UNIVERSITY OF BIRMINGHAM

7th Annual BEAR PGR CONFERENCE 2016

14th December 2016

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Introduction

Each year the University of Birmingham hosts the Birmingham Environment for Academic Research (**BEAR**). This year is the seventh time the conference has been held, and presents a wide variety of research from different schools as well as from internal and external keynote speakers.

The conference originated as a means of providing postgraduate researchers students (PGRS) a relatively 'safe' and familiar environment to present their work before moving on to conferences more specialised to their respective fields. However, the BEAR PGR conference has in fact become a forum for PGRS to present work to their peers around campus and obtain feedback from perspectives from outside of their field.

The BEAR PGR conference has also played host to a number of world-leading academic and industrial delegates. The keynote speakers this year are:

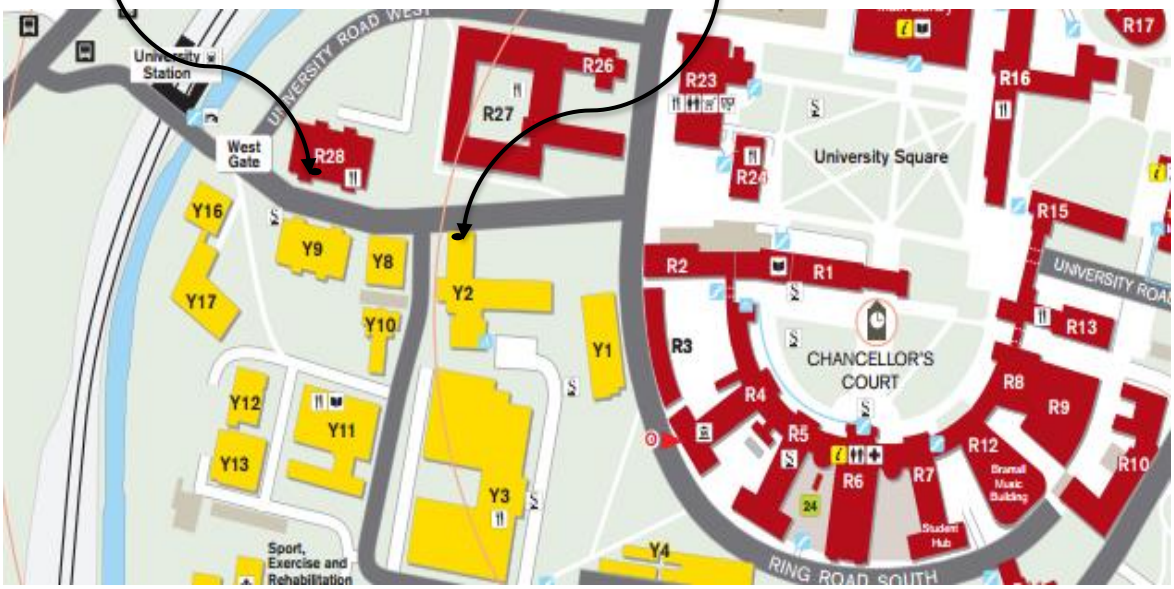
- **Dr. Hauert - a swarm engineer** (University of Bristol)
- **Dr. Glowacki - a computational chemist** (Univeristy of Bristol)
- **Dr. Slater - particle physicist** (University of Birmingham).

This conference is focused on computational analysis, numerical modelling, and HPC. It is open to all disciplines, including STEM, social sciences and humanities. The conference is intended to demonstrate the power and potential uses of the University's HPC (BlueBEAR) and the facilities included in BEAR.

