# Birmingham Environment for Academic Research

Case studies—Volume 1

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# Birmingham Environment for Academic Research

## Case Studies Volume 1

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## Acknowledgements

We would like to thank all the people who contributed to this publication.  Putting this together  pales in comparison with the wondrous research they are doing.

Most of the work is presented at http://www.bear.bham.ac.uk/CaseStudies

Front cover 'Fractal Sqaure Root' created using GIMP.

'The Death of Socrates' Jacques-Louis David (1748-1825), The Metropolitan Museum of Art, image used for 'Optimal voting rules for two-stage committees' by Dr Colin Rowat.

Photo by Flickr user Mukumbura; used under Creative Commons Attribution license for Chunk Learning and Move Prompting Making Moves in Chess by Dr Andrew Cook.

Image of Braid by dow@uoregon.edu for Parallel Computation of Braid Orbits with GAP and SCSCP by Gehao Wang.

## Abstract

These case studies have been brought together to publicise the different types of work that have been carried out on the University's high performance computing facility, known as BlueBEAR. This computer system is part of the Birmingham Environment for Academic Research (BEAR), which helps both staff and students of the University delve deeper into their research than has been possible before.

Traditionally researchers have always had to experiment or to theorise; BlueBEAR can deliver a third option, computer-based modelling. Computer-based modelling is used to underpin experimental and theoretical research. Sometimes computer-based modelling is the only option (e.g. colliding galaxies, nuclear explosions) when safety and cost are prohibitive.

This set of case studies represents only a small part of the vast amount of research that is being done on BlueBEAR and, more generally, around the University of Birmingham as a whole.

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## Contents

## Preface

It is a very great pleasure for me to write an introduction to this booklet on BEAR computing. It contains a very wide range of impressive case studies of some of the computing work performed on BEAR by many researchers, both staff and research students, from across the University. These examples include work from many different disciplines and I am delighted to see that the range of applications being studied on BEAR is still increasing day by day.

I am the Head of the Particle Physics group in the School of Physics and Astronomy and work on the ATLAS experiment at the CERN Large Hadron Collider (LHC). The analysis of billions of proton-proton collisions from the LHC experiments requires the collaborative
use of many different computing facilities from around the world.

A major part of our work to construct this international computing effort and build on the invention of the world-wide web at CERN has
been the development of 'grid computing' where storage and computing resources are shared around the world. This system has taken many years to develop but it is now running very efficiently and allowing us to process and analyse the LHC collision data very soon after it is recorded. In Birmingham we use a Particle Physics cluster and the BEAR cluster to contribute to this work.

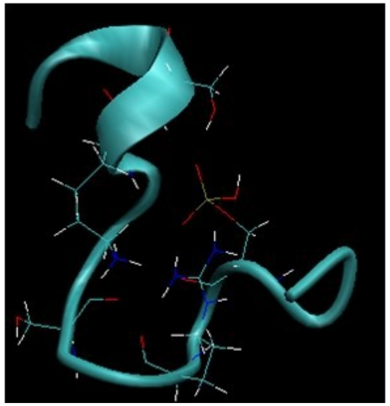
From 2001 we started to construct a network of computers between Particle Physics groups in the UK. At this time it became very clear that outside a few specialist research groups, the general research computing facilities in Birmingham were completely inadequate compared to most other Russell Group Universities in the UK.

Over the next few years we worked with many other Schools across the campus and Information Services to build a case for new University research computing facilities. We felt that unless this investment was made our Phd students and researchers would continue to be at a huge competitive disadvantage in their work.

The University recognised the strength of this case and began to make significant investments to improve the situation. It first invested in a relatively small computer cluster via SRIF funding and followed this by a 2.5 million pounds investment to deliver the much larger BEAR cluster with 1500 cores and 150 TB of disk storage. Very recently it has extended this support by providing an annual investment fund of 300K pounds to update and strengthen our research computing facilities.

