
Birmingham Environment for Academic Research
Case studies—Volume 2
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Birmingham Environment for Academic Research

Case Studies Volume 2

Compiled by
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IT Services
University of Birmingham
March 2014

http://epapers.bham.ac.uk/1887
www.birmingham.ac.uk/bear

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Acknowledgements

We would like to thank all the people who contributed to this publication.

Most of the work is presented at
https://intranet.birmingham.ac.uk/it/teams/infrastructure/fm/bear/projects/index.aspx

Picture of database taken from http://commons.wikimedia.org/wiki/File:Wikiproject_database_icon.png; used under Creative Commons Attribution licence for Analysing datasets from electronic primary care patient records for epidemiological studies by Ronan Ryan.

Abstract

This collection of case studies was brought together to showcase the extent and diversity of research that is being done using the University's high performance computing cluster called BlueBEAR in addition to local compute facilities.

BlueBEAR is a key component of the University of Birmingham's Environment for Academic Research (BEAR), providing compute power and specialist applications free to enable staff and students to delve deeper into their research. Upgraded in 2012/13, the cluster includes some large memory nodes and a GPGPU service alongside standard compute nodes. Visit the web site to see details of the other services available, including Windows HPC www.birmingham.ac.uk/bear .

Theory and experimentation have traditionally been the foundation of research. BEAR now offers additional tools; computer based modeling and simulation, using BlueBEAR and visualisation in BEARView. These new methods can be used to underpin or enhance the physical and theoretical research. Pragmatically, on occasion, computer based modeling is the only way e.g. colliding galaxies, nuclear explosions or pandemics, where factors such as practicality, safety and cost are prohibitive.

We are proud to say that this is just a small set of case studies, taken from the vast and rich vein of research that is being done on BlueBEAR and across the University in general.

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Preface

In the summer of 1987, months before he received the Nobel Prize for his contributions to growth theory, economist Robert Solow famously quipped that, “you can see the computer age everywhere but in the productivity statistics.”

I hope that Solow would regard this second volume of research projects made possible by Birmingham’s BEAR as a convincing refutation of his observation. I also hope that there will not be too many more of these volumes, in the same way that we don’t have case studies of research conducted using the library, or written up with a word processor.

Indeed, the case studies presented here make clear the scope of research now taking place with the assistance of powerful computing clusters: from nanometer scale atomic interactions, through zebrafish embryos to the earth’s climate and – finally – to the dynamics of whole stars, Birmingham’s ongoing investment in high-performance computing is shedding light across the whole spectrum. And in case all this feels a bit too new-fangled, I was pleased to note that the topic receiving perhaps the most research support from BEAR is that great British passion, the railway.

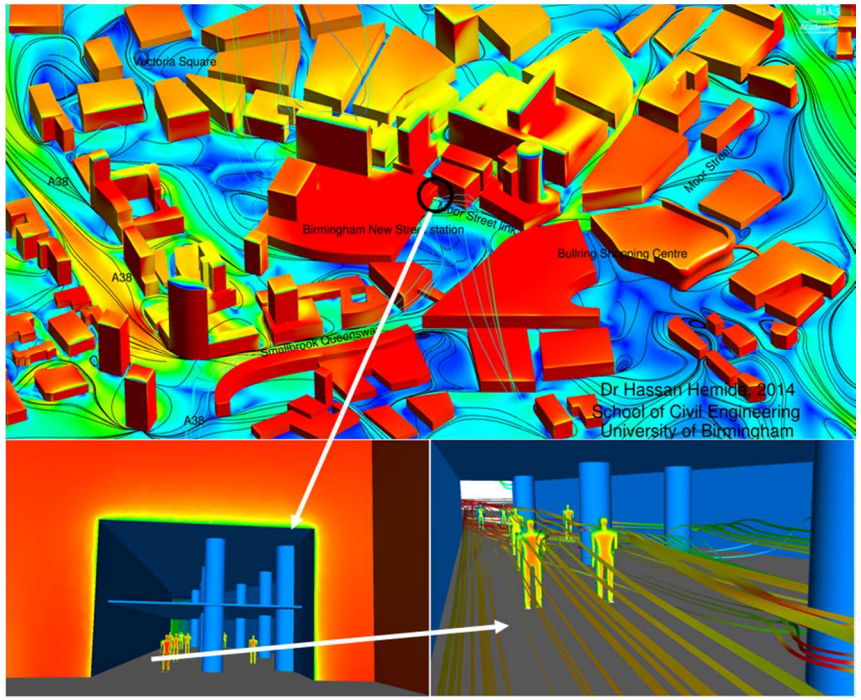
Finally, while Asimov’s portrayal in The Machine That Won The War may be a bit too cynical, he is right to recognise that high performance computers are only as good as the staff to support them. Behind each conclusion reached and high-resolution graphic displayed in the coming pages, they can be found quietly in the background. I am sure that all of BEAR’s users would view their successes as owing as much to John, Carol, Paul, Jon, Simon, Laurence, Earl and Aslam as to BEAR itself.

Dr Colin Rowat
Department of Economics
Chair BEAR Management Group

UNIVERSITY OF BIRMINGHAM

Harvesting wind energy from Birmingham New Street train station

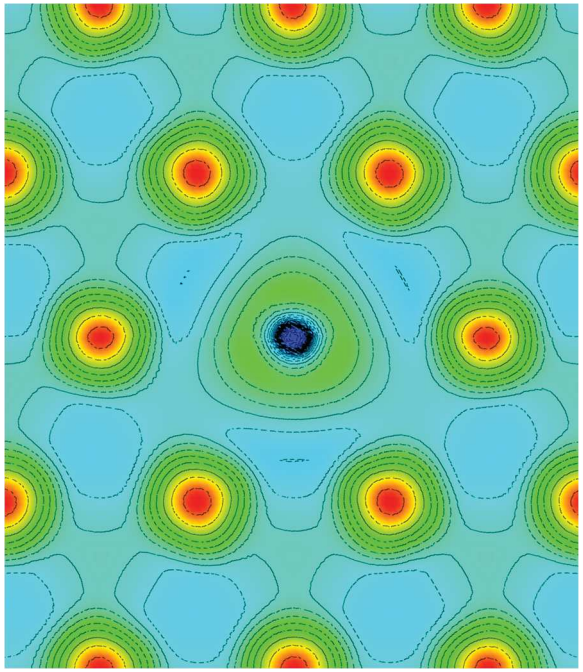
Birmingham New Street train station has been renovated and will be fully opened in 2015 to be a world class transport, shopping and community hub in the heart of the city of Birmingham. The station is expected to be the busiest station outside London and the busiest interchange station in the UK. Once the project is finished in 2015, there will be 36 escalators and 15 new lifts—reaching each platform. These new infrastructures are expected to consume considerable amount of energy. Thus a sustainable and renewable source of clean energy is needed in order to reduce the station CO2 emission.



It is well known that micro wind turbines are an emerging technology for energy generation in urban environment and there is a high potential of harvesting wind energy from around the station using these technology. In particular, it has been noticed a high draft of wind in the Moor Street link (a link between the station and the Moor Street station as part of the renovation project). This research uses the Computational Fluid Dynamics (CFD) as a tool to investigate the possibility of installing micro wind turbines in the link. The wind distribution in the Birmingham City Centre will be obtained including the Moor street link and hence the amount of energy that could be harvesting using the micro wind turbines will be calculated.

Hassan Hemida
School of Civil Engineering

Solute effects on high-temperature properties of Ni-based superalloys



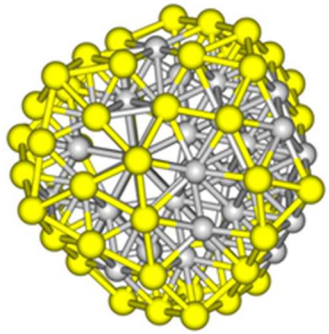
In many applications, the mechanisms that lead small concentrations of solute atoms to dramatically improve the properties of advanced alloys are still unclear. This is the case of rhenium in Ni-based superalloys, or silicon in some Ti-alloys, or many other elements in Mg- and Al-alloys. Understanding these mechanisms is essential to the development of new alloys, and the improvements in performance for these materials lead to many beneficial effects. Gas turbines and jet engines, for example, are limited by the operating temperatures of currently-available Ni-based superalloys, and increasing their operating temperature would result in considerable fuel savings. By some estimates, a 30C increase in operating temperature corresponds to a 1% increase in efficiency, and can lead to £12m savings in fuel alone over the lifetime of a single large gas turbine. Similarly, Ti-alloys capable of withstanding higher temperatures may allow for lighter components in come parts of a jet engine, and weight savings in the jet engine are multiplied four-fold when considering the resulting weight savings in the wings and wing-box structure.

Solute atoms may affect the mechanical properties of alloys in two distinct manners. First, they may change the microstructure of the alloy, promoting or hindering the formation of phases, or affecting the morphology of the microstructure. A change in microstructure results in different dislocation mechanisms and deformation processes. Second, they may directly affect the motion of dislocations. This means that, if an optimal microstructure is selected, the composition of the alloy may be tweaked to improve mechanical properties even further. This is the ultimate research focus of the Mottura group at the University of Birmingham.

In this work, ab initio modelling methods are adopted to simulate how solute atoms affect the motion of dislocations within the microstructure typically observed in single-crystal Ni-based superalloys. Density functional theory is used to investigate the energetics of vacancy diffusion within the microstructure, since vacancy diffusion is believed to affect the rate of dislocation overcoming obstacles in their path. Kinetic Monte Carlo simulations will be adopted to study whether synergetic effects between different solute atoms produce desired mechanisms.

Alessandro Mottura
Department of Metallurgy and Materials

Modelling the structures of bimetallic nanoparticles
Nanoscale Physics Research Laboratory

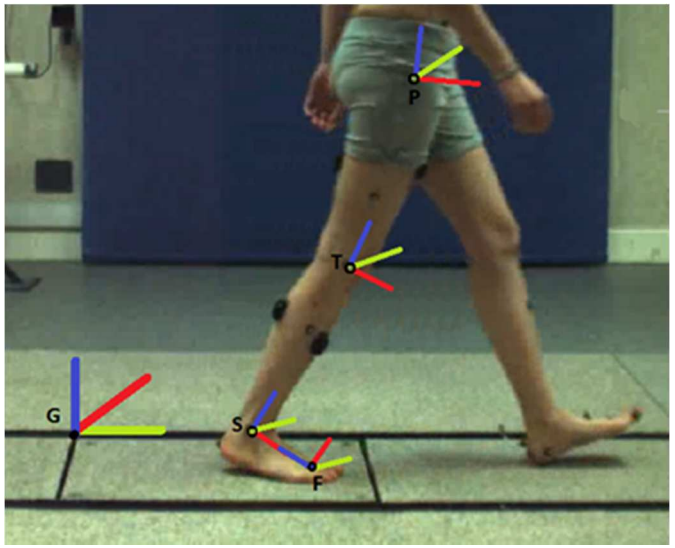


Bimetallic nanoparticles have received considerable attention in the past few years due to their unique performance in fields such as nanocatalysis, optics and medicine. Gold-palladium (AuPd) nanoparticles are one of the most attractive systems, due to their promising activity in catalysis. This superior performance has been attributed to both geometric and electronic effects. A better understanding of the properties of these nanoparticles requires the analysis of metal-metal interactions, segregation and energetics effects at the nanoscale in order to gain insight into possible chemical reaction routes. Theoretically, modelling of bimetallic nanoparticles can be performed either at the empirical level or using first principle approaches based on Density Functional Theory (DFT). Empirical potentials have been widely used to predict the structures and energetics of nanoclusters. However, since important modifications can be introduced by electronic effects, it is important to verify the predictions of empirical potentials using first principles calculations. Theoretical analysis of these nanosystems aims to search for the most stable structures on the potential energy surface, since they are the most promising candidates for the actual nanoparticle structures generated in experiments.

An extensive search of configurational space has been performed using a genetic algorithm coupled with empirical potentials to model the inter-atomic interactions. At the empirical level, we have found that mixed AuPd clusters configurations tend to be more stable than core-shell morphologies. However, the order tends to be reversed at the DFT level, where Pd(core)Au(shell) morphologies are more stable energetically. The process of optimization of chemical ordering has shown that structural motifs such as decahedra, and delete (face centred cubic packed) truncated octahedra have enhanced stability compared to motifs such as icosahedra. We have found this to be in agreement with our experimental analysis, based on the use of Scanning Transmission Electron Microscopy (STEM), of AuPd nanoparticles generated by vapour deposition.

Alina Bruma
School of Physics and Astronomy

Effect of laterality on symmetry/asymmetry of human lower limb based on mechanical model



One of the challenging issues in robotic rehabilitation is mapping the movements of the healthy leg to the affected leg by a robot in bilateral mode. Thus, the consideration of the symmetry/asymmetry between the two lower limbs has a significant effect on the success of the robot-assistive therapeutic treatment.