Conference Venue

Murray Learning Centre [Map: Zone R28]
Upper Ground Room 09 (UG09)]
-Registration & presentations

Centre for Computational Biology (CCB) (Haworth Building) [Map: Zone Y2]
-Poster session & lunch
-Drinks reception



Conference Programme

Time	Event	Location
09:50-10:15	**Registration**	**Murray Learning Centre**
10:15-10:20	**Opening Remarks** Prof. Jean-Baptiste Cazier	
10:20-11:00	**Keynote** Dr. Sabine Hauert *Swarm Engineering*	
11:00-11:20	Rajib Ahmed *Nanophotonic optical devices*	
11:20- 11:40	Dong Li - *Module identification for weighted biological networks*	
11:40 -12:00	Jim Barrett *Gravitational waves and Gaussian processes*	
12:00–13:00	**Lunch and Posters**	**Centre for Computational Biology**
13:00–13:40	**Keynote** Dr. David Glowacki *Computational Chemistry and Cultural Theory*	**Murray Learning Centre**
13:40 –14:00	Shixuan Wang *Detection of a change in panel data*	
14:00 - 14:20	Oji Galadima - *Defect chemistry and properties of mixed Oxide nuclear fuel*	
14:20 - 14:40	Mostapha Ariane - *A mesh-free approach for modelling hydrodynamics*	
14:40 –15:10	**Tea Break**	
15:10 – 15:50	**Keynote** Dr. Mark Slater Research Area: *Particle Physics*	**Murray Learning Centre**
15:50 – 16:00	**Closing Remarks**	
16:00	**Close**	
16:00	**Drinks Reception**	**Centre for Computational Biology**

Keynote Speakers

Dr Sabine Hauert

Sabine Hauert is a Lecturer in Robotics at the University of Bristol. Her research focuses in engineering swarms that work in large numbers (>1000), and at small scales (<1 cm). Swarm strategies are either inspired from nature or are automatically discovered using machine learning and crowdsourcing. Before joining the University of Bristol, Sabine engineered swarms of nanoparticles for cancer treatment at MIT as a Human Frontier Science Program Cross-Disciplinary Fellow, and deployed swarms of flying robots at EPFL.

Sabine is also the President and Co-founder of Robohub.org, a non-profit dedicated to connecting the robotics community to the public. As an expert in science communication, she is often invited to discuss the future of robotics, including in the journal Nature, at the European Parliament, and as a member of the Royal Society's Working Group on Machine Learning.

Abstract

Swarm engineering allows us to design self-organized robotic systems that work in large numbers (>1000), and at small scales (<1 cm). Swarm strategies are either inspired from nature (ant colonies, fish shoals, and bird flocks) or are automatically discovered in simulation using machine learning and crowdsourcing. Demonstrated applications include the deployment of swarms of flying robots to create outdoor communication networks, or the design of nanosystems for biomedical applications. Current work focusses on the design of swarming nanoparticles for cancer applications in simulation and under the microscope on tissue-on-a-chip devices, as well as the design of strategies for our 1000 coin-sized robots at the Bristol Robotics Laboratory. In the future, we aim to use swarm engineering to reverse engineering natural swarm behaviours, further providing inspiration for our robotic systems.

Dr David Glowacki

Dr. David Glowacki graduated from UPenn in 2003, where he obtained an undergraduate degree in chemistry, and did significant coursework in lots of other subjects – mathematics, philosophy, comparative literature, and religions. In 2004 he obtained an MA in cultural theory at the School of Arts, Languages, and Cultures at the University of Manchester (UK).

He completed his PhD in physical chemistry at Leeds University (UK) in 2008. After four years as a post-doc in Bristol, he was awarded a Royal Society Research Fellowship and tenured faculty position in 2013. He has published in several domains: non-equilibrium molecular physics, classical & quantum dynamics, biochemistry, digital aesthetics, interactive art, human-computer interaction, high-performance computing & algorithm development, evolutionary algorithms, religion & power, cultural theory, atmospheric physics, optics, and scientific instrument development. Two of his better known interdisciplinary projects include the multi-award winning 'Danceroom Spectroscopy' digital art installation and the 'Hidden Fields'dance performance. Since 2011, these have been experienced by well over 100,000 people across Europe, the USA, and Asia – featured at a number of prestigious venues like the Barbican Arts Centre (London), the ZKM | Center for Art and Media Technology (Karlsruhe, Germany), the London 2012 Olympics (London, UK), the Stanford University Art Institute (Palo Alto, California), the Bhutan International Festival (Thimphu, Bhutan), and many others.