Professor Pete Watkins
Particle Physics

**Using Molecular Simulation to Interpret Phosphopeptide Structure from Mass Spectrometry**
Centre for Systems Biology



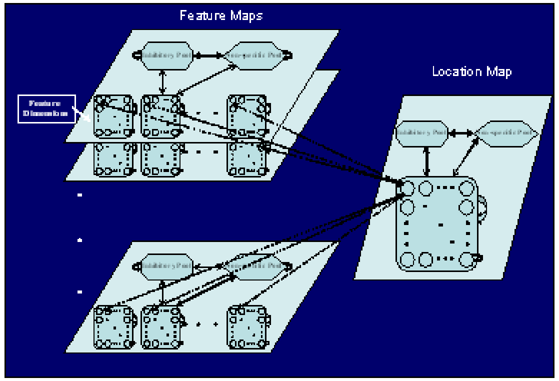
Proteins are the work horses of biology, being the machines responsible for most cellular processes. Once a protein has been initially made by a cell it may undergo further modifications. Phosphorylation is one such modification, being particularly important for cellular message passing, as indicated by the publication of more than 14,000 academic articles on the subject every year. Malfunction of this regulatory process leads to many disease states including cancer, and thus kinase inhibitors, drugs that block phosphorylation, have a market value of about 50 billion dollars annually. Currently, the structural consequences, and hence the mechanisms of action, of protein phosphorylation are poorly defined. If we look more closely at the structural changes associated with phosphorylation, and develop a rule set for how it changes protein structure and function then we will model better the biology of phosphorylation and the diseases associated with the dysregulation of phosphorylation.

Mass spectrometry (MS) has the potential for rapidly probing protein and peptide structures. MS is a technique for identifying the chemical constitution of a protein by fragmenting it and "weighing" the components. More precisely, the ionised fragments are separated according to their mass-to-charge ratios. Since the fragmentation process is dependent on the structure of the protein or peptide, the observed fragments also depend on the structure. Thus, MS is a potential tool for telling us about the structure of proteins, peptides, phosphopetides and phosphophorylated proteins. MS is a particularly appealing technique since it does not have the problems of protein crystallisation inherent in X-ray crystallography or of protein size inherent in NMR, the usual methods used to probe protein structure. This project is developing the application of computational modeling for the interpretation of MS data. Despite the use of simple physical models this is still a computationally intensive

Peter Winn
School of Biosciences

## Lesioning The Spiking Search over Time and Space Model (sSoTS)

This project aims to understand the processes involved in Visual Search by using normal and patients' behavioural data and the sSoTS model.




The visual world contains a vast amount of information, only some of which is relevant to our behaviour; hence, we need a selection mechanism that separates relevant from irrelevant information. Visual selection is associated with the posterior parietal cortex (PPC). Damage to PPC is associated with extinction (after unilateral lesions) amongst other problems in visual selection. Traditionally, in visual search tasks, participants are asked to find a known target item amongst irrelevant distractor items, and the time it takes participants to identify the target is measured (reaction time (RT)).

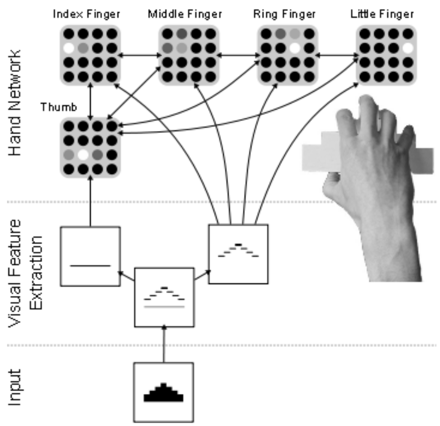
In the cases of extinction, the RT of stimuli presented to the side opposite the brain damage (ipsilesional side) is effected from the stimuli presented in the contralesional side. Here we present simulations of the effect of posterior parietal damage on visual selection using the spiking Search over Time and Space model (sSoTS). The model's predictions are compared with behavioural data from human patients with PPC damage from Glyn Humphreys' lab. The results have shown [1] , that although the model's parameters are set in order to simulate the visual marking effect sSoTS can predict behavioural data in visual extinction paradigms in human patients with PPC damage.

[1] Mavritsaki E., Humphreys G.W., Heinke D. and Deco G. (2009)"Simulating posterior parietal damage in a biologically plausible framework: Neuropsychological

Dr Eirini Mavritsaki
School of Psychology

## Computational model of affordance-based processing

This project aims to understanding how humans reach and grasp objects. This research question is approached through a computational model of neural processes (neural network).