The purpose of this study is to establish the asymmetrical behaviour of the joints between the lower limbs for able-bodied during a gait cycle. Gait analysis performed for 28 healthy adults of both genders. A force plate was used as a target to study the laterality.

Then, the lower limb was modelled as a series of four links representing pelvis, thigh, shank and foot segments, connected by three universal rotary joints representing hip, knee, and ankle joints. Based on kinematic formulation for the proposed lower limb model, MATLAB codes have been developed to read Vicon`s data in order to calculate the joints' angles for the left and right legs.

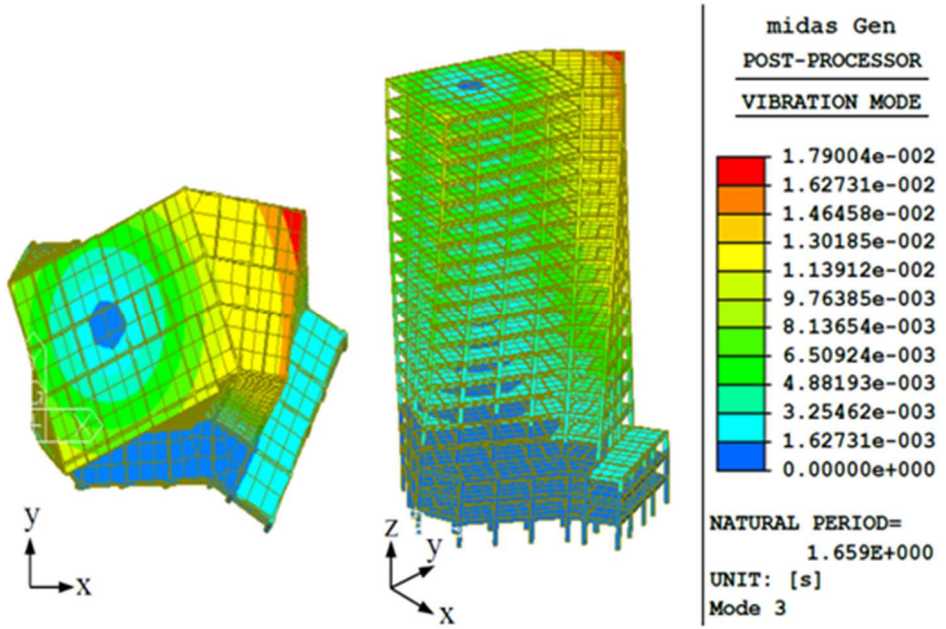
In order to compare the symmetry/asymmetry of joints rotation statistical t-tests were applied using a developed Minitab software. The results have been validated against the measured data using Vicon system based on t-test and $P>0.05$. The $P>0.05$ suggests the presence of relation between laterality and symmetry for the right side of the body. The outcome of this study will provide useful information to design a cognitive control system for the proposed robotic rehabilitation system.

Alireza Rastegarpanah
School of Mechanical Engineering

Effect of the Plan and Mass Irregularities of multi-storey RC Buildings on the Seismic Behaviour of the NSCs

Multi-storey structures with complicated geometries have become widespread due to novel materials, advanced construction techniques and modern architectural requirements. In such structures with plan and/or vertical irregularities, significant torsional effects induced by moderate and strong earthquakes are usually responsible for the damage to the structure and non-structural components (NSCs).

To evaluate the seismic behaviour of the NSCs attached to the P-structures having different cases of plan and/or mass distribution along the height of complicated reinforced concrete (RC) structures, the effect of torsion and the structural ductility of the P-structures were investigated. However, the structural layouts and composite materials used in present-day P-structures are too complicated for an analytical solution to be available and research studies addressing the seismic response of NSCs attached to such P-structures are scarce. One possible solution to bridge the knowledge gap in this area is to use advanced numerical methods such as finite element (FE) analysis. The FE package MIDAS Gen ver. 3.1 is adopted in the nonlinear analyses of the primary-secondary systems.



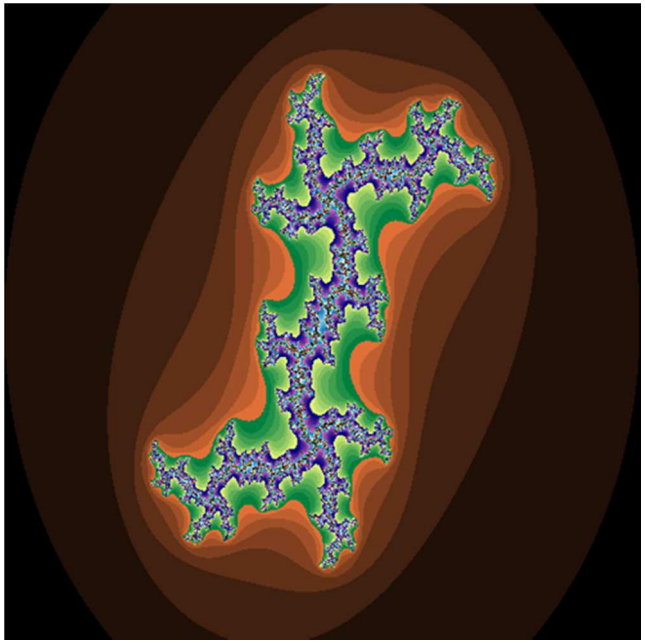
The NSCs considered in the investigation are lightweight acceleration-sensitive mechanical, electrical or medical equipment such as those found in industrial, commercial or healthcare buildings respectively. Normally, only the fundamental modes of such NSCs are of importance therefore they can be modelled as vertical cantilevers fixed at their bases with lumped masses on their free ends.

Comparison between the FE results and EC8 recommendations suggests that, when the fundamental periods and heights of the NSCs match those of the P-structures, EC8 underestimates the dynamic responses of the NSCs mounted on the flexible sides of irregular RC P-structures with a mean predicted-to-numerical ratio in range between 0.42 and 0.72. The perceived cause of this discrepancy is that EC8 does not take into account the amplification in the dynamic response of NSCs caused by the torsional behaviour of RC P-structures.

Ayad Aldeka
School of Civil Engineering

Parametric sweep for Parallel Robot

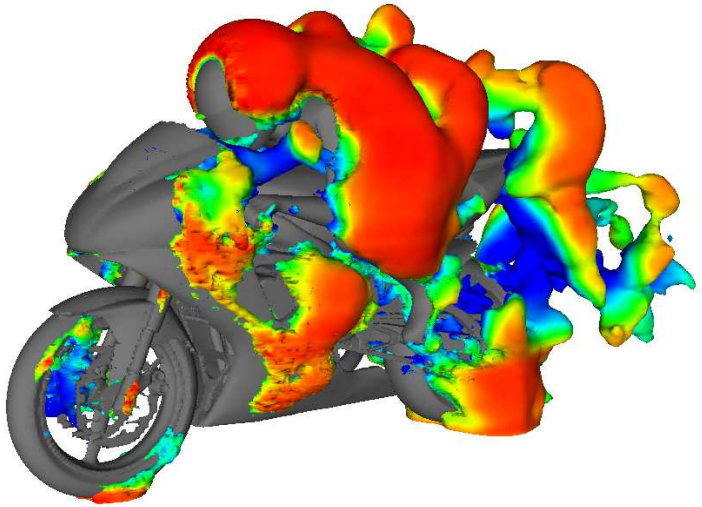
This research is about the verification of non-singularity position for Parallel Robot's end-effectors, or simply known as workspace. It is based on a successful development of a 3d-Python visualization system. Basically, it can perform parametric search based on general test such as cubic and spherical sweep, and also advanced test such as strategic sweep with configurable dimension and direction in the form of controllable test planes.



This plane is indeed a slice of information within the workspace. Various LSystem random generators populate the plane with test positions. The 2D LSystem is positioned and orientated to cover the assumed space covered by the workspace based on rotation around center-point, parallel arrangement to form a cubic grid or interpolation done between various slices. Interpolation builds the relationship between random generated positions to produce 3-Dimensional parametric sweep positions. Other 2D to 3D method has been examined which includes loft, extrusion and quaternion methods. Other advanced methods mentioned in this paper includes spiral 3D, Hilbert 3D and Marching Cube 3D. The workspace validation is done using weighted ranking based on Grassmann and is further extrapolated by using Simplex and Trilinear to verify the condition for 'going into' and' leaving' of a position condition. An example lower limb rehabilitation test result is included to demonstrate the system capability.

Che Zulkhairi Abdullah
School of Mechanical Engineering

Flow investigation around a motorbike in crosswinds



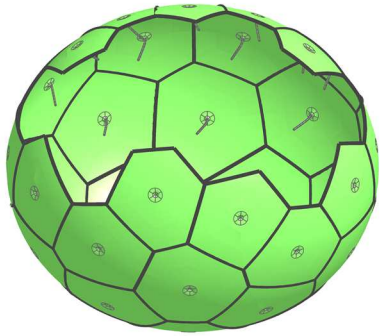
Improving the aerodynamic performance of a motorbike is important to reduce fuel consumption and to improve manoeuvrability. In addition, when cruising into crosswinds the motorbike and rider might experience further aerodynamic forces that could severely influence its stability. Therefore the aim of this study was to investigate the flow structures around a motorbike and the corresponding aerodynamic responses in crosswinds.

Numerical computations were employed to solve the flow around the motorbike subjected to different crosswind yaw angles: 0, 15, 30 and 60°. The Computational Fluid Dynamic (CFD) software on BlueBEAR gave the opportunity to run a large number of parallel computational simulations.

The simulation results allowed investigating the time-averaged and transient flow structures around a motorbike subjected to crosswind. The time histories of the aerodynamic forces were used to reveal the characteristic frequencies of the flow around the motorbike for the different crosswind yaw angles. This analysis showed that stronger vortex shading exists at larger crosswind angles. In conclusion, this study has shown that CFD analysis of a motorcycle in crosswind gives comprehensive information which may lead to improvements in the performance and safety of motorbikes in future.

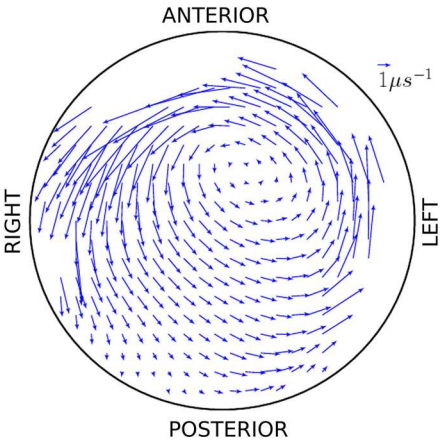
Daniella Fintelman
School of Sport, Exercise and Rehabilitation Sciences

The fluid mechanics of symmetry breaking in the zebrafish embryo.



Most people are familiar with the fact that their heart appears on the left, and this type of organised asymmetry of the internal organs occurs throughout the vertebrates and is necessary for healthy development. But how does the embryo, initially a symmetric clump of cells, know the difference between right and left?

This research focuses on understanding the key initial step in this process: cilia-driven fluid flow. After the front/back and head/tail axes have broken, a microscopic fluid-filled enclosure referred to as the 'node' in mammals, or 'Kupffer's vesicle' in fish appears. This enclosure contains cilia, tiny hair-like structures which are biased to rotate in a particular direction, creating a left-right asymmetric fluid flow. The combination of geometry and fluid mechanics converts molecular chirality (rotational handedness) to lateral asymmetry.



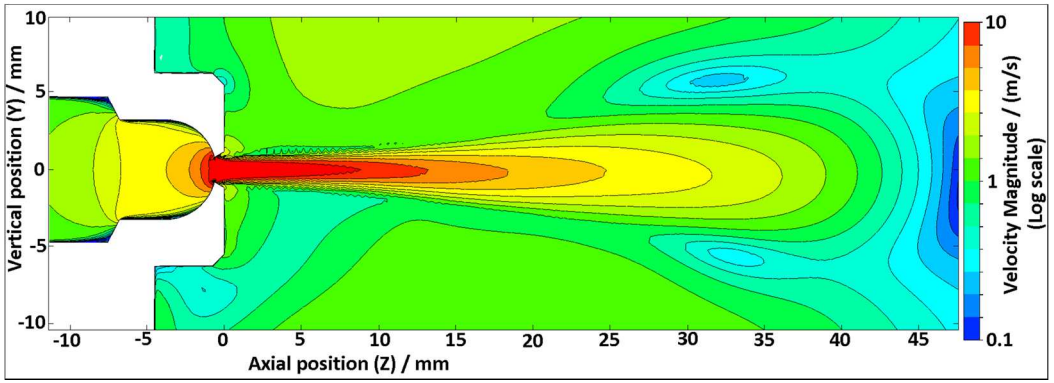
Developmental biologists are particularly interested in studying the process in zebrafish as a model organism. The Kupffer's vesicle in zebrafish exhibits considerable complexity, with great variation in cilia positioning, length and rotational behaviour both within and between embryos. The flow also exhibits considerable three-dimensional spatial and temporal complexity. Dr Susana Lopes and colleagues at the Gulbenkian Institute, Lisbon, Portugal are conducting high speed imaging of both embryos to investigate what properties of the flow are critical to symmetry breaking, and how the flow is converted to asymmetric development - either through transport of signal molecules or through fluid mechanical stresses. Our group in Birmingham has created a mathematical model of the complex three dimensional architecture consisting of approximately 8000 surface elements (as shown in the figure, upper panel), leading to a matrix system with over 600 million entries repeated over hundreds of timesteps for every mesh. The BlueBEAR2 cluster allows us to generate meshes and simulate the fluid flow and particle transport (lower panel) in model Kupffer's vesicles, with many different randomly-generated structures, reflecting the heterogeneity of the natural system. These large scale simulations allow us to define the critical statistical properties underlying normal and abnormal flow.

