High Performance Computing

Annual Symposium

UNIVERSITY OF BATH

8th Annual High Performance Computing (HPC) Symposium

Thursday 6th June 2019

Welcome

Dear Participants,

The Organising Committee are delighted to welcome you to the University of Bath's 8th annual High Performance Computing (HPC) Symposium.

This year, we have four outstanding invited speakers:

- Dr Mike Croucher is a Technical Evangelist at The Numerical Algorithms Group (NAG) with responsibilities that cut across much of the organisation including High Performance and Cloud Computing, research software engineering consultancy, product development and sales and marketing. He has nearly 20 years of experience supporting and developing many aspects of research computing including scientific software, high performance and cloud computing and research software engineering at the Universities of Sheffield, Manchester and Leeds. Dr Croucher will be sharing his experiences with us in how he has worked with research communities to enable them to do computation better.
- Dr Hendrik Van Eerten is a High-Energy Astrophysicist at the University of Bath. His research focuses on using parallel relativistic hydrodynamics simulations though to Bayesian statistics to connect models to astrophysical data as directly as possible. Dr Van Eerten will share how HPC is being used in Astrophysics here at Bath.
- Dr James Price (University of Bristol) is one of the Research Software Engineers (RSEs) who was closely involved in commissioning and acceptance stages for GW4's Tier2 Isambard HPC service. Funded by EPSRC, Isambard is a Cray XC50 system, comprising of 10,496 Marvell Thunder X2 cores and is one of the world's first production Arm-based supercomputers. Dr Price will give an operational update and share the latest performance results.
- Mike Kiernan (*EMEA Team Lead at Microsoft*) specialises in Big Compute and HPC. Mike will give an overview of the research computing tools available in the Azure Cloud with an emphasis on HPC.

To accompany these talks, we have a host of contributions from researchers across the University, delivered as talks and quick-fire introductions to posters. The line-up includes contributions covering machine learning, finite element modelling, algorithmic improvement, in silico clinical trial as well as astrophysics and molecular simulations.

The annual HPC Symposium showcases the breadth of research being carried out by the University's HPC community and has evolved 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 Organising Committee,

Dr Gaël Donval, Chemical Engineering
Dr Ji Wu, Chemistry
Dr Steven Chapman, Computing Services

Programme

The Symposium will take place in 3 West North (3WN) room 2.1 on Thursday 6th June 2019.

09:00 Registration and refreshments in 3WN foyer

09:30 Welcome and introduction
Prof Steve Parker, Chair of the HPC Management Group
Prof Jonathan Knight, Pro-Vice Chancellor for Research

09:45 Session One
Chair: **Dr James Grant**, Research Software Engineer, Computing Services

09:45 Keynote: **Why nobody cares about HPC**
Dr Mike Croucher, Technical Evangelist, Numerical Algorithms Group (NAG)

10:45 Break and poster viewing

11:15 Session Two
Chair:

11:15 **Examining the safety of a novel treatment for knee arthritis – an in silico clinical trial with 3,360 patient models**
Dr Alisdair MacLeod, Dept of Mechanical Engineering

11:30 **Topological Fluid Dynamics**
Dr Anton Souslov, Dept of Physics

11:45 **Efficient methods for calculating free energies and their application to adsorption, defect stability and solid-solid phase transition**
Dr Thomas Underwood, Dept of Chemistry

12:00 **Atom-Level Modelling the Free Energy of Adsorption of Hazardous Compounds at Soil-Water Interfaces**
Leyorla Ohene-Yeboah, Sustainable Chemical Technologies, Dept of Chemistry

12:15 **A Parallel time-evolution algorithm for quantum systems with long-range interactions**
Paul Secular, Dept of Physics and Mathematical Science

12:30 Session Three
Chair: **Dr Benjamin Morgan**, Dept of Chemistry

12:15 **Flash/Poster Session, see page 4**

12:45 Lunch in 3WN Foyer

14:00 Session Four
Chair: **Dr Carolin Villforth**, Dept of Physics

14:00 Keynote: **Astrophysics and Computation at Bath**
Dr Hendrik Van Eerten, Dept of Physics