Abstract

Interactive molecular visualisation and simulation using virtual reality on HPC architectures visualization and simulation of biochemical systems constitute an indispensable strategy for understanding and designing biochemical architectures, furnishing microscopic understanding into both physiology and patho-physiology, helping us to design remedies to tackle disease at the molecular nanoscale. For example, many catalysis & drug-design problems are effectively problems of 'shape-matching' – i.e., attempting to design a small molecular ligand (a drug or substrate) that specifically targets and fits snugly into a larger molecular receptor (a protein or enzyme). Many of these sorts of problems can be likened to a sort of "3D molecular Tetris", but are complicated by the fact that biomolecular systems are flexible objects with 1000s of degrees of freedom and complex intermolecular interactions. Hence, biomolecular 'design space' is enormous – substantially larger than what the best brute-force algorithms can analyse exhaustively. Visualization and simulation approaches have the potential to enable more rational approaches to molecular design in both synthetic biology and pharmaceutical science: by visualizing the atomic details of biomolecular architectures, researchers can make more informed "design decisions" within a massive search space. In this talk, I will outline and demonstrate recent work at that my group has been carried out which fuses virtual reality and machine learning to solve difficult problems in biomolecular design, including both drug binding and protein knotting.

Dr Mark Slater

Mark Slater graduated with a Masters Degree from Cambridge and, after spending a year in the computing industry working on embedded systems and engine control units, returned to Cambridge to undertake a PhD in Particle Physics on the NA48 experiment looking at rare Kaon decays. After completing this degree, he stayed on at Cambridge to work on the Beam Position Monitor systems for a future Linear Collider. He moved to the University of Birmingham in 2007 to take up a Computing and Analysis role on the Atlas experiment. During this time he took on more computing roles both in teaching and code development. He is now working as the System Administrator for the Particle Physics Group cluster as well as doing teaching, code development and analysis support.

Abstract

Modern Experimental Particle Physics is producing more data than ever before by several orders of magnitude. Yearly, the LHC experiments alone produce 30 PetaBytes of raw and processed data, all of which not only must be stored and accessed by physicists from all over the world, but also analysed efficiently. This makes the use of modern coding techniques and frameworks essential as well as the leverage of any computing resources the member institutes can provide. This talk will give a brief overview of the techniques, software and computing models used by the LHC experiments and Particle Physics in general that are enabling the processing of such vast datasets to produce new discoveries such as the Higgs Boson.

Oral Presentation Abstracts

Computational Modelling of Nanophotonic Optical Devices

Rajib Ahmed,[1] and Haider Butt,[*]
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Abstract
Advances in computational capabilities have led to advanced models of optical devices, for verification of their optical properties in a fast, robust, and efficient manner. Computational modelling of the optical devices find applications such as gratings, diffusers, lenses, waveguides, and microring resonators. Here Finite Differential Time Domino (FDTD), Finite Element Method (FEM), and MATLAB codes are used to model and characterize optical properties of these optical device. Finally the results are matched with experiments.

Modules identification for weighted biological networks

Dong Li
School of Computer Science

Abstract:
Physiological and disease processes are typically not driven by a single gene, but multiple genes that interact within molecular modules or pathways. How to identify a group of genes involved in a biological process, i.e. modules identification from biological networks, has become a central task in system biology. Especially when the network is big, modules identification can be computationally intensive. In the past summer, we participated in Disease Module Identification DREAM Challenge and applied several algorithms to find meaningful modules enriched by GWAS datasets. The algorithms and BEAR platform helped us to get tied for second place.
https://www.synapse.org/#!Synapse:syn6156761/wiki/407453

Gravitational Waves and Gaussian Processes - Predicting the Lives of Binary Stars

Jim Barrett[1]
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Abstract

On 14th September 2015 scientists detected gravitational waves for the first time. Around 1.3 billion years ago, two black holes spiralled towards each other and merged, causing ripples in the very fabric of space-time. These ripples travelled through the universe at the speed of light until they reached earth, where they distorted the space inside the Advanced Laser Interferometer Gravitational Wave Observatory (aLIGO) experiment for a fraction of a second. From just this short observation, we have been able to learn a lot about the original black holes. However, this raises an important question; how did the black holes get so close to one another in the first place?