Our published work has already allowed us to reconcile two competing hypotheses on the orientation of cilia around the three dimensional structure. Current work focuses on understanding the role of genes controlling cilia length, and the influence of a subpopulation of cilia observed to have different beating behaviour.

Dave Smith
School of Mathematics

Data analysis for Sonolator results

Determine how the Sonolator makes emulsions and disperses fluids, and apply the findings to industry. CFD simulations are easier to carry out than PIV experiments, but require validation against PIV for confidence in results. ANSYS ICEM was used to build the Sonolator geometry corresponding to PIV experiments. ANSYS CFX programs were used to setup, process and post-process the simulations.



The Particle Image Velocimetry (PIV) Experiments PIV measures flow speeds in the Sonolator. Many photo pairs were taken. Each image pair had delay of ≈5µs. 32x32 pixel squares between image pairs were cross-correlated to give velocity vectors at a point in time . The mean and standard deviation were derived at each point to obtain average flow fields and turbulence profiles. Insight 4G software was used to process raw images, data files processed in MATLAB and Excel.

The CFD results were checked against the PIV results in order to validate that the CFD simulations were accurate. PIV and CFD results were summarised using Excel pivot tables to give velocity vectors every 1/3mm, since original result spacing was less regular. With the same spacing, Excel was used to generate comparison graphs.

David Ryan
School of Chemical Engineering

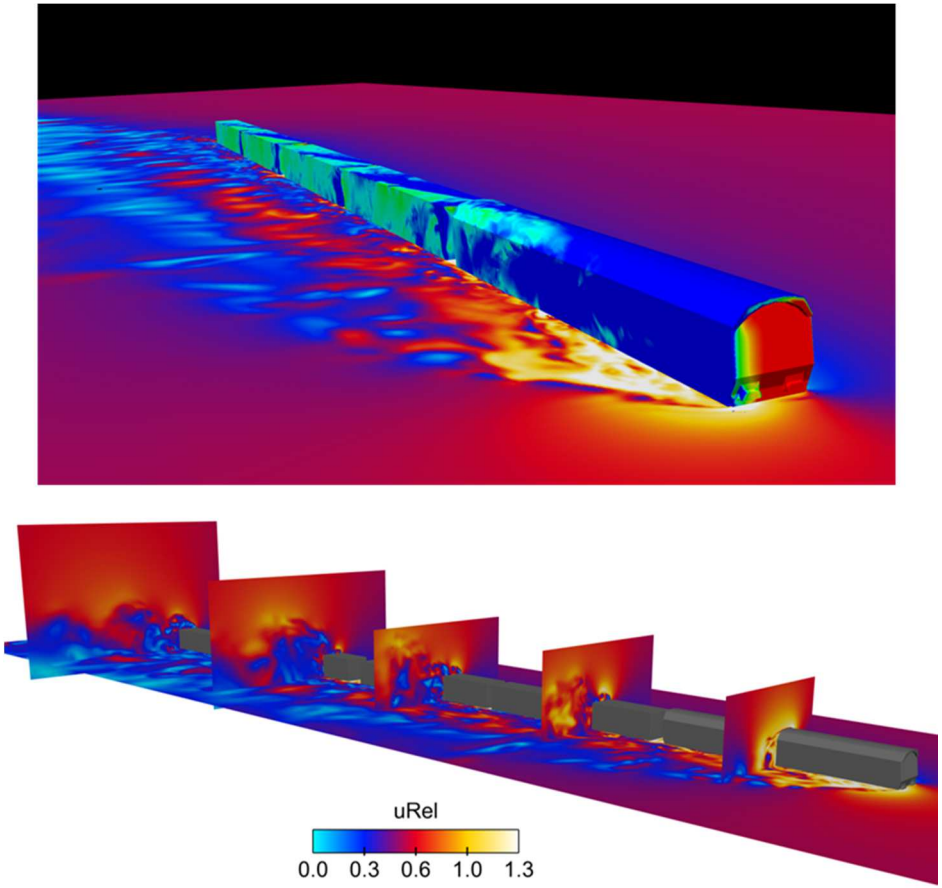
A numerical investigation of the effect of crosswinds on the slipstreams of freight trains

When a train moves through the air, a region of air moves along with it at approximately the same speed; this region is known as the 'slipstream'. Aerodynamic forces increase nearly proportionally to velocity squared ergo any increase in train speed could drastically increase the wind-induced forces on persons and objects, on platforms or at trackside, leading to an increased risk of accidents occurring. Between 1972 and April 2005 there were 25 slipstream-induced incidents in the UK, involving pushchairs, luggage and people.

In experiments freight trains have been found to cause higher slipstream velocities than passenger trains even though they generally travel much slower. Freight trains were also found to be responsible for more object movement incidents than the faster-moving passenger trains.

Crosswinds have been shown to greatly increase the slipstream velocities measured on the leeward side of a freight train which in turn increases the risk to passengers and trackside workers.

A computational fluid dynamics (CFD) study is being conducted to investigate the effect that crosswinds have on the slipstream of a model-scale Class 66 locomotive with four container wagons in tow. These experiments are difficult to conduct at full-scale because of the variability of natural wind. CFD allows for a crosswind to be isolated and its effect on the slipstream behaviour to be better understood.



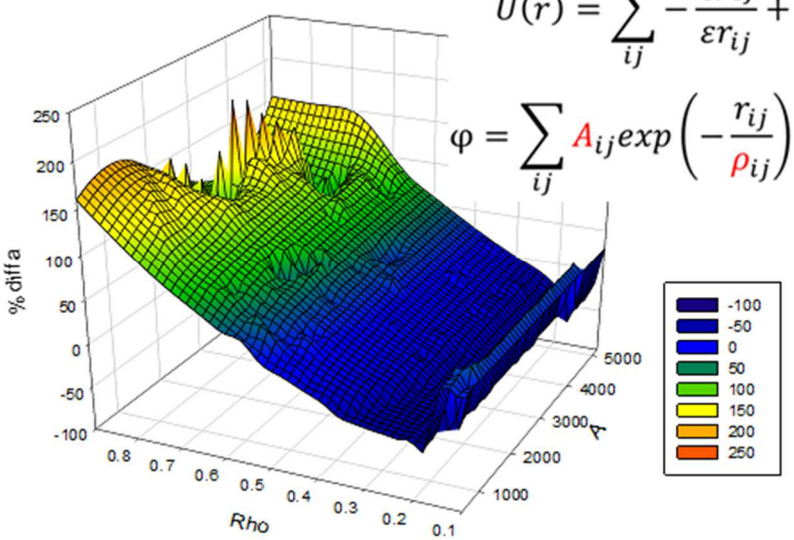
Dominic Flynn
School of Civil Engineering

Investigating radiation damage in materials for high level waste (HLW) immobilisation

In 2010 an estimated 14% of our global electricity production was supplied by nuclear power. The low CO_2 production and good green credentials help hit government targets to reduce emissions of greenhouse gasses. This combined with the high energy density of nuclear fuel relative to fossil fuels makes the expansion of nuclear energy an attractive prospect to meet the worlds growing energy needs.

$$U(r) = \sum_{ij} -\frac{q_i q_j}{\varepsilon r_{ij}} + \varphi$$

$$\varphi = \sum_{ij} A_{ij} exp\left(-\frac{r_{ij}}{\rho_{ij}}\right) - \frac{C_{ij}}{r_{ij}^6}$$



There are many challenges to overcome when considering the expansion of the nuclear industry including; site selection, availability of natural resources and the safety and disposal of increased quantities of radioactive waste. Some components of nuclear waste have half lives in excess of several hundreds of thousands of years. To investigate the stability of candidate wasteforms over these time scales a combination of experimental and computational modelling techniques are required.

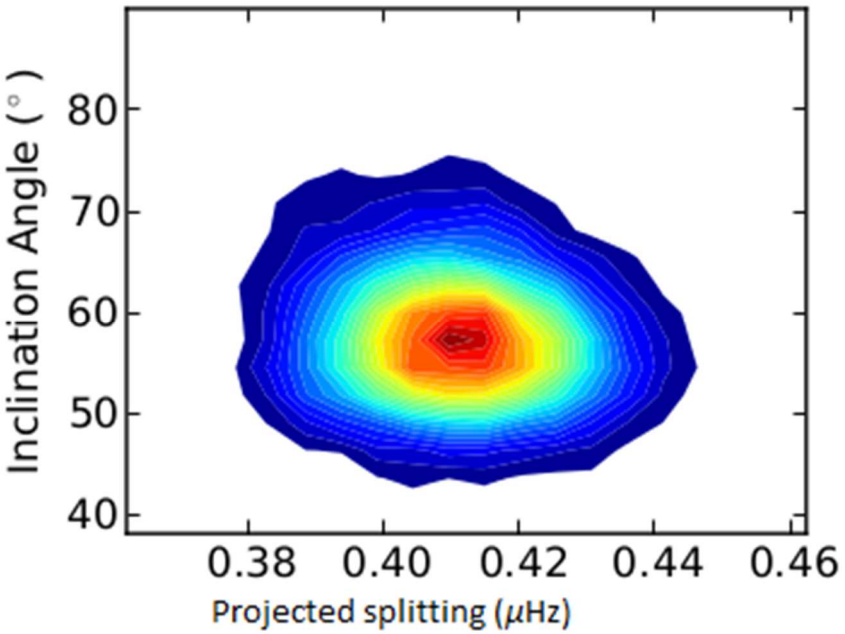
BlueBEAR offers the ability to develop new potential models through large capacity calculations, performing potential sweeps to produce sets of empirically derived potentials for the candidate system. These potentials can then be used to perform a wide range of more computational intensive calculations for example, simulating grain boundaries and surfaces to investigate nucleide migration pathways and leaching behaviour. Alpha decay events can be simulated in a molecular dynamics regime to assess the stability of the system to radiation damage. The damaged structure produced from these simulations can then be validated through comparison to experimentally irradiated samples, analysed by total scattering X-ray diffraction experiments.

Geoff Cutts
School of Chemistry

Measuring rotation in stars using asteroseismology

What is the future of our Sun? We can improve on the crystal ball by using a technique called asteroseismology on stars that are very like our Sun but older. The twin stars, 16 Cyg A and B, are very much like our Sun only around 2 billion years older. By measuring the rotation of these stars we can see the future dynamical state of our own star.

Asteroseismology is an excellent tool for revealing accurate and precise fundamental properties of stars (i.e. their mass, radius, and age) by studying the ways in which a star pulsates. More than that, using asteroseismology we can sense the internal structure and dynamics of a star. Perhaps the most exciting discovery is that we can use asteroseismology to estimate the rotation of many stars.



Sun-like stars have an outer convective envelope that generates broad-band acoustic noise which is trapped inside the star. The trapping of this sound provides the conditions for positive interference that produces delicate pulsations of the whole star - the whole star rings like a bell or a musical instrument. We have used the Kepler Space Telescope to measure the subtle changes in intensity caused by compressed or rarefied gas at the stellar surface, and from differences between prograde and retrograde intensity changes we have estimated the stellar rotation.