14:30 **The star formation history of galaxies that host active galactic nuclei**
Anastasia Efthymiadou, Dept of Physics

14:45 **Autonomous Exploration and Identification of Structure Property Relationships of High Performing COFs using Machine Learning**
Calum Hand, Sustainable Chemical Technologies, Dept of Chemistry

15:00 **Parallelising particle filters with butterfly interactions**
Dr Kari Heine, Dept of Mathematical Sciences

15:15 Break and delegation photograph

15:45 Session Five
Chair: **Prof James Davenport**, Dept of Computer Science

15:45 Invited: **Status and Performance of the Isambard Tier-2 Service**
Dr James Price, Research Software Engineer, University of Bristol

16:00 **Fast electrostatic solvers for kinetic Monte Carlo simulations**
Dr William Saunders, Dept of Physics

16:15 **Efficient solvers for semi-implicit hybridised DG methods in fluid dynamics**
Jack Betteridge, Dept of Mathematical Sciences

16:30 Invited: **HPC and Research Computing in Azure**
Mike Kiernan, EMEA Lead for Microsoft Big Compute and HPC

17:00 Presentation of prizes

17:05 Close of meeting
Prof Steve Parker, Chair of the HPC Management Group

17:10 Pizza reception in 3WN Foyer

Posters

Dedicated session for researchers to give a three-minute introduction to themselves and their poster.

1. Automated First-Principles Exploration of Anionic Redox Cathode Materials
   Alexander Squires, Dept of Chemistry

2. Parallel cross interpolation for high-precision calculation of high-dimensional integrals
   Dr Sergey Dolgov, Dept of Mathematical Sciences

3. Size-dependent adsorption and framework flexibility in DUT-8(Ni)
   Megan Thompson, Dept of Chemical Engineering

4. Co-Adsorption of Heavy metal Cations and Phosphate on Goethite-Water Interfaces
   Wenkai Zhang, Dept of Chemistry

List of attendees

First Name	Surname	Department / Organisation
Petros	Ampatzidis	Dept of Architecture and Civil Engineering
Elizabeth	Arter	Bath Institute for Mathematical Innovation
Jack	Betteridge	Dept of Mathematical Sciences
Mark	Cahill	Dept of Computer Science
Steven	Chapman	Computing Services
Dewan	Chowdhury	Dept of Physics
Stephen	Collinson	Computing Services
Matt	Cowley	Dept of Chemistry
Mike	Croucher	NAG
James	Davenport	Dept of Computer Science
Jacob	Dean	Dept of Chemistry
Sergey	Dolgov	Dept of Mathematical Sciences
Gaël	Donval	Dept of Chemical Engineering
Anastasia	Efthymiadou	Dept of Physics
Chloe	Ferris	Computing Services
James	Grant	Computing Services
Calum	Hand	Dept of Chemistry
Kari	Heine	Dept of Mathematical Sciences
James	Hook	Dept of Mathematical Sciences
Roger	Jardine	Computing Services
Nathaniel	Kelly	Dept of Mechanical Engineering
Mike	Kiernan	Microsoft
Matthew	Lennox	Dept of Chemical Engineering
Alisdair	MacLeod	Dept of Mechanical Engineering
Joe	Manning	Dept of Chemical Engineering
Roshan	Mathew	Computing Services
Benjamin	Morgan	Dept of Chemistry
Lucy	Morgan	Dept of Chemistry
Eike	Mueller	Dept of Mathematical Sciences
Leyorla	Ohene-Yeboah	Dept of Chemistry
Steve	Parker	Dept of Chemistry
Jospeh	Paul-Taylor	Dept of Chemistry
Tom	Pennington	Dept of Mathematical Sciences
James	Price	University of Bristol
Matt	Richards	Computing Services
Will	Saunders	Dept of Physics
Paul	Secular	Dept of Physics
Ryan	Sharpe	Dept of Chemistry
Alexander	Smith	Dept of Physics
Thijs	Smolders	Dept of Physics
Anton	Souslov	Dept of Physics
Alex	Squires	Dept of Chemistry
Megan	Stalker	Dept of Chemistry

