Welcome

Dear Participants,

We, the Scientific Organising Committee, are delighted to welcome you to the 5th Annual University of Bath HPC Symposium.

This year, we have a full programme, with keynotes from Dr Tom Conner from the CLIMB project and Andy Mallinson from Intel alongside a diverse programme of talks from across the University departments.

Tom will take us through the development of a cloud infrastructure to provide bioinformaticians with new tools for their research, giving access to software HPC resources on demand and better facilitating the sharing of research data. Andy will give us an introduction to Intel's many integrated core (MIC) architecture, a coprocessor card with many lightweight cores optimised for vector operations. The Xeon Phi is relatively new but fast gaining in popularity, Andy will provide some programming tips for the current-generation hardware and talk us through Intel's roadmap for future developments.

The schedule for the day includes contributions from Physics and Maths, Chemistry and Engineering, covering a wide range of topics from molecular dynamics and quantum-chemical simulations through to high-level finite-element methods to solve engineering problems.

The University's second-generation HPC cluster, Balena, has been up and running for over a year now, and is seeing full utilisation. With 3,072 CPU cores and a peak CPU LINPACK performance of 57.5 TFLOPS, compared to the 800 cores and 6.9 TFLOPS of her predecessor, Aquila, Balena provides a substantially higher throughput and has both the capacity and the capability to take on much more ambitious projects. In addition to the traditional core architecture of compute nodes and a 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, as well as a remote visualisation service for graphically-intensive applications and dedicated high-performance storage.

This year's Symposium will showcase the breadth of research being carried out by the University's HPC community, and we hope will provide a forum for discussion and new collaborations.

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

Yours faithfully,

The Scientific Organising Committee

Dr Steven Chapman, HPC Manager, Computing Services
Dr Jonathan Skelton, Department of Chemistry

Programme

The Symposium will take place in Chancellors' Building, Room CB2.6 on Thursday 9th June 2016

09:00 Registration and refreshments

09:30 Welcome and introduction
Prof Jonathan Knight, Pro-Vice-Chancellor (Research)

09:40 Session one
Chair: **Prof Aron Walsh,** Dept of Chemistry

09:40 Quick fire poster talks (see page 4)

10:15 Session two
Chair: **Dr Andrew Rhead**, Dept of Mechanical Engineering

10:15 **Performance Portable Molecular Dynamics**
William Saunders, Dept of Mathematical Sciences

10:30 **Firedrake: automating the finite element method by composing abstractions**
Dr Andrew McRae, Dept of Mathematical Sciences

10:45 Delegation photograph in atrium outside CB2.6

10:50 Break and poster viewing

11:30 Keynote one
Chair: **Prof James Davenport**, Dept of Computer Science

11:30 Pathways for multicore computing with Intel Xeon Phi
Andrew Mallinson, Intel

12:30 Lunch - Chancellors' Building level 2 atrium

13:45 Session two continued
Chair: **Dr Andrew Rhead**, Dept of Mechanical Engineering

13:45 **Multiscale modelling of aerospace composites**
Dr Anne Reinarz, Dept of Mathematical Sciences and Dept Mechanical Engineering

14:00 **Particle Methods and Parallel Computing Algorithms for Simulation of Quasi-brittle Structures**
Dr H. David Miranda, Dept of Architecture and Civil Engineering

14:15 Keynote two

Chair: **Prof Sam Sheppard**, Director of Bioinformatics, Dept of Biology and Biochemistry

14:15 **The Cloud Infrastructure for Microbial Bioinformatics; overcoming barriers to software use and data sharing in biology**

Dr Thomas Connor, Cardiff University

15:15 Break

15:45 Session three

Chair: **Dr Benjamin Morgan**, Dept of Chemistry

15:45 **Noisy level set topology optimization**

Dr Lester Hedges, Dept of Physics

16:00 **Throwing away the lock and key - A rigid framework look at antibodies (using FRODA)**

Thomas J. McManus, Dept of Physics

16:15 **Self-consistent hybrid functional calculations: Implications for structural and electronic properties of oxide semiconductors**

