the data are described. Calculation examples, describing a good fitting with the classical theory of linear elasticity and the ability to reproduce cracking patterns are presented. The simple but highly computational intensive algorithm may lead to better predictions than other more mathematical based methods such as the Finite Element Method, while addressing materials subjected cracking. A better predictive capacity may lead to improvements in research and application of brittle materials, higher construction quality in civil engineering and mitigation of environmental issues.

Keywords – *Parallel computing, MPI, particle systems, explicit methods, structures, materials*

Session three

Chair: Prof Nigel Wilding, Dept of Physics

3.1 Global Estimation of Air Quality

Presented by: Matthew Thomas, Dept of Mathematical Sciences

Calculating the burden of disease attributed to air pollution requires accurate estimation of population level exposures to pollutants. Although coverage of ground monitoring networks is increasing, these data are insufficient to independently estimate exposures globally. Information from other sources, such as satellite retrievals, chemical transport models and land use covariates must therefore be used in combination with ground monitoring data. Each of these data sources will have their own biases and uncertainties that may vary over space. Set within a Bayesian hierarchical modelling framework, the recently developed Data Integration Model for Air Quality (DIMAQ) integrates data from multiple sources and allows spatially-varying relationships between ground measurements and other factors that estimate fine particulate matter (PM_{2.5}) concentrations. The outputs of the model are estimated exposures that can be combined with population estimates to produce population-level distributions of exposures for each country. DIMAQ was used to estimate exposures of PM_{2.5}, together with associated measures of uncertainty, on a high-resolution grid (~11 km × 11 km) covering the entire globe for use in the 2016 WHO report 'Ambient air pollution: A global assessment of exposure and burden of disease', and in the 2015 and 2016 updates of the Global Burden of Disease.

For 2015, 92% of the world's population lived in areas that exceeded the WHO 10 µg/m³ guideline. Fifty percent of the global population resided in areas with PM_{2.5} concentrations above the WHO Interim Target 1 (IT-1 of 35 µg/m³); 64% lived in areas exceeding IT-2 (25 µg/m³); and 81% lived in areas exceeding IT-3 (15 µg/m³). Nearly all (86%) of the most extreme concentrations (above 75 µg/m³) were experienced by populations in China, India, Pakistan, and Bangladesh.

Keywords – *SAMBa, Air Quality, Bayesian*

3.2 Delivering a DLMONTE Workshop on Balena

Presented by: Dr James Grant, Dept of Chemistry

As part of our project developing DLMONTE for Monte Carlo simulation we delivered a workshop for prospective users at Bath in April 2017. Here I will discuss the reasons behind our decision to use Balena for the material and discuss the pros and cons of this approach. I will cover the setting up of the environment, how we chose to deliver material, the different resources we required and how the process was supported by the HPC team. Finally I will discuss the challenges faced, how we addressed these and considerations for future courses.

Keywords – *Balena, Workshop, DLMONTE*

Session four

Chair: Dr Benjamin Morgan, Dept of Chemistry

4.1 Hydrogen Defects in Hyperstoichiometric Uranium Dioxide

Presented by: Joseph Flitcroft, Dept of Chemistry

Co-author: S.C. Parker¹, M. Storr², M. Molinari¹, N. Brincat²

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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 defect energetics and formation of H interstitial species in UO_2 .

The trapping of hydrogen defects plays a critical role in determining the macroscopic materials of functional materials. DFT (GGA+U) has been used to investigate the effect of varying hydrogen defect concentration on oxygen defect clusters properties and stability in UO_{2+x} . Furthermore, a model is proposed to identify reversible and irreversible hydrogen traps. This will be beneficial in modelling the corrosion of uranium metal, where the diffusion of hydrogen through the UO_2 surface layer may form the pyrophoric uranium hydride at the metal-oxide interface, posing safety concerns for long term materials stability and storage.