First Name	Surname	Department / Organisation
Adam	Symington	Dept of Chemistry
Oliver	Thomasson	School of Management
Megan	Thompson	Dept of Chemical Engineering
Piers	Townsend	Dept of Chemistry
Tom	Underwood	Dept of Chemistry
Hendrik	Van Eerten	Dept of Physics
Carolin	Villforth	Dept of Physics
Esther	Walton	Dept of Psychology
Yiming	Wang	Dept of Computer Science
Ian	Williams	Dept of Chemistry
Christopher	Woods	University of Bristol
Ji	Wu	Dept of Chemistry
Wenkai	Zhang	Dept of Chemistry

Submitted Talk Abstracts

Session Two

Examining the safety of a novel treatment for knee arthritis – an in silico clinical trial with 3360 patient models

Presented by: Dr Alisdair MacLeod, Dept of Mechanical Engineering
Co-authors: A. Casonato, A. Toms, H.S. Gill

Computational modelling and simulations offer a unique ability to virtually perform multiple surgeries on the same individual to compare the functional and structural outcome of the interventions. We present an in silico clinical trial, performed using Balena HPC, whose objective was to evaluate the safety equivalence between a novel high tibial osteotomy (HTO) procedure and a well-established existing method. Ethical approval was obtained for the in silico clinical trial (REC reference: 17/HRA/0033). The two arms of this in silico trial were (1) HTO using the well-established Tomofix™ Osteotomy System; (2) HTO using the Tailored Osteotomy for Knee Alignment (TOKA®) – a novel patient-specific procedure. Virtual HTO surgery was performed on 30 patients using their lower limb CT scans (Royal Exeter and Devon NHS, UK). Finite element models (ANSYS 18.0, ANSYS inc.) were developed including several key input parameters: the screw configuration for each implant, material properties of the bone, and muscle and joint forces for different daily living activities. The key output results were the maximum stress within the plate, the maximum strain at each bone-screw interface and the movement at the osteotomy site. Paired Wilcoxon and chi-squared tests were used to evaluate the differences between the two devices. A total of 3360 models were solved to date, with 840 more in progress. We developed python-based input generation and submission scripts and a unix and matlab results extraction codes. These results will be used to provide safety evidence in the planned NHS clinical trial later this year.

Keywords: Biomechanics, orthopaedics, osteotomy, stress, implant

Topological fluid dynamics

Presented by: Dr Anton Souslov, Dept of Physics

Active liquids are composed of self-driven microbots that endow the liquid with a unique set of mechanical characteristics. In this talk, I will explore how to use finite-element methods such as COMSOL Multiphysics to simulate flows and density waves in continuum models of active fluids. These simulations guide the design of materials exhibiting topological states. For example, topological edge waves arise in a rotating fluid as a result of the Coriolis force that breaks Galilean invariance and opens a gap at low frequency. The number and spatial profile of topological edge states depends on an anomalous response coefficient called odd (or Hall) viscosity. As the sign of odd viscosity changes, an unusual topological phase transition occurs without closing the bulk band gap.

Keywords: Finite-element method, active-fluid dynamics, acoustics, COMSOL Multiphysics

Efficient methods for calculating free energies and their application to adsorption, defect stability and solid-solid phase transitions

Presented by: Dr Thomas Underwood, Dept of Chemistry
Co-authors: Leyorla Ohene-Yeboah, Vincent Ballenegger, Heather Wiebe, Graeme Ackland, Nigel Wilding, Steve Parker

'Free energy' is an important concept in physics and chemistry. The free energy of a state of a system is a measure of how likely the system is to be in that state. Here 'state' could mean a number of things, e.g. the crystal structure, or the position of one or more molecules. For example, the preferred crystal structure of a solid is that with the lowest free energy; and the likelihood of a molecule binding to a ligand or surface reflects the free energy difference between the bound and unbound states of the molecule. There is hence considerable interest in being able to calculate accurate free energies using computer simulation. Unfortunately, such calculations are extremely challenging. Evaluating a free energy entails calculating the energy of a vast number of configurations of the system; where the more configurations included in the calculation, the more precise the calculated free energy will be. Thus precise free energy calculations are extremely computationally demanding, and reaching the precision desired for practical purposes is often intractable. The situation could be improved by if more efficient computational methods for evaluating free energies were developed, especially methods which can make the most of modern HPC resources. We have developed new methods and software for calculating free energies, and applied them to a variety of problems, including: adsorption of small molecules in solution on a clay surface; determining the stability of grain boundaries; and pinpointing solid-solid phase transitions in porous materials and quantum crystals. Here, we provide an overview of this recent work, with a focus on the improvements to the methods and software which have realised significant speed-ups in our calculations.