"Compact Object Mergers: Population Astrophysics and Statistics" (COMPAS) is software we have been developing at Birmingham to answer exactly this question. COMPAS focusses on a process known as isolated binary evolution, where basic idea is to put two stars orbiting one another and let them evolve. The stars will interact with one another through a variety of physical processes and, if the right combination of processes occur, they may form a pair of black holes which would merge and be detectable here on earth.

The problem is that such systems are incredibly rare. It can take many CPU hours to build up a statistically meaningful sample of interesting objects. If we want to explore modifications to our models, the problem quickly becomes computationally intractable. I have been exploring the application of various machine learning and statistical techniques to create an emulator; an algorithm which is able to predict the outcomes of simulations we haven't run yet, given the ones we have.

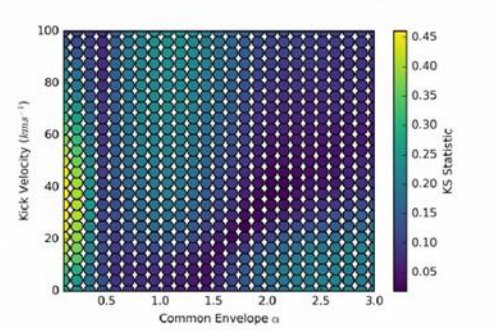

Figure 1: Plot showing how the distribution of a well measured combination of the black hole masses changes with two different physical parameters

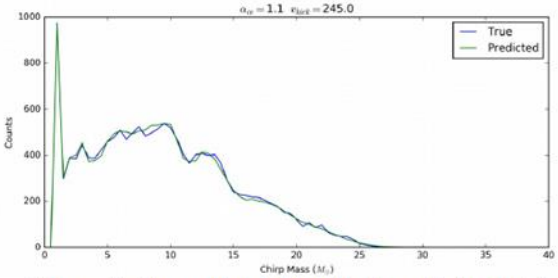

Figure 2: An emulated distribution of simulated binaries. The x-axis shows a well measured combination of masses and the y-axis shows the number of systems in that bin

Detection of a Change in Panel Data

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Lajos Horva'th
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Abstract

In this paper we provide a new procedure to test a change in the panel data model $y_{i,t} = \mathbf{x}_{i,t}^T(\boldsymbol{\beta}_i + \boldsymbol{\delta}_i I\{t \geq t_0\}) + e_{i,t}$, $1 \leq i \leq N$ and $1 \leq t \leq T$ under the no change null hypothesis against the alternative that the regressor in the i[th] panel changes from $\boldsymbol{\beta}_i$ to $\boldsymbol{\beta}_i + \boldsymbol{\delta}_i$ at unknown time t_0. We only assume that $N \to \infty$, but T is fixed. For Monte Carlo simulation, the wild bootstrap is employed to obtain the distribution functions of the test statistics. The simulation shows the test has the right rejection rate under the null and the power under the alternative. We apply our method to find changes in the US mutual funds performance.

Atomistic Simulation of the Defect Chemistry and Properties of Mixed Oxide Nuclear Fuel

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Abstract

An investigation of intrinsic point defects of nuclear fuel using the Buckingham potentials [1] and the Mott-Littleton methods was carried out using General utility program lattice (GULP) codes and the Shell model [2] [3]. The mean field approach [1] was used to conduct various simulations replicating pure uranium dioxide UO2, Mixed oxide fuel MOX UxPu1-xO2 and pure plutonium dioxide PuO2. The mean field approach was found to be the most efficient way of finding the mechanical and physical properties of any crystal structure.
Findings from the simulations showed that the mechanical properties of nuclear fuel all have a linear trend with an increase in plutonium concentration which verifies the Vegard's law. More so, the binding energy of the material was calculated and found that the defects formed prefer to remain as cluster defects rather than point defects. The fission products generated upon irradiation of the nuclear fuel pellets was investigated for Barium Ba and

Strontium Sr this is shown in figure 2. It was found that when these products are generated in the nuclear fuel Sr remain as an interstitial and Ba as vacancy. However, this method fails when investigating the defect energy of the crystal structure as shown in figure 1.