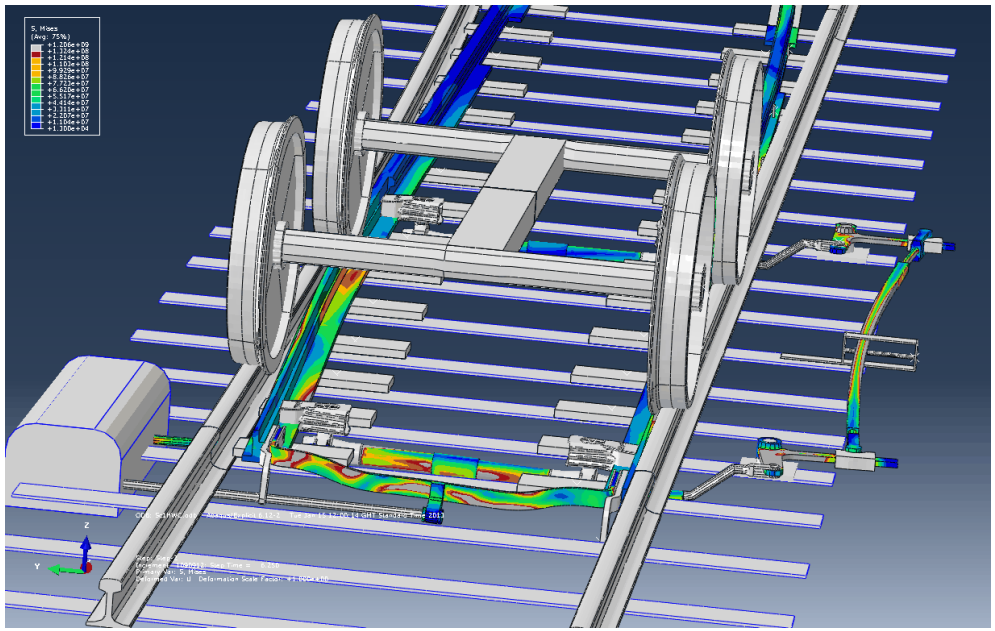
Estimating stellar rotation using asteroseismology is a computationally intensive task. We used BlueBEAR to run optimised Markov chain Monte Carlo algorithms with hundreds of free parameters to estimate the posterior probability distributions of the stellar period of rotation and the angle of inclination with respect to the line of sight. The results provided excellent constraint on rotation of the two stars.

We used our results to calculate the tidal time scale on which the large gaseous planet orbiting 16 Cyg B would tidally lock and the time scale on which the planet-star orbit would circularise. In addition, we were able to test relations of gyrochronology (the relationship between stellar mass, age, and period) producing a “decisive" result in a Bayesian model comparison.

Guy Davies
School of Physics and Astronomy

FEA of Rail Switches
Railway Research Centre

Current standards of switches require the locking force to have a maximum limit, such that should a train run through the switches whilst they are locked, the locking mechanism shall give way to allow the wheel flange to pass between the switch and stock rail without derailing. Two types of point operating equipment's (POE) running the switch were investigated: HW and the RCPL types.



The University of Birmingham has developed a finite element, FE, model capable of modelling the full switch. This model is used to investigate the performance of the switch for different run-through scenarios. The classifications of the rail switch are as follow C-type, left handed, shallow depth, RCPL and HW POE

The FE results show that a significant plastic deformation occurs on the stretcher bar and its attaching components such as bracket and drive bar as a result of the run-through scenario . These deformations are due to the rigid connection between the stretcher bar and the switch blade. Thus a new design of the stretcher is proposed by NR that allows for rotation between the stretcher bar and the blade reducing unnecessary stress in the mechanism.

The new mechanism contains:
* Polyurethane blocks allow for further movement to remove the rigidity from the mechanism.
* Increased diameter of the stretcher bar that gives greater strength.

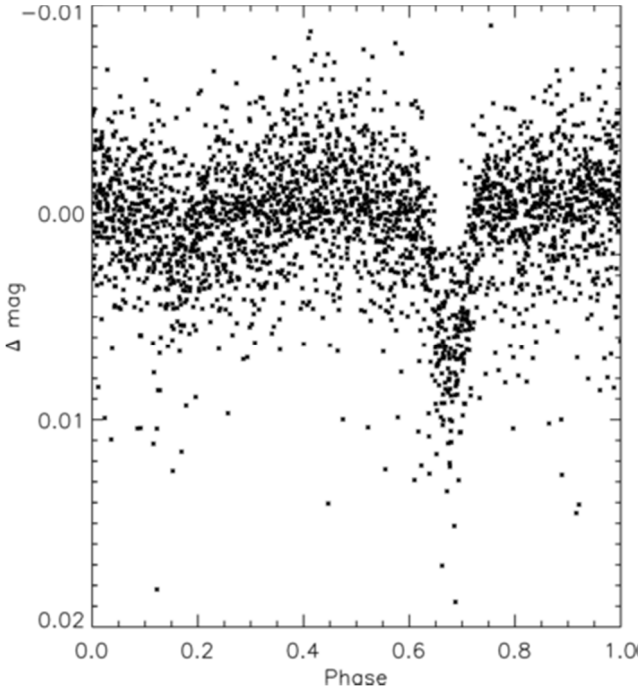
The initial results shows that a high degree of buckling occurs in the channel rod but no significant deformation has been observed in the stretcher bar.

Hassan Hemida
School of Civil Engineering

Stellar Light curves from the STEREO satellites

The two STEREO satellites are designed to monitor the Sun and to study material ejected from the surface of the Sun in 3 dimensions. The satellites do this by continually taking CCD images of the region near the Sun. A by-product of this is that we can monitor a large number (many tens of thousands) of stars for changes in brightness, to look for new variable stars, study the behaviour of known variable stars and even transiting extrasolar planets (that is planets orbiting other stars, where a small dip in light from the star is caused by the planet passing in front of the star.

This is a very considerable data analysis task - there are many tens of thousands of images to process, and often thousands of star in each image. Processing of the CCD frames to produce the light curves can be done in a parallel fashion and the multiple processors and large memory of Blue-Bear has been very important to this work. We have to perform accurate photometry (that is, measure the brightness of each star) and correct for any systematic trends in the data. The goal is to reduce the systematic (mainly associated with the instrument) noise levels down to as low a level as possible, in order to see small variations in the brightness of as many stars as possible.

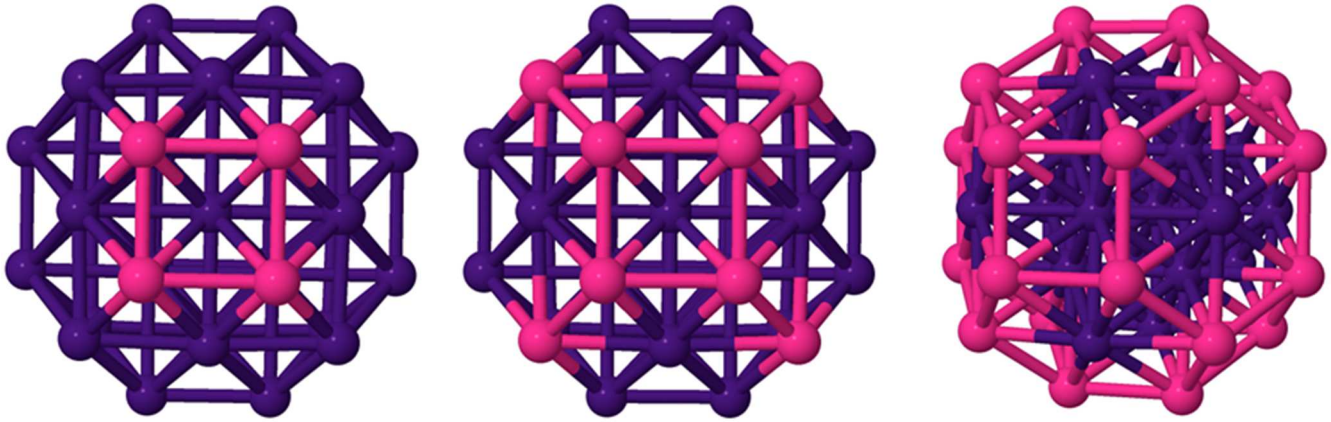


A sample light curve of a star, generated using BlueBEAR and STEREO data, showing a dip in brightness, caused by a transiting object. STEREO has found a number of these objects that are the subject of further study

Ian Stevens
School of Physics & Astronomy

The Free Energy Concentration Expansion Method for the Prediction of Compositional Order in Palladium-Iridium Nanoalloys

The free energy concentration method (FCEM) is a statistical mechanical method for the prediction of compositional structure in nanoalloys, capable of the compositional characterisation of clusters of up to 1000 atoms. The energetics required by FCEM are provided by the extraction of coordination dependent bond energy variations (CBEV) from six density functional theory (DFT) computed surface energies. The resources provided by BlueBEAR has aided in the computation of new energetics for the improvement and expansion of the model. DFT calculations were carried out using Vienna Ab-initio Simulation Package (VASP).



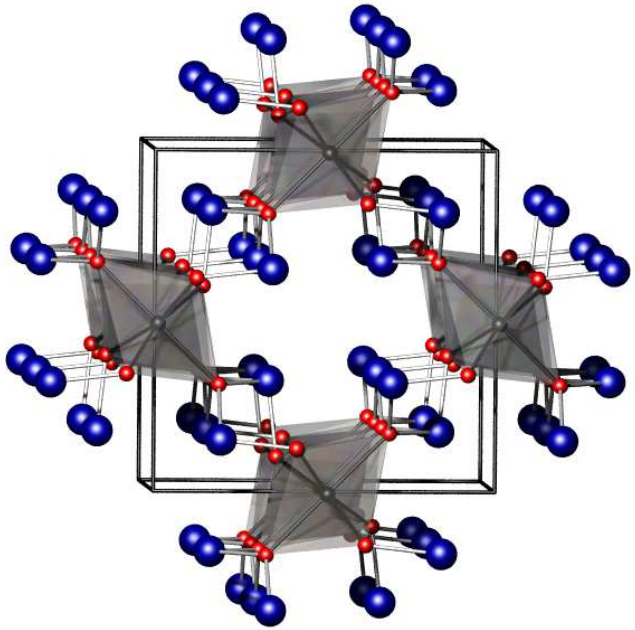
These newly computed energetics have allowed the calculation of compositional structure in a variety of palladium-iridium nanoalloys. BlueBEAR has been used to evaluate these predictions through comparison with predictions made using the Birmingham Cluster Genetic Algorithm. Structures from both methods were evaluated directly through DFT calculations. CBEV/FCEM calculations showed a high degree of accuracy, especially for larger sizes.

In the future the predictions made by CBEV/FCEM will be used as a starting point for the study of catalytic activity in palladium-iridium nanoalloys.

Jack Davis
School of Chemistry

Computational study of magnetic ordering in low-dimensional crystals

Magnetism is a complex phenomenon, and experimental results are often difficult to fully explain. As such, the use of computational modelling can be used to enhance our understanding of these problems, and potentially direct research into new materials for use in magnetic devices (such as computer hard drives). One active area of research is low-dimensional materials, where magnetic interactions occur primarily in one direction within the solid. If the properties of such materials can be chemically adjusted, such materials could be used in a wide variety of applications to provide 'directional' magnetism.



This research focuses on the low-dimensional mineral Schafarzikite and the associated magnetic properties of some related compounds. The BlueBEAR cluster has enabled us to perform Density Functional Theory (DFT) calculations of potential magnetic structures, and used these results to help rationalise experimental data. Additionally, the DFT results have successfully predicted previously unknown magnetic behaviour for one of these compounds, which have been validated by experiment.

Overall, the results have improved our understanding of magnetism in these compounds, allowing us to guide future research towards technologically useful modifications in these materials.

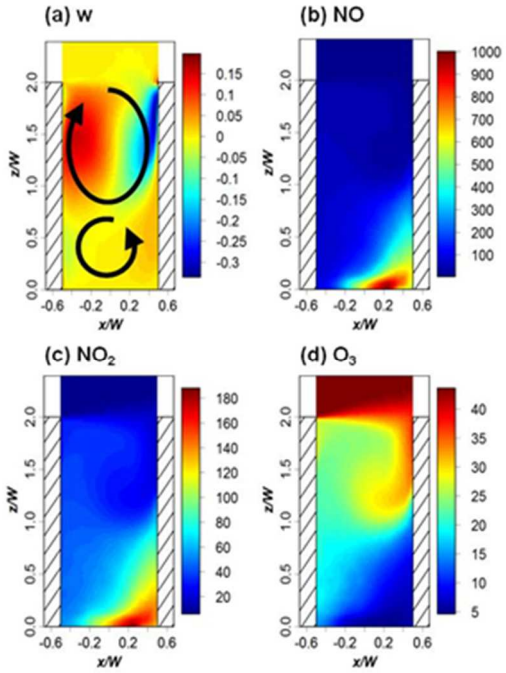
James Cumby
School of Chemistry

Turbulent and photochemical processes in a deep street canyon: a Large-Eddy Simulation

A street canyon is a typical restricted site in urban areas with buildings along both sides of the street. Released from the ground level, traffic emissions (e.g. NOx,VOCs and CO) are dominant air pollutant sources into urban street canyons where air ventilation is very poor. Air pollutant concentrations within a street canyon are determined by the mixing with the background air, vehicular emissions and photochemical processing of air pollutants.