Keywords: Monte Carlo, free energy, statistical mechanics, computational chemistry, adsorption, phase transition

Atom-Level Modelling the Free Energy of Adsorption of Hazardous Compounds at Soil-Water Interfaces

Presented by: Leyorla Ohene-Yeboah, Sustainable Chemical Technologies, Dept of Chemistry
Co-authors: Tom L. Underwood, Jonathan M. Skelton, Steve C. Parker

The accumulation and persistence of hazardous compounds (HCs) in the environment has emerged as an adverse effect of human behaviour. HCs emerge from a variety of sources, including contaminants in personal care products, pesticides and manufacturing wastes. Some of these compounds have been shown to cause adverse effects in aquatic organisms, as well as increase the risk of developing thyroid disorders, tumours and diabetes in humans [1] In this study, we aim to build on the foundations of our understanding of how HCs interact with the environment. We use atomistic simulation methods to determine the physicochemical factors controlling the distribution of pollutants and their metabolites in aqueous and terrestrial environments. This enables us to identify sustainable ways of control the transport of HCs and remediate their effect. Our initial studies focused on the adsorption of HCs on model surfaces found in soil, such as the clays, sodium montmorillonite and pyrophyllite, ubiquitous silica and a model organic surface. We used a combination of dispersion corrected DFT and classical MD methods to calculate the binding free energy and identify favourable sites for HC adsorption on these organic and inorganic surfaces in vacuum and water. We then moved towards calculating the free energy of adsorption of these HCs at the mineral-water interfaces. The calculations proved too difficult using conventional simulation methods; hence we applied a new

Monte-Carlo-based approach which allows the calculation to be efficiently parallelized [2]. By calculating the free energies of adsorption, we obtain insights into the behaviour of HCs at the soil-water interface and help to identify and potentially remediate highly persistent HCs.

[1] Petrie, B. et al.(2014) Water Res., 72, 3–27
[2] Brukhno, A.V., (2019) Molecular Simulation, pp.1-21

Keywords: computational chemistry, MPI, parallelization, hpc

A Parallel time-evolution algorithm for quantum systems with long-range interactions

Presented by: **Paul Secular**, Dept of Physics and Mathematical Science
Co-authors: Nikita Gourianov (Oxford), Michael Lubasch (Oxford), Sergey Dolgov (Bath), Stephen Clark (Bristol), Dieter Jaksch (Oxford)

In this talk I present a brand-new parallel algorithm for simulating the dynamics of quantum particles with long-range interactions. Quantum mechanics suffers from a curse of dimensionality meaning it is hard to simulate more than just a few particles. Full-scale quantum computers may be a solution but are still a long way off. In the meantime, it is essential that we use classical computers to their full capacity. To harness the potential of HPC requires parallel algorithms, which are not always easy to develop. My work involves the simulation of strongly-interacting quantum particles confined to a crystal lattice. Two of the leading approaches are Quantum Monte Carlo and Tensor Network Theory (most famously the DMRG algorithm). Condensed matter physicists are particularly interested in electrons, but unfortunately the same property of electrons that gives rise to the Pauli Exclusion Principle also leads to a numerical "sign" problem which plagues Quantum Monte Carlo methods. Tensor Network algorithms do not suffer from this problem but do not scale as well to 2 or 3 spatial dimensions. For one dimensional systems, tensor network methods are quasi-exact. By their nature, Monte Carlo algorithms are "embarrassingly parallel" (in other words, trivial to parallelise). However, it is far more challenging to find parallel tensor network algorithms, and very few are known. Inspired by the Parallel DMRG algorithm [1], we have developed a parallel version of the Time-Dependent Variational Principle algorithm described in [2], which allows us to simulate the dynamics of quantum lattice systems with long-range interactions. In order to test the accuracy of the method we have so far applied this to two paradigmatic models of magnets in one-dimension: the long-range Ising model and the long-range XY model.