Dr Daniel Fritsch, Dept of Chemistry

16:30 **Computational screening of all inorganic materials**

Dr Keith T. Butler, Dept of Chemistry

16:45 **Fast(ish) multipole methods for transient wave fields**

Dr Michael Carley, Dept of Mechanical Engineering

17:00 Presentation of prizes

17:00 Pizza reception in Chancellors' level 2 atrium

18:00 Close of meeting

Posters

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

1. Atomistic Simulation of Oxide Interfaces in Materials for Energy Technologies
   Joel Statham, Dept of Chemistry

2. Realistic Computer Simulations of Metal-Organic Frameworks: From Lattice Vibrations to Heteroepitaxy
   Jessica K. Bristow, Dept of Chemistry

3. Efficient Simulation of Rare Events
   Tobias Brewer, Dept of Physics

4. DFT investigation of the relative stability of Magnesium Carbonate Minerals
   Joshua Tse, Dept of Chemistry

5. Using HPC to Explore Hydrogen Behaviour in $UO_{2\pm x}$
   J. M. Flitcroft, Dept of Chemistry

6. Ferroelectric properties of hybrid organic-inorganic perovskites
   Dr Katrine L. Svane, Dept of Chemistry

7. Ab initio lattice dynamics for materials science: application to the tin sulfides
   Dr Jonathan Skelton, Dept of Chemistry

8. Modeling distributed computing processes as max-plus linear dynamical systems
   Dr James Hook, Dept of Mathematical Sciences

List of attendees

First Name	Surname	Department / Organisation
Stefano	Angioni	Computing Services
Jakub	Baran	Dept of Chemistry
David	Bird	Faculty of Science
Russell	Bradford	Dept of Computer Science
Tobias	Brewer	Dept of Physics
Jessica	Bristow	Dept of Chemistry
Iain	Burns	Other Organisation
Keith	Butler	Dept of Chemistry
Michael	Carley	Dept of Mechanical Engineering
Martha	Carpinteyro	Dept of Economics
James	Cave	Dept of Physics
Steven	Chapman	Computing Services
Hungru	Chen	Dept of Chemistry
Thomas	Connor	Cardiff University
Stephen	Cook	Dept of Mathematical Sciences
Zhuangzhu	Dai	Dept of Electronic and Electrical Engineering
James	Davenport	Dept of Computer Science
Huan	Doan	Dept of Chemical Engineering
James	Edwards	Dept of Mathematical Sciences
Gunes	Erdogan	School of Management
Richard	Evans	Library
Joseph	Flitcroft	Dept of Chemistry
Daniel	Fosas	Dept of Architecture and Civil Engineering
Daniel	Fritsch	Dept of Chemistry
Jonathan	G-H-Cater	Dept of Electronic and Electrical Engineering
James	Grant	Dept of Chemistry
Lester	Hedges	Dept of Physics
James	Hook	Dept of Mathematical Sciences
Antal A.	Jarai	Dept of Mathematical Sciences
Roger	Jardine	Computing Services
Surendra	Kaushik	cplx
Andrew	Mallinson	Intel Corp
Roshan	Mathew	Computing Services
James	McClung	ClusterVision
Thomas	McManus	Dept of Physics
Andrew	McRae	Dept of Mathematical Sciences
David	Miranda	Dept of Architecture and Civil Engineering
Benjamin	Morgan	Dept of Chemistry

First Name	Surname	Department / Organisation
Steve	Parker	Dept of Chemistry
Julio	Perez	Dept of Chemical Engineering
Anne	Reinarz	Dept of Mathematical Sciences
Andrew	Rhead	Dept of Mechanical Engineering
Matt	Richards	Computing Services
William	Saunders	Dept of Mathematical Sciences
Neys	Schreiner	Dept of Mechanical Engineering
Sam	Sheppard	Dept of Biology and Biochemistry
Jonathan	Skelton	Dept of Chemistry
Alexander	Smith	Dept of Physics
Joel	Statham	Dept of Chemistry
Katrine	Svane	Dept of Chemistry
Ian	Thompson	Dept of Physics
Joshua	Tse	Dept of Chemistry
Thomai	Tsiftsi	Dept of Mathematical Sciences
Alison	Walker	Dept of Physics
Aron	Walsh	Dept of Chemistry
Robert	Watson	Dept of Electronic and Electrical Engineering
Jim	Webb	Dept of Physics
Lucy	whalley	Dept of Chemistry
Mike	Wilson	Dept of Mechanical Engineering