Keywords - *Computational Chemistry, DFT, Hydride, Hydroxyl, UO_2 , Oxidation, Trapping*

4.2 Migration of Interstitial ions in Inorganic Perovskites

Presented by: Dibya Ghosh, Dept of Physics

Hybrid as well as inorganic lead halide perovskite (APbX_3) materials recently have attracted considerable attention due to their exceptional performance as an absorber materials in solar-cell device architecture, leading to high power conversion efficiency. Despite the outstanding material properties, structural instability in working condition, hinder their large-scale commercialisation. Defect mediated migration of constituent halide ions is one the major problems to be solved in this regard.[1] In the present work, migration pathway of less studied however frequently appearing defect, interstitial halide ions in mixed-anion inorganic perovskites at finite temperature and pressure have been investigated using ab initio molecular dynamics simulations.[2] It appears that migration of these defects strongly depend on various factors such as the size and concentration of migrating ions as well as chemical nature of host inorganic frames. Smaller anions, such as, chlorine migrate fast through iodide-based perovskites by both sequential hopping and ion-exchange mechanism. Further, at high concentration of interstitial defects, polyhalide chains can form spontaneously and migrate inside these perovskites. All these insights will help to gain a fundamental understanding about the migration behaviour of interstitial ions and can further suggest ways to suppress their movement at ambient condition.

1. Yuan et. al., *Acc. Chem. Res.*, 2016, 49, 286
2. Dastidar et. al., *Nano Lett.*, 2016, 16, 3563

4.3 Higher-order DG discretisations on modern architectures with applications in NWP

Presented by: **Jack Betteridge**, Dept of Mathematical Sciences

Co-author: *Eike Müller and Ivan Graham*

Many research problems in science and engineering rely on the solution of partial differential equations (PDEs) on a large scale and at a high resolution; one example is numerical weather prediction (NWP). This requires the use of modern high performance computing (HPC) technology and corresponding modern discretisation techniques. To make optimal use of the computational hardware, those methods have to be implemented using the latest software packages.

I will discuss the use of discontinuous Galerkin (DG) methods for solving advection type PDEs in the *dune* software framework. DG methods have been studied since the 1960's, but are becoming more popular for applications due to properties that make them efficient on modern HPC architectures. The method itself conserves certain physical quantities and has a high rate of convergence. These are desirable properties, since fewer degrees of freedom are required to reach a given error tolerance. Furthermore, on modern CPUs calculations can be performed quickly, but memory access is an order of magnitude slower. The high arithmetic intensity of higher-order DG methods allows for the computational capacity of these architectures to be exploited.

My numerical results for both a stationary and a time dependent advection problem demonstrate the high accuracy and computational efficiency of the method.

Keywords – *Partial Differential Equations, Discontinuous Galerkin, High-order, Numerical Weather Prediction*

4.4 Matrix-free block smoothers for higher-order DG methods

Presented by: **Dr Eike Müller**, Dept of Mathematical Sciences

Co-author: *Peter Bastian, Steffen Müthing, Marian Piatkowski (Heidelberg University)*

Efficient and suitably preconditioned iterative solvers for elliptic partial differential equations (PDEs) of the convection-diffusion type are used in all fields of science and engineering. To achieve optimal performance, solvers have to exploit the high arithmetic intensity of modern manycore CPUs. The computationally most expensive components of the solver are the repeated application of the linear operator and the preconditioner solve. For discretisations based on higher-order Discontinuous Galerkin methods, sum-factorisation techniques result in a dramatic reduction of the computational complexity for the matrix-free operator application. However, an algorithmically optimal *hp*-multigrid preconditioner also requires the repeated inversion of dense block-matrices in the DG smoother. The explicit assembly and direct solution of those block-matrices with a bandwidth-bound LU- or Cholesky-factorisation counteracts any gains from the efficient operator application. Here we present an alternative, fully matrix-free implementation of DG block-smoothers. By inverting the block-matrices iteratively, it is possible to harness the full computational power of the CPU. We implemented a hybrid multigrid algorithm for high order DG discretisations in the EXADUNE framework. The effectiveness of this approach is demonstrated by solving a set of representative elliptic PDEs of increasing complexity.

Keywords – *Partial Differential Equations, Discontinuous Galerkin*

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Notes