In this study, the Large-Eddy Simulation (LES) methodology coupled with a reduced chemical mechanism is developed at the University of Birmingham to investigate characteristics of turbulent mixing and photochemical processes in a deep street canyon (e.g. with H/W=2) using the Computational Fluid Dynamics (CFD) software package (OpenFOAM) in BlueBEAR.

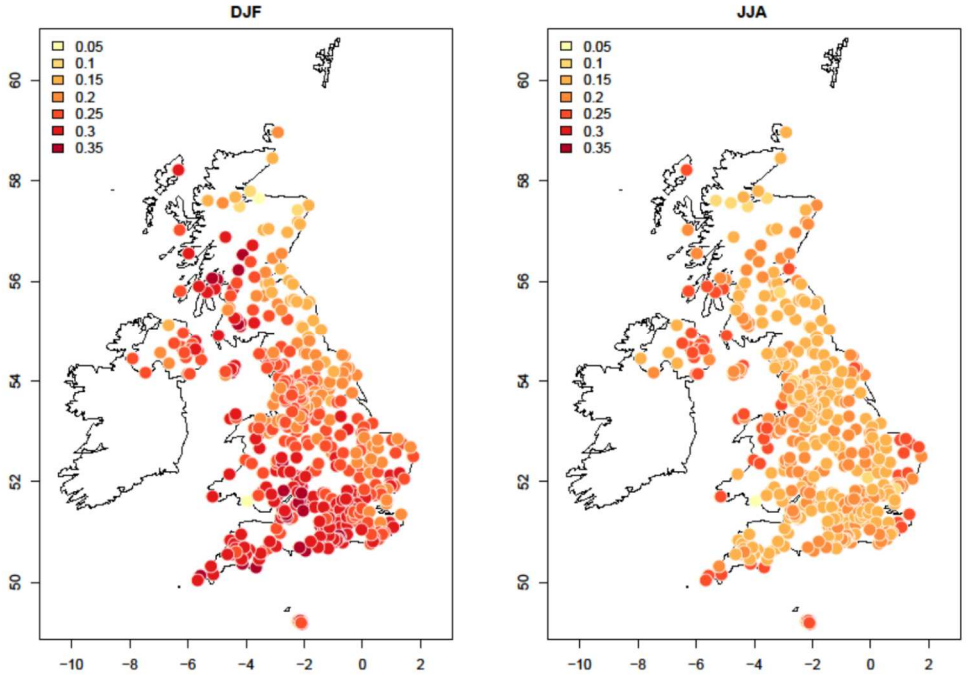
The preliminary results show that the concentrations of air pollutants vary significantly in space and time within the street canyon due to the existence of unsteady multiple vortices. High levels of pollutants can occur at the pedestrian height near the windward side. There is also evidence of separated chemical regimes in the deep canyon: the top part of canyon significantly affected by the background chemical composition and the bottom part significantly affected by the emissions. This study can provide a better understanding of the segregation effects caused by the multiple vortices on the nonlinear photochemical processes and the characteristics of air pollution within a deep street canyon.



Jian Zhong
School of Geography, Earth and Environmental Sciences

Statistical correction of extreme rainfall from global climate models

Extreme rainfall events constitute major natural hazards. Reliable estimates of rainfall changes are required at local scales where impacts are most keenly felt. However, the limited spatial resolution and the systematic errors of rainfall simulated in General Circulation Models (GCMs) make direct estimates of future daily rainfall from GCMs unrealistic. For this reason, high-resolution estimates are often made using GCM-driven Regional Climate Models (RCMs) over a limited area (i.e. Europe). While able to simulate rainfall characteristics at smaller scales, RCMs do not represent local variables and remain limited by systematic errors and biases. Furthermore, as RCMs are computationally expensive and their application is only justified when RCM output exhibits consistent improvement over GCM output.

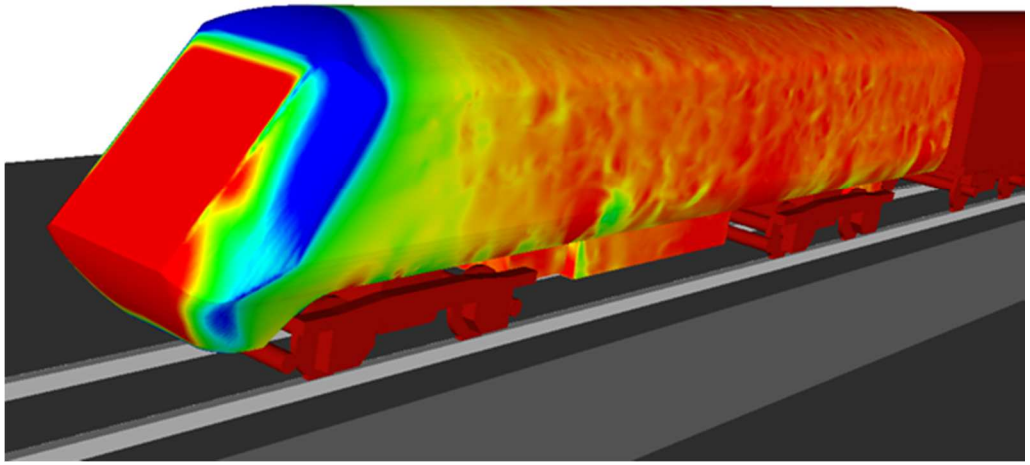


As part of the international research project PLEIADES (funded by the Volkswagen Foundation) we aim to develop a statistical correction approach to downscale GCM-simulated daily rainfall distributions to the point scale. Skilful downscaling models will be applied to GCM simulations for the 21st century in order to produce more meaningful projections of local- and regional-scale precipitation, including extreme events. Another key component of the project is to compare statistically corrected GCMs with statistically corrected RCMs, and to determine whether it is possible to quantify the value added by RCMs in the downscaling process. This is an important question in Climate Science but our approach represents the first time that a comparison of statistically corrected simulations has been made.

Jonathan Eden
School of Geography, Earth and Environmental Sciences

Comparison of RANS and DES results to Wind-tunnel Data for the Surface Pressures upon a Class 43 High Speed Train

This project investigates the application of multiple Reynolds Averaged Navier-Stokes (RANS) turbulence models and two Detached Eddy Simulation (DES) approaches to external aerodynamic flow around a 1/25th scale class 43 HST model. The RANS approach relies upon modelling the turbulence within the flow whilst the DES approach is a hybrid of simulation and modelling. The research is conducted as part of the measurement of train aerodynamic phenomena in operational conditions research project.



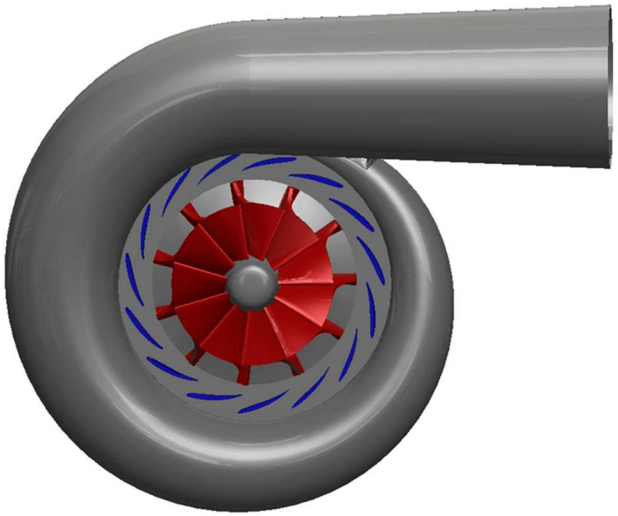
By using BlueBEAR the research is able to be conducted on a high accuracy geometry that matches wind-tunnel tests using both the RANS and Considerably more demanding DES approaches. In order to run the RANS approaches around 48 hours was required on 16 processors. The DES based approaches required upwards of 240 hours using 80 processors.

Results show that the best prediction of surface pressures over the trains engine car are achieved using the DES based approaches. These approaches gave the best prediction of pressure peaks particularly around the trains nose region and fell within the margin of error from the wind-tunnel test more than the RANS approach with any of the turbulence models.

Justin Morden
Department of Civil Engineering

Design and experimental study of a small scale radial turbine for organic Rankine cycle

The aim of this project is to develop a highly efficient and compact radial turbine for waste heat recovery of low-grade heat resources using organic Rankine cycle.



In the complete design process of radial turbine after one-dimensional modeling, it is necessary to evaluate the aerodynamics of the flow field within the turbine blade passages in order to optimize the three-dimensional geometry of blades.

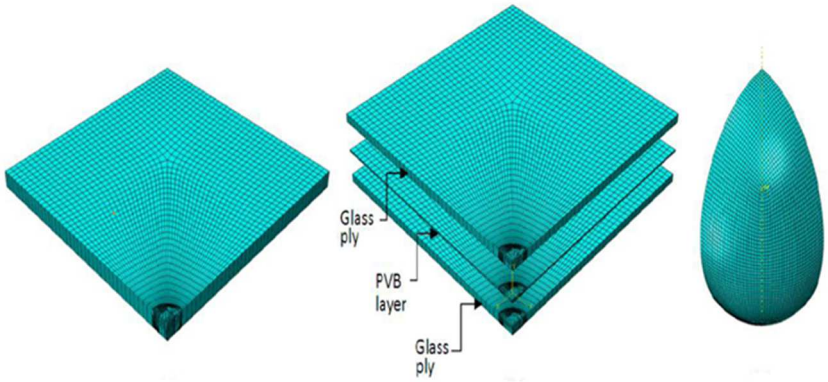
Flow in radial turbines is among the most complex flows that encountered in fluid dynamic problems. The flow is highly three-dimensional, viscous and turbulent with transonic or supersonic conditions in most cases. In addition, flow separation, tip clearance effects and time-dependent interactions of adjacent nozzle and rotor blade rows make the flow behaviour even more complex.

In this regard, CFD (Computational Fluid Dynamics) with full three-dimensional, viscose Navier-Stokes equation plays an important role in simulating the complex flow. CFD is used to make the detailed prediction of the flow filed and to highlight the regions of poor performance caused by flow separation, incidence effects, secondary flows, tip clearance and flow blockage at leading and trailing edges. Then the three-dimensional geometry of turbine in terms of volute, nozzle and rotor is modified to directly address those undesirable effects and improve the efficiency.

Kiyarash Rahbar
School of Mechanical Engineering

Low-velocity impact analysis of monolithic glass using 3D Finite Element Method (FEM) to Low-velocity impact analysis of monolithic and laminated glass using 3D Finite Element Method (FEM)

Low velocity drop ball impact response of monolithic and laminated glasses was studied using analytical and Finite Element (FE) methods. Material linear elastic and damage responses were considered throughout the numerical analysis. The performance of monolithic and laminated plate glasses subjected to the impact loads in normal and oblique angles was thoroughly examined.

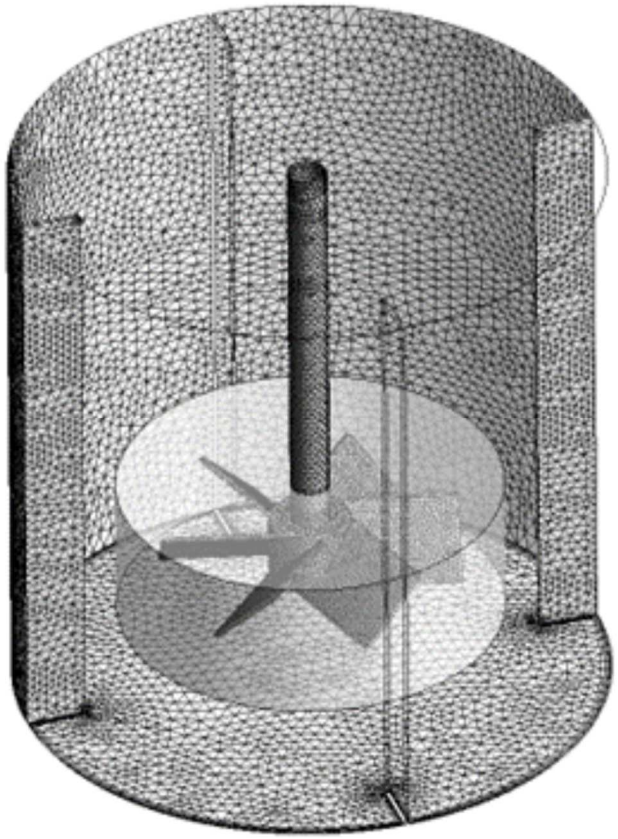


In this study, the verification of the analytical and numerical models has been conducted by using one of the previous investigation results. The adopted analytical models include the spring-mass model, energy balance model and wave propagation method for the infinite thick plates, respectively.