Abstracts

Keynote

K.1 Pathways for multicore computing with Intel Xeon Phi

Presented by: **Andrew Mallinson**, Intel

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

K.2 The Cloud Infrastructure for Microbial Bioinformatics; overcoming barriers to software use and data sharing in biology

Presented by: **Dr Thomas Connor**, Cardiff University

Chair: **Prof Sam Sheppard**, Director of Bioinformatics, Dept of Biology and Biochemistry

Genome sequencing has made it possible to examine fundamental biological questions over vast scales; from bacteria to man. Since the first bacterial genome was published 20 years ago, research focused around bacterial pathogens has been at the very vanguard of the revolution that has transformed biology into a data rich, data intensive field of science. With this transformation come key challenges around the provision of infrastructure and the training of researchers in order to make the most of the datasets that we can now routinely generate. In 2014 the Medical Research Council made a ~£50m investment in "big data" to support the development of new research e-infrastructures. The £8.5m CLoud Infrastructure for Microbial Bioinformatics (CLIMB) was the only award to a consortium focused on the needs of researchers interested in bacterial genomics and is one the largest investments in microbial bioinformatics ever made. CLIMB will provide bioinformatics infrastructure as a service to the entire academic UK medical microbial community. CLIMB will provide a single sign-on, distributed computing and storage infrastructure – providing a one-stop-shop for both analysis and training. This talk will introduce CLIMB, and how cloud approaches are being used to overcome key issues that exist for most biologists today.

Session one

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

1.1 Atomistic Simulation of Oxide Interfaces in Materials for Energy Technologies

Presented by: **Joel Statham**, Dept of Chemistry
Co-authors: *Marco Molinari, Stephen Parker*

Materials used for energy generation applications normally have a complex microstructure and the resulting interfaces profoundly affect their properties. In this project we are developing tools for generating such interfaces at the atomic level. Initially, we are focussing on the fluorite- perovskite system, e.g. CeO_2 || $SrTiO_3$, where the aim is to be able to assess the importance of the hetero-interfaces on the transport properties. High performance computing (HPC) is essential when investigating the structure and transport properties of interfaces due to the number, size and complexity of such systems. Currently we have begun an optimization procedure by using a combination of potential-based energy minimisation in a perfectly parallel mode by displacing one over the other and minimising each displacement to obtain a preliminary energy landscape, and then at each of the minima carry out molecular dynamics (MD) simulations to anneal the interfaces by first raising the temperature to 3000K and then cool systematically back to room temperature. We have just begun large scale simulations to test this approach and obtained the number of nodes/cores with respect to efficiency and time. From the structural models obtained, our test step is to investigate how the interface controls transport properties such as oxygen migration, thermal and electrical conductivity and again we show that the simulations require access to HPC resources.

Keywords – *Interface, fluorite-perovskite system, high performance computing, molecular dynamics*

1.2 Realistic Computer Simulations of Metal-Organic Frameworks: From Lattice Vibrations to Heteroepitaxy

Presented by: **Jessica K. Bristow**, Dept of Chemistry
Co-authors: *Julian D. Gale, Aron Walsh*

The prediction of solid-state properties is becoming evermore prevalent for understanding the chemical and physical behaviour of metal organic frameworks. While in the past, the primary interest was in gas absorption, new applications areas including photocatalysis, ferroelectrics and optoelectronics are attracting increasing attention.

Materials modelling approaches vary according to the properties of interest. Classical forcefield methods allow large-scale simulations and have been used in screening procedures for the identification of functional topologies for applications such as gas adsorption capacities. Electronic structure methods, such as Density Functional Theory (DFT), allow the prediction of electronic properties such as band gap, frontier orbital composition and magnetic interactions.

Firstly, we present the development of an accurate and robust forcefield (VMOF) that is capable of reproducing not only structure but also vibrational properties. Temperature dependent properties such as heat capacity, Gibbs free energy, bulk modulus and Grüneisen parameter can be predicted

across all MOF topologies. Negative thermal expansion is found to be well described within the quasi-harmonic approximation.