[1] EM Stoudenmire and SR White (2013) Phys Rev B 87, 155137
[2] J Haegeman, C Lubich, I Oseledets, B Vandereycken, and F Verstraete (2016) Phys Rev B 94, 165116

Keywords: computational physics, MPI, tensor networks, matrix product states, DMRG, time evolution, parallel algorithm, quantum mechanics, condensed matter

Session Four

Atom-Level Modelling the Free Energy of Adsorption of Hazardous Compounds at Soil-Water Interfaces

Presented by: **Anastasia Efthymiadou**, Dept of Physics
Co-authors: Carolin Villforth, Vivienne Wild, Paul Hewett

Galaxies are systems of billions of stars, gas, dust and dark matter bound all together by gravitational attraction. Most of the heaviest galaxies contain a very massive black hole at their centres, known as the supermassive black hole. Those black holes are fed by cold gas through accretion. When a supermassive black hole undergoes a period of fast accretion it appears as an Active Galactic Nucleus (AGN). Cold gas is also consumed in star formation, a procedure through which a galaxy grows. Light from stars, gas, dust, star formation, fast accretion onto the black hole (AGN) and other processes constitutes the spectrum of a galaxy, which carries all sort of information. When a galaxy hosts an AGN it appears as a point source as the AGN outshines the light originating from the stars residing within the galaxy. Therefore, it is very difficult to extract any information about the properties of the stars. We study the star formation history of galaxies that host AGN. We decompose the complex active galaxy spectrum using 19 spectral components in Bayesian MCMC fitting. Some components describe the light resulting from the AGN and others that of the stars. We are then able to remove the AGN spectrum and recover the star light spectrum with the aim of estimating the age of the stars within the galaxy.

Keywords: Bayesian MCMC fitting in Astrophysics

Autonomous Exploration and Identification of Structure Property Relationships of High Performing COFs using Machine Learning

Presented by: **Calum Hand,** Sustainable Chemical Technologies, Dept of Chemistry
Co-authors: James Hook, Gaël Donval, Matthew Lennox, Tina Düren

Methane is currently being investigated as an alternative transport fuel with a particular focus on storing it in nanoporous solids. With 100,000s of different porous materials to choose from, simulations are invaluable to identify promising candidates. Most studies to date use a brute force screening approach requiring thousands of potential materials to be simulated and assessed which is computationally expensive. This work demonstrates the successful use of machine learning models to assess COFs as methane storage materials and develop structure property relationships at reduced computational cost.

Keywords: Monte Carlo, COF, methane, alternative, machine learning, decission tree,

Parallelising particle filters with butterfly interactions

Presented by: **Dr Kari Heine**, Dept of Mathematical Sciences
Co-authors: Nick Whiteley, A. Taylan Cemgil

Bootstrap particle filter (BPF) is the corner stone of many algorithms used for solving generally intractable inference problems in Hidden Markov models. The long term stability of BPF arises from particle interactions that typically make parallel implementations of BPF nontrivial. We propose a method whereby the particle interaction is done in several stages. With the proposed method, full

interaction can be accomplished even if we allow only pairwise communications between processing elements at each stage. We show that our method preserves the consistency and the long term stability of the BPF. The proposed method was tested numerically on the HPC framework Balena at the University of Bath and it displayed notable gain in performance compared to other state of the art methods in certain scenarios. It should also be noted that the proposed methodology lends itself to further considerations on the gain in efficiency in different computer network topologies, such as hypercubes.

Keywords: Particle filter, sequential Monte Carlo, HMM

Session Five

Fast electrostatic solvers for kinetic Monte Carlo simulations

Presented by: Dr William Saunders, Dept of Physics
Co-authors: Eike Müller, James Grant

Kinetic Monte Carlo (KMC) is an important computational tool in theoretical physics and chemistry. KMC permits the description of time dependent dynamical processes and is not restricted to systems in equilibrium. Compared to Molecular Dynamics, it allows simulations over significantly longer timescales. Recently KMC been applied successfully in modelling of novel energy materials such as Lithium-ion batteries and organic/perovskite solar cells. KMC considers interacting particles which can hop between localised sites in a material. The transition rates for these hops depend on the change in total potential energy of the system. For charged particles this requires the frequent calculation of electrostatic interactions, which is usually the bottleneck of the simulation. We recently developed a new variant of the Fast Multipole Method by Greengard and Rokhlin which ameliorates this issue by dramatically reducing computational costs. Our algorithm scales linearly in the number of charges for each KMC step, something which had not been deemed to be possible before. In this talk we provide an overview of the KMC algorithm and methods to compute the electrostatic interactions. Furthermore we present initial performance results on Balena and Isambard.