The results from the wave propagation analytical method found a good agreement with open literature results and it was recommended for future impact predictions. The prediction results obtained include the time histories for impactor-glasses contact force, displacement and velocity during impact under various parameters, such as impact velocity, impact mass and glass plate and PVB interlayer thicknesses. A three-dimensional (3D) finite element method (FEM) is used to model and simulate impact response of both monolithic and laminated glass. The finite element (FE) commercial software package ABAQUS was used in the numerical simulation. The numerical model geometry obtained as a symmetric and full section, which incorporated 8-nodes linear solid (Brick) elements with reduce integration method.

Kuruvita Arachchige Don Lasitha Priyanga Karunarathna
School of Civil Engineering

CFD Modelling of Complex Fluid Flow and Mixing in Stirred Vessels Challenge



The suspension of solids in stirred vessels is an operation which is widely encountered in industry including food, crystallization, catalysts, minerals, pharmaceuticals and chemical/nuclear reactors. Numerous difficult mixing problems are found with solid-liquid processing which pose a formidable challenge to industry. The methods generally used for designing stirred vessels for solid-liquid mixing tend to be based on global empirical data. A localized hydrodynamic approach provides a better more efficient basis for design since it enables a detailed description of the multiphase flow structure. However, few measurement techniques exist which can provide reliable data of this kind.

The commercial CFD code ANSYS CFX 12.0 at the BlueBEAR cluster was used to simulate solid-liquid suspensions in a mechanically agitated vessel. The multi-fluid Eulerian-Eulerian model was used such that the liquid and solid phases were both treated as continua. All CFD modelling steps including the build-up of stirred tank configuration, mesh generation, equation solving and data post-processing were conducted on the BlueBEAR cluster.

The two-phase flow field was accurately predicted by CFD as validated by experimental data obtained from a technique of positron emission particle tracking. Predictions of the spatial solids distribution were good except near the base of the vessel and underneath the agitator where they were overestimated; this still requires improvement of the solid-liquid interaction models

Li Liu
School of Chemical Engineering

Atomistic Simulation of Nuclear Materials

Nuclear energy research in the UK is currently undergoing a renaissance due to the need to reduce reliance on carbon -based fuels and meet the country's CO_2 emission reduction commitments.

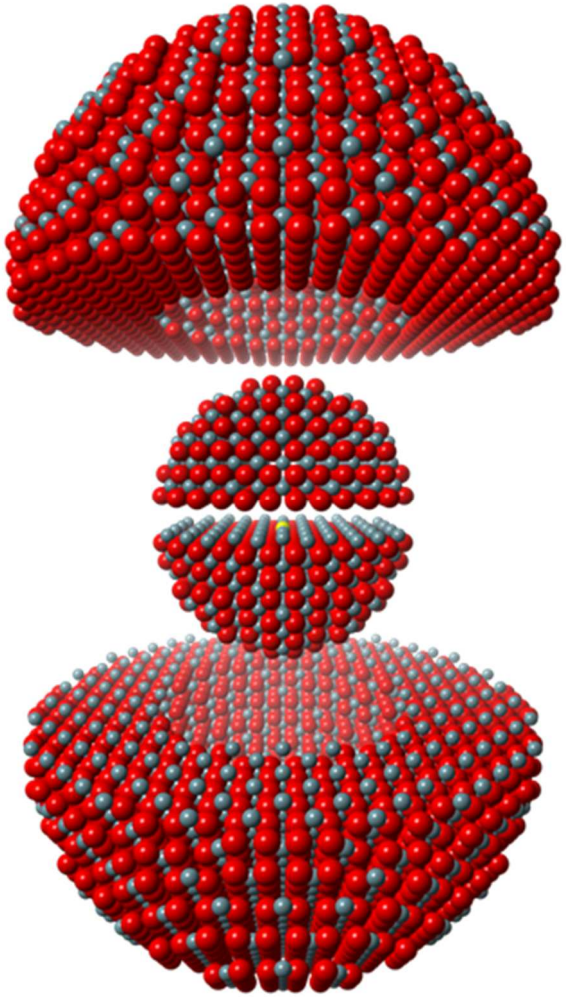
Computational simulation extends our understanding of the structure, stability and reactivity of solid state materials at the atomic level and BlueBEAR High Performance Computing services provide the facility to perform these calculations efficiently in terms of both scale and quantity.

Two main topics of research within the nuclear fuel cycle include the following:

Fuel Performance : Modelling the defect chemistry within the bulk and at surfaces (which control many important material properties) of current (UO_2) and potential future (MOX and ThO_2) fuel ceramics at the atomistic level provides insight into the prediction of ageing effects and fuel performance within reactor cores.

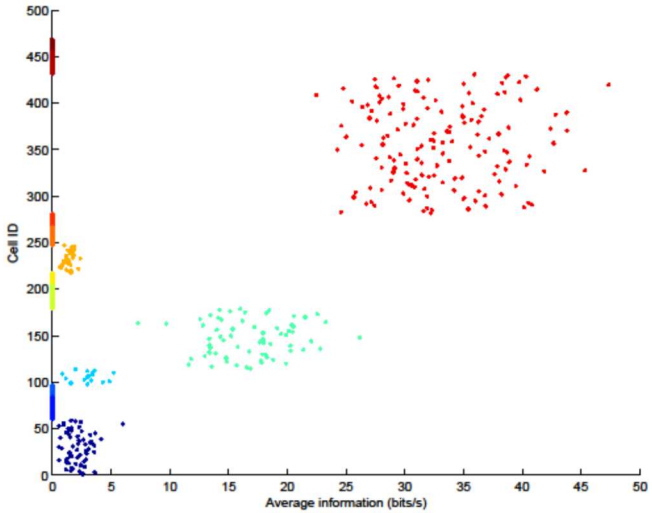
Nuclear Waste : Once spent fuel is reprocessed and radioactive fission products isolated, the 'safe and secure' immobilization of high level radioactive waste in a form suitable for final disposal is of paramount concern. Simulations predict properties of candidate ceramic compositions as host matrices including tolerance to radiation damage and radionuclide transport characteristics.

Mark Read
School of Chemistry



Information-selectivity of Alzheimer's disease progression

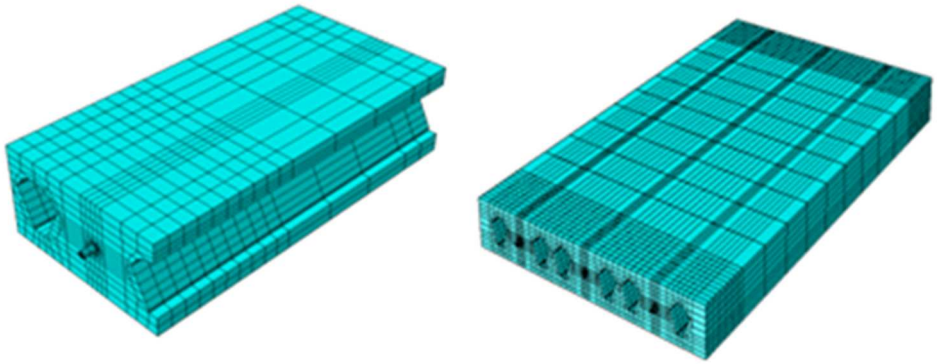
Current treatments for Alzheimer's disease only attempt to mask symptoms and delay death, rather than targeting the underlying causes of the disease. The work presented here revealed a mechanism by which Alzheimer's disease, through hijacking the brain's normal synaptic regulatory mechanisms, may selectively target the neurons with least importance to the network after disease onset, thereby sparing the most important neurons until the later stages. Whilst this means that the cognitive symptoms (such as reduced memory) do not appear until long after disease onset, this is actually a major problem as it means that the presence of the disease is hidden from view, and clinical treatment cannot begin until it is already too late to make any difference.



Through use of large-scale two-day simulations on BlueBEAR, individual neurons in a simulated neocortical neural network were profiled for their information contribution to the rest of the network, and then observed as they succumbed to the spread of the disease. These simulations confirmed the existence of a relationship between information contribution of a neuron, and its time of death due to Alzheimer's disease pathology. The results additionally hinted at a novel method of treatment for the underlying mechanisms driving the disease, using long-term low-level electrostimulation to act on the brain's normal regulatory processes and reduce their susceptibility to Alzheimer's disease.

Mark Rowan
School of Computer Science

Numerical Evaluation of Codified Design Methods for Progressive Collapse Resistance of Precast Concrete Cross Wall Structures



Progressive collapse of building structures typically occurs when an abnormal loading condition causes a sudden loss in the structural capacity of one or more critical members, which leads to a chain reaction of failure and ultimately catastrophic collapse. The tensile tie force (TF) method is one of the main design approaches for considering progressive collapse. As this method does not take into account factors such as dynamic effect, the load redistribution mechanism, the effect of steel-concrete interfacial properties, or the size and embedment length of tie bars on bond behaviour, it can be considered as a simplified method; hence a thorough examination of the adequacy of this method is needed.

This project is to undertake such a study including numerical evaluation of the codified methods of progressive collapses for precast concrete cross wall buildings. To this end, detailed three-dimensional finite element models of the pull out behaviour of reinforcement bars/strands in the keyway of precast concrete blocks and of the ductility behaviour of floor to floor joints subjected to uniform and line loads exerted from upper walls were developed. Through a calibration process for laboratory tests of pull out damage to precast concrete blocks carried out through present study and by the Portland Cement Association (PCA), the interfacial bond properties were established using numerical modelling. The same modelling method was then used in the subsequent three dimensional non-linear numerical analyses to
simulate the ductility behaviour of precast concrete floor-to-floor joints in the absence of underlying wall supports.

The numerical analyses showed a close agreement between FE analyses and test results. The tie force developed during the collapse process was particularly examined. Discrepancies in the tie force between the numerical and the codified specifications have suggested an underestimate of tie force in the TF method that may lead to an unsafe design. Finally, an improved model based on the numerical results has also been proposed to address this problem.

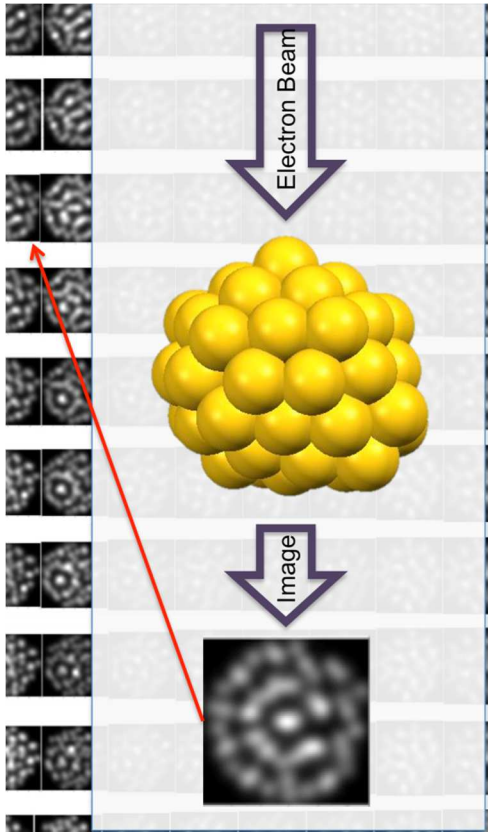
MoslehTohidi
School of Civil Engineering

Simulated image atlas of Au55 chiral nanoclusters using multislice method

From quantum size effects to the demonstration of outstanding properties in catalysis, photonic, and electronic applications, research of nanoclusters is crucial for our understanding of why and how nanostructures are different from bulk materials in many aspects. As their size are in the nanometer range, the structure of nanoclusters would not be as ordered as crystalline material, yet they are not individual atoms either, but the structure of these fine particles has a strong connection to their unusual properties. To probe their structure, we employ aberration-corrected scanning transmission electron microscopy that could provide us with resolution of sub-Angstrom level on these nanoclusters of only tens to a hundred Angstroms in diameter.

However, structure of clusters cannot be resolved solely by high-resolution images, because STEM images are 2D projections of electron-atom interaction with 3D structure of clusters. To solve this problem, we conduct image simulation based on multislice method. Multislice method treats the interaction as electrons interacting with slices of the 3D structure and calculates the interaction with each slice individually in orders. We generate simulated image atlas of given theoretical models through multislice method from various directions of the cluster. We then will match each experimental image with simulated images in the atlas.

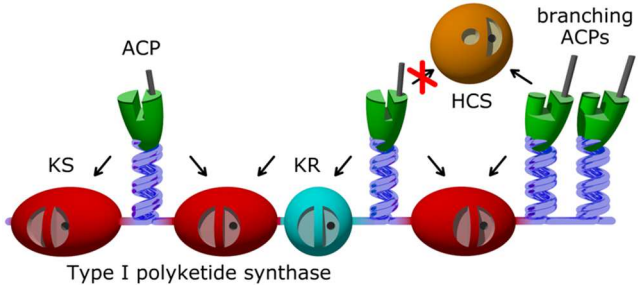
In this research, we find the positive match between experimental images of size-selected Au55 clusters and simulated images calculated from a DFT theoretically predicted Au55 chiral model.