Secondly, we present the heteroeptixy of MOFs on metal oxide surfaces with both electronic structure and forcefield methods. We first identify low-mismatch oxide-MOF combinations, and focus on the binding of MOF-5 on the surface of TiO_2. The interface structure and thermodynamics will be discussed, which sheds light on recent experimental reports of eptiaxial growth.

Keywords – *Computational Chemistry, materials modeling, large scale simulations*

1.3 Efficient Simulation of Rare Events

Presented by: **Tobias Brewer**, Dept of Physics

Whether it's an avalanche, a tsunami or a highly improbable genetic mutation, we know that rare events can have dramatic effects. It is, therefore, essential for us to know just how rare that rare events really are. To do this we use an algorithm (Lecomte, Tailleur *2007*) in which many systems are evolved simultaneously and large deviations theory is used to quantify the probability of unlikely events. The more systems that we use, the rarer the events that we can consider. HPC techniques allow us to significantly increase the number of systems that we can simulate in a short period of time.

Thus far, we have primarily utilised OpenMP and MPI to parallelise C++ codes. These codes model simple systems of interacting particles on 1-D lattices. OpenMP has given us impressive speed-ups with an efficiency of 90% on 16 threads. We have been able to achieve larger speed-up's by employing MPI on 4 nodes, although working on multiple nodes incurs significantly lower efficiencies. We are in the early stages of extending the project to include the usage of Intel Xeon Phi cards and this will be a key area of research going forward. We have also found Allinea to be of use for profiling the code to determine the overheads and waiting times associated with parallelisation.

Keywords – *Large Deviation Theory, Theoretical Physics, OpenMP, MPI, C++, Intel Xeon Phi Cards, Allinea*

1.4 DFT investigation of the relative stability of Magnesium Carbonate Minerals

Presented by: **J. Tse**, Dept of Chemistry
Co-authors: *J.R.Grant, M.Molinari and S.C.Parker*

A combination of quantum and potential based methods have been used to model Hydrated Magnesium Carbonate minerals. The challenge is to find the order of stability of Mg containing minerals at different H_2O and CO_2 partial pressures. Brucite and Hydromagnesite are of particular interest as they potentially trap radionuclides in nuclear waste repositories. HPC is a safe and effective tool to assess the structure, stability and interaction of these minerals with radionuclides. Standard DFT does not include long range dispersion forces. However, it is widely recognised as being essential

for the correct treatment of intermolecular interactions. We compared four commonly used approaches (Grimme D3, optB88-vdW, optB86b-vdW and uncorrected DFT) which were run in the VASP code on Balena. Analysis showed optB88-vdW gives a better representation of crystal structure and formation energy for these minerals.

Evaluating the relative stability as a function of chemical potential we can generate a phase diagram, which illustrate the most stable phase at different conditions. At atmospheric conditions (350ppm CO_2, 32mbar H_2O at 0K), Lansfordite is the most thermodynamically stable phase. Having shown that the functional optB88 reproduces experimental values, we will apply this method to calculate the sorption behaviour of species on mineral surfaces.

Keywords – *Computational Chemistry, HPC, Magnesium Minerals, Radionuclide*

1.5 Using HPC to Explore Hydrogen Behaviour in $UO_{2\pm x}$

Presented by: **J. M. Flitcroft**, Dept of Chemistry
Co-authors: M. Molinari1, N. A. Brincat2, N.R. Williams2, M. T. Storr2 and S. C. Parker1
[1]Department of Chemistry, University of Bath, Bath, BA2 7AY, UK
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UO_2 is generally a passivating layer over uranium metal, which reduces the rate at which hydriding occurs. However, hydriding of the underlying metal still occurs. The UO_2 layer is generally a non-stoichiometric phase, such as U_4O_9 and U_3O_7, as UO_2 prefers hyperstoichiometry. These non-stoichiometric phases contain a range of oxygen defects clusters. Therefore knowledge of the behaviour of hydrogen's interaction with oxygen defect clusters, is important.

The aim of the project is to explore the structure, stability and transport of hydro- gen species in uranium based matrixes. As there is a lack of experimental data, in part due to the difficulty of determining how hydrogen behaves, and the dangers associated with the handling of uranium materials, HPC provides a safe and efficient route for investigating these properties.