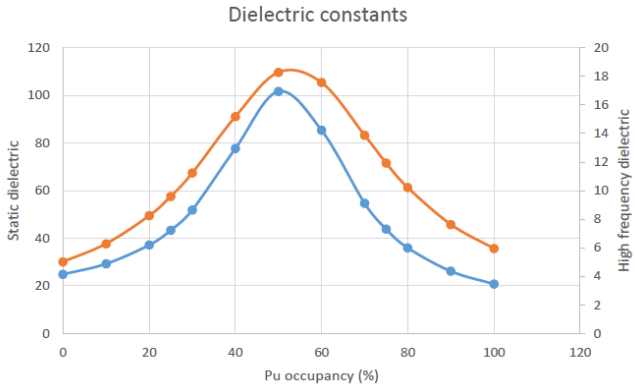

Figure 1 dielectric property of uranium dioxide.

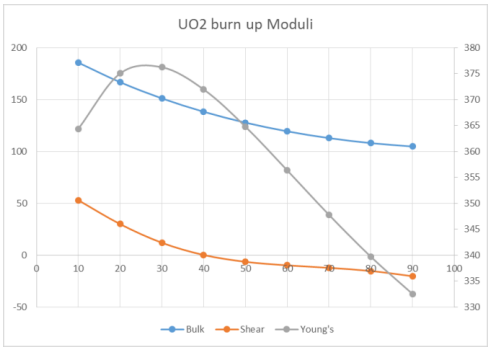

Figure 2 Burnup moduli of a nuclear fuel.

References

[1] D. S. Mark and R. A. Jackson, "Derivation of enhance potentials for uranium dioxide and the calculation of lattice intrinsic defects properties," *Journal of Nuclear Materials*, vol. **406**, pp. 293-303, 2010.
[2] K. Govers, L. Lemehov, M. Hou and M. Verwerft, "Comparison of interatomic potentials for UO2 Part I: Static calculations," *Journal of Nuclear Material*, vol. **366**, pp. 161-177, 2007.
[3] J. D. Gale and A. L. Rohl, "The General Utility Lattice Program (GULP) , Molecular Simulation," *Journal of Molecular Simulation*, vol. **29**, no. 5, pp. 291-341, 2003.

Discrete multi-physics: a mesh-free approach for modelling the hydrodynamics in flexible biological valves including the formation of solid aggregates

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Introduction

Computational fluid dynamic (CFD) simulations of biological valves have steadily improved over the years; however, procedures accounting for the formation of actual solid aggregates, such as calcifications or clots, have not been implemented yet. At the same time, researchers have also devised mathematical models for clot formation and growth; however, these models have been developed independently and are not usually associated to the dynamics of the valve.

Mesh-free methods are usually considered viable alternatives to traditional modelling, but have never enjoyed the same popularity of mesh-based techniques. Many mesh-free methods have been developed only in relatively recent years and offer, to the potential user, less available information, experience and software. On the other hand, a specific sub-set of mesh-free algorithm (e.g. the Coarse-grained Molecular Dynamics (CGMD) and the Smoothed Particle Hydrodynamics (SPH)) share a common particle-based framework that makes particularly easy their linkage in multi physics problems.
Our discrete multi-physics approach is based on the so-called discrete multi-hybrid system (DMHS). This technique combines various mathematical models to achieve a representation of fluid-structure interactions and solid-liquid systems. Here, we apply the same approach to biological valves including the formation of solid aggregates in the flow and at the membrane surface.

Methods

In this study, models for solid contact, or for fluctuating hydrodynamics are not necessary; consequently, the coupling is limited to SPH (liquid phase) and CGMD (solid phase).