Keywords: computational physics, computational chemistry, MPI, OpenMP

Efficient solvers for semi-implicit hybridised DG methods in fluid dynamics

Presented by: Jack Betteridge, Dept of Mathematical Sciences
Co-authors: Thomas Gibson, Ivan Graham, Lawrence Mitchell, Eike Müller

For problems in Numerical Weather Prediction (NWP), time to solution is a critical factor. Semi-implicit time-stepping methods can speed up geophysical fluid dynamics simulations by taking larger time-steps than explicit methods. This is possible because they treat the fast (but physically less important) waves implicitly, and the time-step size is not restricted by the CFL condition for these waves. One disadvantage of this method is that an expensive linear solve must be performed at every time step, however, using an effective preconditioner for an iterative method significantly reduces the computational cost of this solve, making a semi-implicit scheme faster overall. Higher-order

Discontinuous Galerkin (DG) methods are known for having high arithmetic intensity making them well suited for modern HPC hardware, but are difficult to precondition due to the large number of coupled degrees of freedom. By using a hybridised DG method we can eliminate the original coupling and instead couple the equations to a smaller global system on the trace space, which is easier to precondition. This is achieved by considering the numerical flux variables which only lie on the facets of the mesh. We build on recent work[1] in this area by solving the resultant system using a non-nested geometric multigrid technique instead[2]. We discretise and solve the non-linear shallow water equations, an important model system in geophysical fluid dynamics, and demonstrate the effectiveness of the multigrid preconditioner for a semi-implicit IMEX time-stepper. The method is implemented in the SLATE language, which is part of the Firedrake project. Firedrake is a Python framework for solving finite element problems via code generation.

[1] Kang, Shinhoo and Giraldo, Francis X and Bui-Thanh, Tan. IMEX HDG-DG: a coupled implicit hybridized discontinuous Galerkin (HDG) and explicit discontinuous Galerkin (DG) approach for shallow water systems arXiv preprint arXiv:1711.02751, 2017
[2] Cockburn, Bernardo and Dubois, Olivier and Gopalakrishnan, Jay and Tan, Shuguang. Multigrid for an HDG method IMA Journal of Numerical Analysis 34(4):1386–1425, 2014

Keywords: Numerical Weather Prediction, Efficient solvers, Hybridised DG, Firedrake, Shallow Water Equations, Code Generation

Submitted Flash Poster Abstracts

Automated First-Principles Exploration of Anionic Redox Cathode Materials

Presented by: **Alexander Squires**, Dept of Chemistry
Co-authors: Dan Davies, Ben Morgan

Anion redox (AR) batteries are one of the most exciting developments in electrochemical energy storage in the 21st Century; however, higher performance materials are required to make this technology a reality. One clear strategy for developing new AR battery materials is varying the transition metal present in archetypal AR cathode materials. This will affect the relative positions of the energy levels within the structure, directly impacting on the likelihood of AR taking place. We intend to systematically vary the metal to build up a clear picture of how this new library of compounds will perform in AR batteries. An issue with exploring such a vast combinatorial space is that each calculation is so unique that the time spent by researchers setting up, "babysitting", analysing and collating results from each one presents a serious bottleneck. Our current working level of theory combined with modern computing capability means that in principle we can carry out many thousands of accurate calculations systematically. We hope to use such techniques to examine electronic structure properties of these potential AR materials in an attempt to validate various metrics that have been proposed within the literature to screen for new potential anionic redox materials.