Nan Jian
School of Physics & Astronomy

New Synthetic Biology rule to modify Antibiotics

A collaborative research project between research groups at the Universities of Bristol, Birmingham and Leuven (Belgium) has decoded a key step in antibiotic production by bacteria, underpinning the development of new antibiotics to tackle the global threat from multiply resistant superbugs like MRSA and E. coli. Many important drugs, including antibiotics, are created by bacteria in a similar way (e.g. mupirocin, erythromycin, rifamycin). The discovery brings us a step closer to controlling these biochemical pathways to produce novel molecules. For example, antibiotics might be modified to bypass the resistance mechanism that superbugs use to survive in their presence.



Type I polyketide synthase

The process by which these complex chemicals are made is very much like a production line, with the molecule being extended piece by piece as it is passed along a huge, multi-functional protein. Key components of this process are the carrier proteins which transport the chemical along the production line. The research team here identified a code in the amino acids that form the small carrier proteins. The research team comprises structural biologists, protein modellers, chemists and microbial geneticists who worked out what parts of the carrier protein allows the modification machinery to identify and insert changes in precise areas of complex antibiotic structures. The code they identified consists of amino acids in the core of the protein as well as on its surface and applies to essentially all the biosynthetic factories of this type in any organism. The accompanying cartoon shows how the special carriers can dock with the modifying enzymes as an additional function the typical carriers do not have.

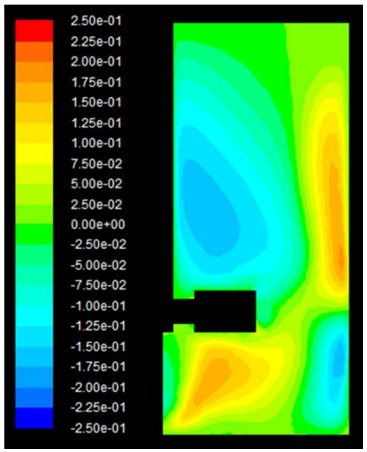
The computational analysis, partly performed on the University of Birmingham's BlueBEAR cluster consisted of statistical analysis of the patterns of amino acids in the different proteins, and simulations of the motion of the atoms in different carrier proteins, which allowed the identification of the key molecular interactions responsible for the recognition of the modifying enzyme (HCS) by the carrier protein (ACP).

Laboratory tests showed that the carrier domains that have the correct code can be moved between systems but also that there are variants that allow two different modifications to be introduced at different positions in the same system. This shows how this sort of modification can be directed when we are designing new synthetic pathways to make drugs against the increasingly problematic Enterobacteriaceae like Escherichia coli and Klebsiella pneumoniae.

The work was funded by the UK Biotechnology and Biological Sciences and Engineering and Physical Sciences Research Councils (BBSRC and EPSRC respectively) as well as the Darwin Trust of Edinburgh and the European Union, the researchers' work paves the way for using synthetic biology create novel antibiotics that may help to solve the growing problem of bacterial infections that are resistant to essentially all antibiotics.

Peter Winn
School of Biosciences

Identifying mixing regimes in anaerobic digesters that optimise renewable gas production

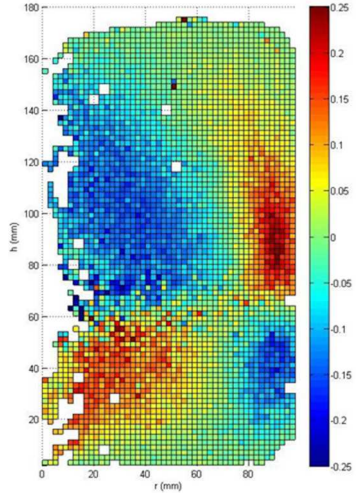


Anaerobic digestion is one of the final stages in wastewater treatment in which sewage sludge, the by-product of the earlier treatment processes, is broken down in the absence of oxygen, to produce biogas, which can be used as a renewable energy source and digested sludge, which can be used as a fertiliser. Mixing is required to bring the micro-organisms and the food sources in the sludge into contact. However, there is a cost to mixing and no clear consensus on the effect of mixing on biogas production.

Experimental work was carried out to assess the effects of mixing speed in a lab-scale mechanically mixed digester. Four digesters were mixed at different rotational speeds and the gas volume produced from each of the digester was recorded.

Computational Fluid Dynamics (CFD) models of a lab-scale mechanically mixed digester were set up to study the flow patterns within the digester at a range of mixing speeds (top). These were validated against results from Positron Emission Particle Tracking (PEPT) experiments, whereby a single radioactive particle is tracked as it moves through the digester (bottom). This allows a clear picture of the areas of high and low turbulence in the digester to be built up.

By taking samples of sludge from the digester in both areas of high and low turbulence, the microbiological communities in these areas can be analysed using quantitative polymerase chain reaction (qPCR) to determine what types of methane-producing micro-organisms are present in different regions. By pairing this information with the mixing patterns in the digester, established using CFD models, and the overall gas production from the digester, determined experimentally, the effects of mixing on anaerobic digester microbiology and hence gas production can be better understood.

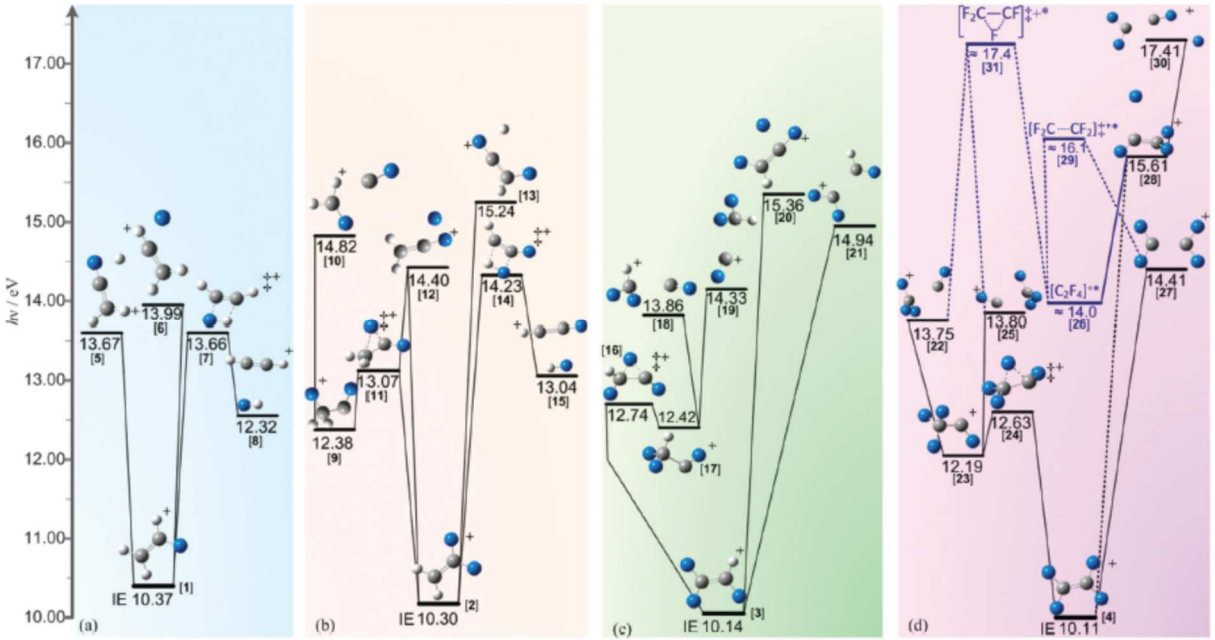


This understanding will allow designers and operators to strike a balance between the cost of mixing and the value of the biogas produced by anaerobic digesters and thereby optimise digester mixing.

Rebecca Sindall
School of Civil Engineering

Dissociation dynamics of fluorinated ethene cations ; experiment and theory

We have studied the dissociative photoionisation of the parent cation of four fluorinated ethene molecules; C2H3F, 1,1-C2H2F2, C2HF3 and C2F4. We study the trend of the changing mechanism as H atoms are replaced by electron-withdrawing F atoms. Experiments were performed at the vacuum-ultraviolet beamline of the 3rd generation synchrotron Swiss Light Source at the Paul Scherrer Institute. Complementary ab initio calculations were performed using the Gaussian 03 and 09 computational chemistry suites mounted on the BlueBEAR at the University of Birmingham. The results were published in Phys. Chem. Chem. Phys., (2012) 14, 3935-3948 (also at http://eprints.bham.ac.uk/1006) and formed a major component of the PhD thesis of Jonelle Harvey (http://etheses.bham.ac.uk/4290).



Gaussian 03 / B3LYP (denoted G3B3 in the paper above) density functional theory calculations were carried out at the minima of the potential energy curves and the saddle points in order to determine ab initio energetics for the different dissociative photoionisation channels of C2HxF4-x+, where x = 0,1,2,3. The results are shown in the Figure, where the IE denotes the experimental ionisation energy of the parent molecule in units of electron Volts (eV). Continuous lines show observed reactions, dashed lines indicate reactions not observed in the dissociative photoionisation mechanisms. Five channels are observed: HF loss, F loss, cleavage of the C-C bond after H- or F-atom migration across the bond, and direct cleavage of the C=C bond. The lowest-energy dissociative photoionisation pathway of both C2H3F and 1,1-C2H2F2 involve loss of the HF molecule, where slow dissociation over a reverse activation barrier is followed by a large release of kinetic energy. By contrast, the first dissociative photoionisation pathway for both C2HF3 and C2F4 involves an F-atom migration across the C=C bond, resulting in dissociation of C2HF3+ to CHF2+ + CF, and of C2F4+ to CF3+ + CF. A definitive solution to the longstanding problem of the determination of the adiabatic ionisation energy of the CF3 free radical has been solved, and its value is 9.090 ± 0.015 eV.

Richard Tuckett and Jonelle Harvey
School of Chemistry

Analysing datasets from electronic primary care patient records for epidemiological studies

The Health Improvement Network (THIN) database is a large UK general practice database which contains anonymised longitudinal patient records from over 500 practices (about 6% of the population). This data is used to answer research questions on epidemiology, clinical practice and health care utilisation

There have been many studies conducted using the THIN database, which are

- Patient factors influencing the prescribing of lipid lowering drugs for primary prevention of cardiovascular disease in UK general practice: a national retrospective cohort study PLoS One
- Patterns of warfarin use in subgroups of patients with atrial fibrillation: a cross-sectional analysis of 430 general practices in the United Kingdom PLoS One
- The diagnostic performance of scoring systems to identify symptomatic colorectal cancer compared to current referral guidance Gut.
- The risk of colorectal cancer with symptoms at different ages and between the sexes: a case-control study BMC Medicine
- The importance of anaemia in diagnosing colorectal cancer: a case-control study using electronic primary care records. British Journal of Cancer.

One major advantage of THIN Data is the ability to gain access to supplementary anonymised medical records to confirm diagnoses recorded electronically and to elicit further information on patients.

Ronan Ryan
Primary Care Clinical Sciences

Numerical studies of the enhancement of particle motion in cylinder

The fluidity of non-Newtonian fluids can be enhanced by vibrational motion. This phenomenon is well known in some industries: such as the building and confectionery industries and has been exploited for many years, but mainly on an empirical basis. In this paper, we report on one case with application of ANSYS CFX: the effects of vibration on the motion of particles in fluids of non-Newtonian rheology, which is relevant to problems of solid-liquid flow, particle settling and disengagement of entrapped bubbles in complex fluids.

Difficulty in this study is that drag force between solid particle and liquid is important, which results in unsuitability of immersed rigid body method and multiphase modelling. Therefore, dynamic mesh method is applied to this study. Additionally, a fine boundary mesh layer near solid particle is very necessary for this case because of requirement of accurate modelling of drag force.

CFD-predicted solution shows that particle begins settling after a very short duration and then reached falls at a constant velocity. It is accordance with published work, confirming the reliability of our model.