DFT has been used, on Balena, to investigate a range of hydrogen species in $UO_{1.97-2.156}$. Interstitial hydrogen can exist as a proton (as part of a hydroxyl group) and hydride. This demonstrates the complexity of the energy landscape and the challenges in evaluating the diffusion pathway of hydrogen in UO_2. Hence, the requirement of HPC resources, such as supplied by Balena.

Keywords – *HPC, Uranium Oxides, Hydrogen, Hydroxyl, Hydride*

1.6 Ferroelectric properties of hybrid organic-inorganic perovskites

Presented by: **Katrine L. Svane**, Dept of Chemistry
Co-authors: *Aron Walsh*

We use density functional theory to investigate the ferroelectric properties of hybrid organic-inorganic perovskites. This class of materials, generally consisting of a negatively charged cage structure with a small organic cation in the cavities, contains several multiferroic compounds as well as a number of room temperature ferroelectrics. The ferroelectric polarisation arises from an ordering of the organic cations within the cavities, resulting in an asymmetric positioning of the positive charge relative to the negatively charged cage. Here we compare two different approaches, based on Berry phase calculations and Wannier functions, respectively, for calculation of the polarization density. Since hybrid materials are mechanically softer than typical inorganic ferroelectrics, the effect of phonons is of particular interest. We therefore investigate the temperature- and time-dependence of the ferroelectric ordering, showing that the magnitude of the polarisation is very sensitive to the geometry, leading to large variations on the picosecond timescale.

Keywords – *Computational Chemistry, Wannier functions, Ferroelectrics*

1.7 Ab initio simulation of vibrational spectra: application to materials characterization

Presented by: **J. M. Skelton**, Dept of Chemistry
Co-authors: *L. A. Burton, A. J. Jackson and A. Walsh*

Identifying efficient, sustainable and cost-effective functional materials for the generation of "green" energy is an active challenge in contemporary materials science. The tin sulphides (Sn_xS_y), which include the SnS, SnS_2 and Sn_2S_3 phases, have long been regarded as promising potential photovoltaic (PV) absorbers, but practical high-efficiency devices have yet to be realised. Among the core issues is the difficulty of preparing phase-pure materials, and impurities have been demonstrated to have a detrimental effect on PV performance.

Vibrational (infrared/Raman) spectroscopy is a standard and widely-available tool for materials characterisation, and is well suited to rapidly assessing the purity of materials e.g. prepared with different synthetic techniques. Obtaining high-quality reference spectra is experimentally challenging, however, requiring careful sample preparation and specialist measurement equipment.

Previous work has shown that first-principles modeling techniques can be used to simulate vibrational spectra with quantitative accuracy, representing a powerful tool for materials modeling and a fruitful area of overlap between experiment and theory.

This talk will present a recent modeling study of the infrared and Raman spectra of the three tin sulphides, using the framework of *ab initio* lattice dynamics. Particular emphasis will be placed on the techniques involved, which span several different levels of approximation and computational requirements ranging from a single multicore workstation to a high-performance HPC cluster such as Balena.

Keywords – *computational chemistry, materials modeling, density-functional theory, ab initio lattice-dynamics calculations*

Session two

Chair: **Dr Andrew Rhead**, Dept of Mechanical Engineering

2.1 Performance Portable Molecular Dynamics

Presented by: **William Saunders**, Dept of Mathematical Sciences

Co-author: *Dr Eike Mueller, Dr James Grant, Prof Rob Scheichl, Prof Steve Parker*

Molecular simulations in Computational Chemistry and Physics model interactions between many particles to infer information at the macroscopic level. Researchers often wish to perform many simulations with large numbers of particles to inform theoretical and experimental science, hence codes must be efficient and parallel. Furthermore the large datasets produced during simulations must be analysed within the simulation itself or as a post processing stage.

A variety of codes exist to provide highly parallel libraries for generic computation of Molecular Dynamics. However existing codes are not performance portable and must be reimplemented for each new hardware architecture requiring substantial knowledge in both the physical domain and the computer science domain. A similar barrier is faced by members of the research community who wish to perform customised simulations which are beyond the scope of existing codes or develop codes for computationally intensive analysis.