Keywords: Computational Chemistry, Automation, High-Throughput, Density Functional Theory

Parallel cross interpolation for high-precision calculation of high-dimensional integrals

Presented by: **Dr Sergey Dolgov**, Dept of Mathematical Sciences
Co-authors: Dmitry Savostyanov (U. Brighton)

We propose a parallel version of the tensor cross interpolation algorithm and apply it to calculate high-dimensional integrals motivated by the Ising model in quantum physics. The cross method approximates the given function in a low-rank tensor decomposition using univariate fibers with adaptively calculated positions. We implement a hybrid parallel code with distributed MPI computations of different tensor factors, and shared OpenMP computations of elements in each factor. We observe a fast superlinear convergence with respect to the number of samples, and almost ideal strong scalability up to hundreds of processes or threads.

Keywords: MPI, OpenMP, Ising model, high-dimensional approximation, tensor decompositions, parallel renormalisation group

Size-dependent adsorption and framework flexibility in DUT-8(Ni)

Presented by: **Megan Thompson**, Dept of Chemical Engineering
Co-authors: Claire Hobday, Tina Düren

Metal-organic frameworks often exhibit guest-induced framework flexibility due to weak coordination bonds between secondary building units. Such MOFs spark interest for sensory and drug delivery devices, but the phase-transition pressure is not well understood. The adsorption

properties of these MOFs are normally determined for large, bulk crystals and in simulations using perfect, periodic models. However, for many applications MOF nanoparticles are preferable as their smaller size improves mass transfer and the ease of incorporation into the system. But how does the particle size and shape influence the uptake of guest molecules and framework flexibility? This work uses molecular simulations to investigate the size-dependent adsorption and framework flexibility in DUT-8(Ni). DUT-8(Ni) is peculiar in that its micron-sized crystals exhibit a breathing effect, whereas its nanoparticles remain rigid in their open pore configuration. A combination of grand-canonical Monte Carlo simulations and density functional theory optimisations has been used to develop a thorough understanding of this size dependent phase transition.

Keywords: computational chemistry

Co-Adsorption of Heavy metal Cations and Phosphate on Goethite-Water Interfaces

Presented by: Wenkai Zhang, Dept of Chemistry
Co-authors: T.L.Underwood, J.Liu, M.Molinari, S.C.Parker, R.L.Zhu

Cadmium is highly toxic to human beings and many other organisms. We consider goethite α-FeO(OH), as an natural adsorbent not only for its ability to trap Cd(II) but also for its abundance in the earth's crust and as a good model system for computational investigations. Co-adsorption between phosphate and Cd(II) was discovered experimentally with ferrihydrite surfaces, a precursor of goethite (Liu et al., 2018). We strongly suspected that a similar relationship will be found on goethite surfaces as well. Hence we combine computational simulations with experimental studies to investigate the anticipated co-adsorption behaviour. We have simulated the structures of five common surfaces of goethite: {100}, {110} and {021}; studied their surface characteristics; and proposed likely adsorption mechanisms. Then, we performed atomic simulations with Monte Carlo simulations (Brukhna et al., 2019) to mimic a mixture of Cd(II) and phosphate at fixed chemical potentials. The result from the simulations allowed us to evaluate the effect of surface composition on the free-energies of adsorption. The laboratory works utilised spectroscopic (i.e UV-Vis, atomic absorption, etc.) and microscopic analysis to confirmed that co-adsorption occurs and provides an enhancement of the immobilisation of Cd(II) on goethite. The comparison between experimental work and simulations have given us more comprehensive understanding towards the synergistic adsorption of Cd(II) with phosphate on goethite surfaces.

Keywords: computational chemistry, environment, geochemistry

Acknowledgements

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

Thank you to James Grant and the Doctoral College for holding three HPC workshops in the lead up to this event.

Thank you to the prize committee for judging the contributions and awarding the prizes.

Special thanks go to the members of Organising Committee and HPC Team for their invaluable input during the planning stages and in coordinating the event:

Dr Steven Chapman, Computing Services
Dr Gaël Donval, Chemical Engineering
Dr Ji Wu, Chemistry
Dr James Grant, Computing Services
Roshan Mathew, Computing Services
Chloe Ferris, Computing Services

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: go.bath.ac.uk/hpc

You can also follow us on Twitter: @BathHPC