Kernel interpolation [1]:

$$f(r_i) = \sum_j m_j \frac{f_j}{\rho_j} W(r_i - r_j, h) \quad (1)$$

Bending and spring network [2]:

$$U_{bond} = k_b(r - r_0)^2 \quad (2)$$

$$U_{angle} = k_a(\theta - \theta_0)^2 \quad (3)$$

Results

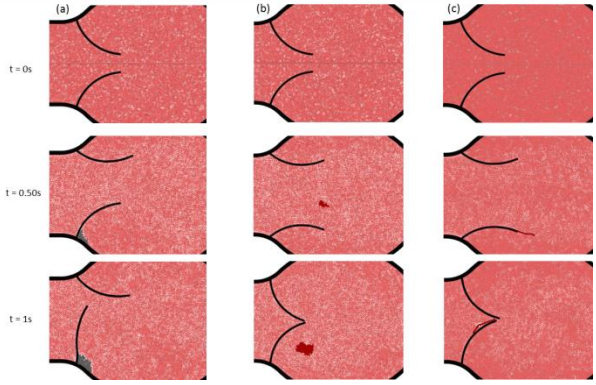

Fig 1. Formation of solid aggregates in biological valves: (a) 'calcification', (b) 'free clot' (c) and 'filiform clot'.

Discussion

Discrete multi-physics can tackle, with relatively little effort, problems that are considered very challenging with mesh-based multi-physics. By taking advantage of its mesh-free nature, this approach demonstrated the capability to easily implement each node (Particle) separately and thus to realistically mimic deformation of leaflets, in particular during a backward flow.
Moreover in certain circumstances, it is more than a mere alternative to traditional modelling. To the best of our knowledge, this is the first study to directly account for the hydrodynamics, the membrane deformation and the formation of solid aggregates at the same time and, as such, it has the potential to open a new prospective to the modelling of biological valves.

References

Monaghan, J. Computational Physics, 399-406, 1994.
Alexiadis A. (2015a), PLoS ONE 10: e0124678.

Participated posters topics

1- A. A. Tomlinson and N. K. Wilkin

What do Plant Stems and Repulsive Particles on a Cylinder Have in Common?

2- A.A. Tolipov, Dr.Khamis Essa

Development of a Finite Element (FE) model for a Multi-Point Forming (MPF) of a sheet metal using a mesh-type elastic cushion

3- Can Bıyık, Professor Miles Tight, Dr Michael Burrow

A comparative research on perceptions of future sustainable transport interventions among different groups in Turkey

4- George Rowley

Optical detection of corrosion on intermediate level nuclear waste containers

5- Guanbo Jia, Shan He, Xin Yao and Peter Tino

Overlapping Community Detection in Complex Networks Using Differential Evolution and Multimodal Optimization

6- Jack Gartlan and Prof. Nicola Wilkin

Gravity's Rainbow

7- John Hey, Emily Doyle, Yuting Chen and Roy L. Johnston

Structures and energy landscapes of micro-hydrated Sulfite and Chlorate clusters

8- Kanika Gupta, Dr. Mark S.D. Read and Prof. Colin Greaves

Simulation Techniques for Modelling Schafarzikite and Related Materials

9- Maha Al Mumiaz

Modelling the Impact of Road Construction on Lands Values

10- Mohamed Elflah and Marios Theofanous

Structural Performance of stainless steel beam to column joints

11- Nathan Palmer

Computational Modelling of PuO2 Structure and Defects

12- Richard Bassett, Xiaoming Cai, Lee Chapman, Clare Heaviside, John E. Thornes

Semi-idealised urban heat advection simulations using the Weather Research & Forecasting mesoscale model

13- S. Al-Najjar, N. Nirmalkar, M. Barigou

Mass transfer from spherical particles in tandem arrangement in Visco-Plastic Fluids

14- Saif Alzabeebee, David N Chapman1 and Asaad Faramarzi

Numerical Investigation of the Bedding Factors for Concrete Pipes under Deep Burial Conditions

15- Z. T. Al-Sharify and M. Barigou

Using CFD simulations and Positron Emission Particle Tracking to Study the Mixing of Shear Thickening Fluids in Stirred Tank.