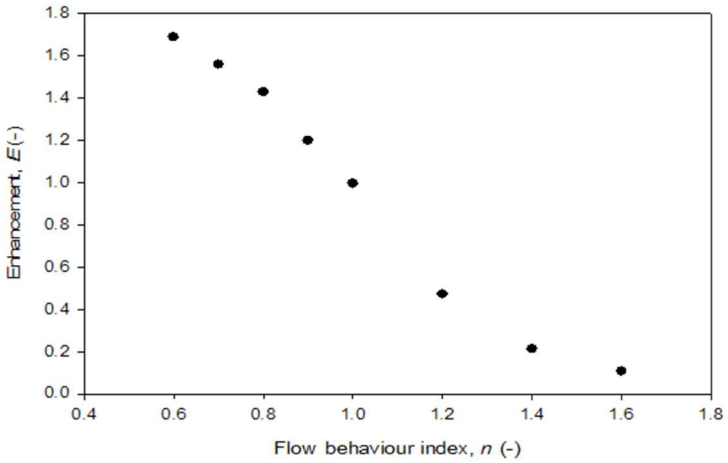


Figure: Effect of flow behaviour index on terminal velocities enhancement in power law fluids subjected to vibration:

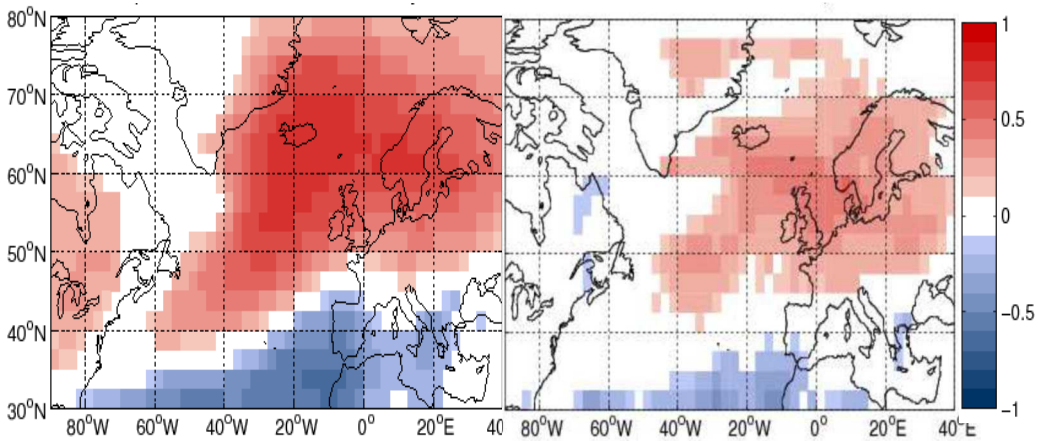
From the figure, which shows the effect of flow behaviour index on terminal velocities enhancement in power law fluids subjected to vibration, it can be concluded that particle's motion in Newtonian fluid cannot be changed by superimposed vibration. But it can be accelerated in shear-thinning fluids and retarded in shear-thickening fluids. With the increase in flow behaviour index for shear-thickening fluids and decrease in shear-thinning fluids, the acceleration and retardation effects are less and less obvious.

Shuai Tian
School of Chemical Engineering

20th Century Storminess: Developing a coherent understanding of long-term trends and decadal variability

Severe extra-tropical cyclones are the major meteorological hazard in Europe. Recent scientific research, investigating the 20th Century Reanalysis for the last century revealed that North-Atlantic/European storminess might be underlying a long-term positive trend with unprecedented high values in recent decades. These results are partly contradictory to studies analysing local station observations (e.g. in the Netherlands). Questions concerning the coherence of different storminess measures are not answered yet

Severe surface wind storms are substantially influenced by mid- and upper-tropospheric growth factors. Some of the main factors include divergence and vorticity advection in the upper troposphere, latent heat release, low static stability and baroclinic waves in the mid troposphere. In this study we examine these potential growth factors for extra-tropical cyclones and coherent physical mechanisms leading to extreme wind speeds on a synoptic as well as decadal time scale. We will further focus on the role of large-scale precursor conditions for wind storms (e.g. NAO, AMO etc.). We thus aim to develop a comprehensive understanding of storm variability for the last century.



Correlation of the NAO (first of EOF of detrended MSLP anomalies) with track density (left) and footprint (right) of cyclones. The footprint is measured with the Storm Severity Index. Results for winter months from October to March from 1871-2008 are shown

First results for the 20th Century Reanalysis from 1871 to 2008 show the expected relationship between large-scale conditions over the North Atlantic and high wind speeds over Europe. Using an objective algorithm to identify and track cyclones and their associated wind fields, we find high correlations between the North Atlantic Oscillation (NAO) and storminess for large parts of Northern and Western Europe.

Simon Wild
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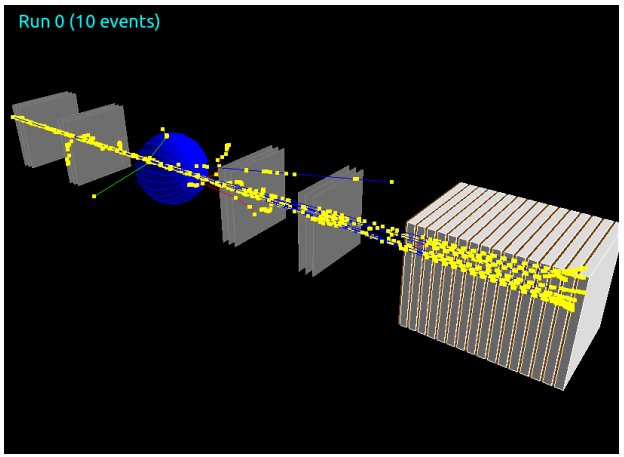
Monte Carlo modelling of a novel proton Computed Tomography device



Cancer is responsible for 1 in 8 deaths worldwide with 300,000 new cases diagnosed in the UK alone each year. There is no single cure for cancer and most patients receive a combination of radiotherapy, chemotherapy and surgery. In 2013 the UK Government committed funds to build two proton therapy centres in the UK to further enhance the UKs standing as a world leader in the fight against cancer.

Proton therapy is different to conventional radiotherapy as it uses positively charged particles (protons from the heart of a hydrogen atom) to deposit energy in the cancer rather than massless, chargeless photons. A proton will deposit a small amount of energy along most of its path and the reminder amount at the end of its range. This is known as the Bragg Peak. The Bragg Peak is a powerful tool in the treatment of cancer as it minimises the dose to healthy tissue whilst maximising the dose to the tumour.

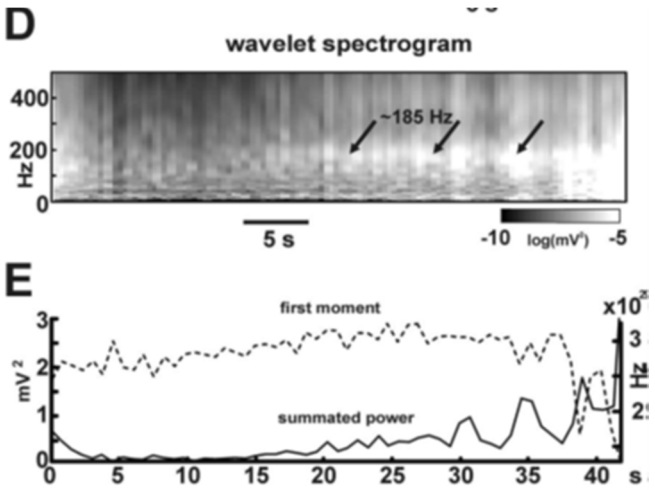
Protons have a finite range, which varies depending on the tissue characteristics they traverse, and the position of the Bragg Peak within the tumour can be tuned by varying the initial proton energy which enters the patient. To do this accurately we must know the composition of bone, fat, muscle and other tissues within the patient as the protons deposit energy differently in all of these. Conventionally this information is gathered using a Computed Tomography (CT) scan of the patient. However, a conventional CT scan uses photons rather than protons to image the patient. A conversion factor is then applied to convert the information (Hounsfield numbers) obtained from the photon images to the proton stopping powers of the various tissues inside the patient, which in turn relate to the proton energy lost during its flight path. These conversion factors lead to uncertainties in the proton stopping powers and can add complications to the proton therapy treatment plans due to the uncertainty in the range of the protons. The range uncertainties could result in either underdosing the tumour or overdosing an adjacent critical healthy organ, both of which will compromise the treatment outcome.

It is the aim of the PRaVDA Consortium to design, build, and test a device which will allow a CT scan to be obtained using protons directly and removing the need for the conversion. As protons are positively charged they will undergo Coulomb Scattering within the patient, which changes the protons energy and direction. The PRaVDA device will need to be able to accurately measure the direction of the protons both into and out of the patient to account for the scattering and their residual energy using a specially designed Range Telescope.

The BlueBEAR system has been used for Monte Carlo modelling of the properties of such a device to ensure we can achieve our final goal of producing a proton CT image. To date around 15,000,000,000 protons have been modelled, using approximately 30,000 hours of CPU time and 4 TBytes of data. Obviously, without use of the BlueBEAR system this work would not have been possible and we would like to extend our gratitude for being allowed to use the service.

Tony Price
School of Physics and Astronomy

High frequency activity preceding epileptic seizures



Brain comprises of 100 billion basic elements, the neurons. By the accurate cooperation and delicate balanced activities between neurons, we live are all the individuals are unique. Nevertheless, small defects in brains might cause psychiatric problems or even physical malfunctions.

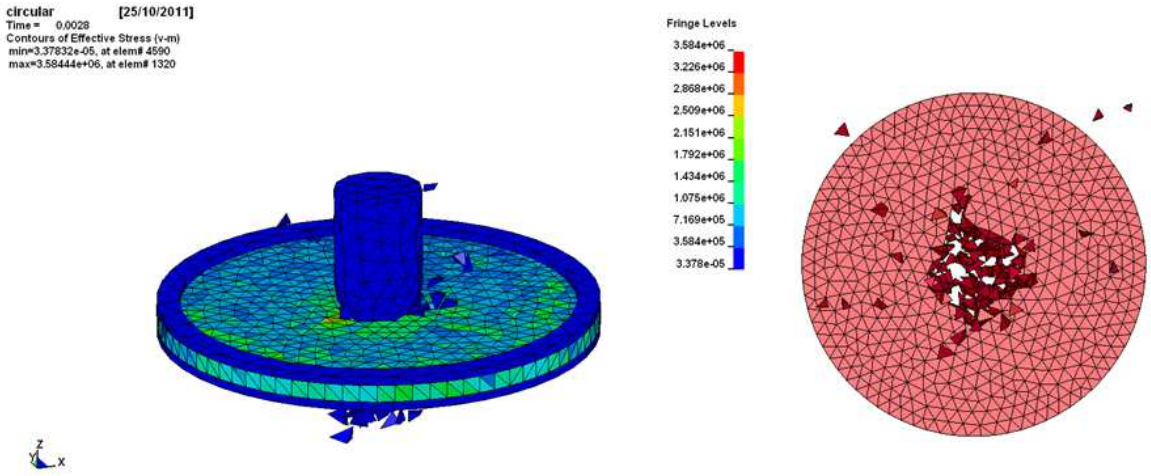
Epilepsy is one of the most common brain diseases, and our research focus; we investigate epilepsy mainly in rodent models or in rodent brain tissues. Brain waves are electrical summations of the neuronal activities we can record from both experimental conditions, and the transformations of the brain waves generally reflect the underlying changes of the neuronal activities and functions.

Although commercialised software quickly gives us glances of these changes, they are limited and insufficient. What we really need is a flexible and customised analysing strategy, and only MATLAB platform fulfils our requirements. Wavelet and Fourier transforms are commonly used in our researches, and MATLAB helps us tracing the dynamic alterations of the brain waves in every second or even tens milliseconds. Besides, MATLAB grants us the abilities to simultaneously handle correlations between many events (single neuron activities or particular brain waves), especially when a script was made the massive data can be analysed quickly and automatically. Last but not least, MATLAB flexibly generates high quality plots, that many of our published figures were amended from MATLAB's products.

Wei-Chih Chang
Neuronal Networks Group

FEM/DEM modelling of hard body impact on glass and laminated glass

Glass and laminated glass are widely used as structural members in civil engineering. To investigate how they fracture under hard body impact as well as the subsequent fragmentation, the combined finite-discrete element method (FEM/DEM) incorporating finite elements into discrete elements was employed.



In order to accurately describe the fracture behaviour of glass and laminated glass, appropriate damage models are needed in this research. A mode I fracture model was extended for glass by changing the strain softening curve to a bilinear-like exponential decay shape. To better understand the mixed-mode damage, a simple Mode (I + II) elasto-plastic fracture model (E-P model) was developed for the glass and the interface in the laminated glass.

The models are all implemented into the FEM/DEM program and be verified with test data and other numerical results. Parametric studies on these models were performed by using the extensive supply of CPUs of the BlueBEAR clusters. This HPC facility provided an excellent platform for doing jobs requiring considerable number of CPUs, regardless of serial or parallel program it is. The results obtained from this research showed the better energy absorption capacity and safety of the laminated glass over the monolithic glass. It also showed that the FEM/DEM modelling and the developed damage models (both Mode I and E-P models) are applicable and can provide realistic simulations.

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