We present a novel technique to develop highly parallel codes for general Molecular Dynamics computations that does not require detailed knowledge of computing hardware from domain specialists. Following the successful approach of PyOP2 and Firedrake in the Partial Differential Equation world we implement an abstraction which separates the concerns of the domain specialist from those of the computer scientist. The result is a framework where a high level language is used to describe computational work in the science domain that is interpreted to generate efficient and parallel code for a target architecture.

Keywords – *Computational Chemistry, GPUs, MPI, CPUs, Python*

2.2 Firedrake: automating the finite element method by composing abstractions

Presented by: **Andrew McRae**, Dept of Mathematical Sciences

A lot of scientific research depends on the ability to efficiently simulate physical systems modelled by partial differential equations. However, it is rare that a single person is knowledgeable in everything from numerical analysis to parallel computing, in addition to their domain of expertise.

Firedrake, developed largely at Imperial College London, is a library for the highly-automated solution of PDEs using the finite element method. For maximum ease of use, the user code is written in Python, allowing problems to be specified in a form that is close to the underlying maths. Corresponding efficient C 'kernels' are automatically generated and executed, with data movement handled by generated 'wrapper' code. Firedrake is suitable for both small and large-scale programs;

parallelisation is handled automatically, and we have run on over 24,000 cores on the national supercomputer ARCHER.

Keywords – *Python, finite element, PDEs, domain-specific languages, automatic code generation*

2.3 Multiscale modelling of aerospace composites

Presented by: **Dr Anne Reinarz**, Dept of Mathematical Sciences and Dept Mechanical Engineering
Co-author: Rob Scheichl (Math), Victor Bayona Revilla (Math), Richard Butler (Mech. Eng.)

Our goal is to model deformations of composite materials used in aerospace engineering. Due to their layered and strongly anisotropic structure these composites require sophisticated numerical tools.

To implement an efficient and highly parallel model we use DUNE (Distributed and Unified Numerics Environment), a C++ library for solving PDEs. DUNE has been shown to allow parallel efficiency on hundreds of thousands of compute cores.

During the manufacture of composite materials certain defects are expected to appear and need to be included into the model. To model these defects' impact on peak stresses we use uncertainty quantification. This requires us to run the model repeatedly placing particular importance on the efficiency of the solver. Therefore, we are developing a multilevel iterative solver with log-linear complexity specifically tailored to our application.

Keywords – *Finite Elements, DUNE, MPI, Aerospace composites, elasticity*

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

Presented by: **Dr H. 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: **Dr Benjamin Morgan**, Dept of Chemistry

3.1 Noisy level set topology optimisation

Presented by: **Dr Lester Hedges**, Dept of Physics
Co-author: Robert Jack (Bath), Alicia Kim (University of California, San Diego)

Level set toplogy optmisation is a method for finding "optimal" structural deisgns that satisfy a set of constraints, e.g. finding the structure that is as stiff as possible while using a fixed amount of material. Although widely used, soutions obtained by the method are highly dependent on the initial trial design and little is known about the shape of the design landscape. For example, is the converged design a true global minimum? Using techniques from statistical mechanics we attempt to introduce noise to the level set method. This allows us to sample an ensemble of designs and explore the design landscape.

Keywords – *Computational Physics, Structural Optimisation*

3.2 Throwing away the lock and key - A rigid framework look at antibodies (using FRODA)

Presented by: **Thomas J. McManus**, Dept of Physics

The Framework Rigidity Optimized Dynamic Algorithm (FRODA) surfaced in 2005 as an accurate method for modelling the internal mobility of proteins [1], by reproducing barnase structures in close agreement with NMR, using a set of rules based on purely steric interactions. It was also shown to be successful in finding pathways from one known confirmation of a protein structure to another by combining directional and random biases in the propagation of a protein structure throughout space. For this reason it is my belief that FRODA can be utilized to classify, or at least screen, the rules which govern the confirmation of an antibody's hypervariable Complimentary Determining Regions (CDRs) and thus which polypeptide sequences can be certain to interact with a given target antigen binding site. Moreover the spatial behavior of antibodies as a whole is an, as of yet, rather mysterious and unsolved problem. Angular allowances along the joints between variable (VH / VL) and crystalline (Fc) regimes, and in particular at the hinge region separating the Fc and Fab sections of the heavy chain, could hold the answer as to why these systems behave in their manner. It is our belief that through analysis of these parameters, based on an elastic modelling network which can explore globally favorable motions of the system, and observation of the pathways taken by these global motions we

can start to undercover some of the secrets behind these molecules that still lay hidden 30 years into the field's discovery.

Keywords – *Computational Physics, Computational Biology, FRODA, Antibody, CDRs*

3.3 Self-consistent hybrid functional calculations: Implications for structural and electronic properties of oxide semiconductors

Presented by: Dr Daniel Fritsch, Dept of Chemistry
Co-authors: *Benjamin Morgan, and Aron Walsh*

Density functional theory has proven hugely successful in the calculation of structural properties of condensed matter systems and the electronic properties of simple metals. Band gaps of semiconductors and insulators, however, are often severely underestimated due to the limitations of existing approximate exchange-correlation functionals. Considerable improvements are possible by including a fraction of Hartree-Fock exchange, constructing a so-called "hybrid" functional. The precise proportion of Hartree-Fock exchange is typically treated as an empirical parameter chosen by intuition and experimental calibration.

This empiricism can be avoided with a self-consistent hybrid functional approach for condensed systems [1], which allows parameter-free hybrid functional investigations. Using this approach, we report on the implications for structural and electronic properties of oxide semiconductors, with ZnO, SnO2, and MgO as specific examples. Structural and electronic properties will be compared to theoretical and experimental data, showing considerable improvement with respect to previous approaches.

[1] J. H. Skone, M. Govoni, and G. Galli, Phys. Rev. B 89, 195112 (2014).

Keywords – *Computational Chemistry, Hybrid Functionals, Oxides*

3.4 Computational screening of all inorganic materials

Presented by: **Dr Keith T. Butler**, Dept of Chemistry
Co-authors: Adam J. Jackson, Daniel W. Davies, Joshua Evans, Andy Morrison, Jonathan M. Skelton, Jarvist M. Frost, Aron Walsh

Forming a four component compound from the first 103 elements of the periodic table results in excess of 10^{12} combinations. Such a materials space is intractable to high-throughput experiment or first-principles computation. We have developed a procedure to address this problem. Through the application of simple chemical principles we have explored this vast compositional hyperspace for new, useful materials.

In this talk I will introduce the python based SMACT (Semiconducting Materials from Analogy and Chemical Theory) package, which we have developed for the past three years. The package applies simple textbook chemical rules to filter through vast numbers of compounds. The simplicity of the package means that developers have included undergraduate Masters students and sixth-form placement students, their contributions to the code will be explained. The vast task of exploring 10^{12} combinations also demonstrates the value of code profiling and optimisation; I will explain how one search procedure was reduced from a three week runtime to 45 minute runtime, by careful optimisation and parallelisation. Finally I will present an application focused screening, which has predicted several promising, hitherto unknown, materials for solar driven water splitting.

Keywords – *High-throughput screening, materials design, Python*

3.5 Fast(ish) multipole methods for transient wave fields

Presented by: **Dr Michael Carley**, Dept of Mechanical Engineering

The Fast Multipole Method (FMM) is a method of choice for solving problems with large numbers of elements in areas such as acoustics, electromagnetism, optics, and fluid dynamics. At present, it is mainly limited to static or harmonic (single frequency) calculations, but is not directly applicable to calculations of transient radiation such as those which arise in computing noise from random or non-periodic sources in a number of engineering applications such as aeroacoustics. This talk will present recent work on developing methods for transient radiation calculations based on the use of time-domain spherical harmonics, which have the important property of guaranteeing causality, a property not shared by the alternative technique of plane wave expansions. Results of computational tests will be presented and applications will be discussed.

Keywords - *Fast Multipole Method, spherical harmonics, wave equation, transient radiation*

Acknowledgements

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

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

Steven Chapman
Jonathan Skelton
Roshan Mathew

We are also grateful to our ground crew for their help and hard work on the day.

Finally, thank you to you, the attendees, for your participation and for truly making the Symposium a real success.

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

You can also follow us on Twitter: @BathHPC

Notes