Classically the execution of actions with objects has been explained by a two-stage process: object recognition and parameterization of actions. However recent experimental evidence suggests that parallel to this two-stage process actions are also determined by visual information without the "detour" of object recognition (affordance-based processing). The computer model in this project implements the extraction of such object affordances.

The model has been successfully implemented. We were able to demonstrate that the model successfully extracts affordances. The simulation results were also experimentally validated.

Christoph Boehme
School of Psychology

### Optimal voting rules for two-stage committees

In many environments, committees are required to make both preliminary and subsequent, final decisions: bills must typically survive two parliamentary votes to be adopted; couples typically are first engaged before marrying; employees may be probationary hired before being granted a permanent position. Within such environments, committee members must decide how to vote: adopting a candidate at the preliminary stage allows the committee to glean more information about them; turning the candidate down at either stage allows the committee to search for a new candidate. What voting rules should a committee adopt at the preliminary and final stages if it wishes to efficiently trade off its impatience against a desire to make the right decision?

Each of the voting rules considered reduces to a polynomial equation. As these are typically above fifth order, they are not – by Galois' theory – solvable in radicals. We therefore use Magma to implement techniques from algebraic geometry, allowing us to solve for those points at which the yields of two voting rules perform equally. By testing the voting rules against these solutions, we may determine the domain over which any particular rule is optimal.

Committees that are patient, or which are highly able to glean information from probationary candidates should adopt a rising threshold rule, under which the probationary threshold is easy to leap, but the final one difficult. Committees that are either impatient or less able to glean information from probationary candidates should make both thresholds low. These results therefore provide a consistent theoretical underpinning for intuition. We also find, less intuitively, that a committee's performance can deteriorate if its ability to glean information from candidates improves: optimistic committee members may be more willing to initially vote in favour of an option, in the hope that their pessimistic colleagues will be convinced by the candidate's performance; insofar as this delays the committee's

Dr Colin Rowat
Department of Economics

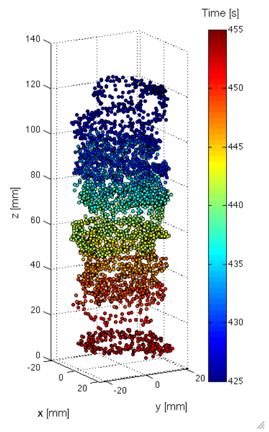
## Medieval Warfare on the Grid


This project uses agent-based modelling in a distributed environment to help understand how medieval states moved and fed armies.

The movement of large numbers of people across a pre-industrial landscape presents a series of significant logistical challenges. When logistical systems broke down, armies failed and states sometimes collapsed. Given its importance to the state and its inhabitants, medieval military logistics has been slow to utilise computer modelling techniques in order to understand the complex processes involved. This project takes as a case study the march of the Byzantine army to the battle of Manzikert in AD1071 and models the army on a 1:1 basis, tracing the movement and status of each individual. The Byzantine army probably numbered over 40,000 and travelled more than 700 miles from Constantinople to Manzikert through the Mediterranean summer. By modelling different scenarios regarding the size and composition of the army, the different possible routes and differing levels of food availability the project seeks to generate a set of plausible parameters within which the fragmentary historical record can be placed. These results can then be rendered in both 2d and 3d images or animations, enabling them to be more easily understood by people unused to traditional agent-based modelling outputs.

Phil Murgatroyd
Institute of Archaeology and Antiquities

## An experimental and numerical fluid dynamic study of a Pin-Stirrer Heat Exchanger




Tackling obesity in modern society requires advanced technology. New, engineered healthier food can be obtained by rethinking the formulation. This opens the way to a new and exiting discipline, Food Engineering. The primary challenge is to replace the unhealthy constituents with designed alternatives, without altering the sensory perception of the product.

A way of achieving this is to gain a deeper understanding of the current food processing technology and its effect on the final food properties. The Pin Stirrer Heat Exchanger (PSHE), is the standard for the production of margarine, although very little is known about the internal extremely complex mixing structures.

BlueBEAR offered the unique opportunity to use an extensive computational capacity to simulate with Ansys CFX the entire PSHE. Furthermore, because the simulations were intended as a shortcut to screen different PSHE designs, experimental validation was needed. Custom developed MATLAB codes were used under BlueBEAR to process the large amount of data obtained from Position Emission Particle Tracking experiments (PEPT). In conclusion, thanks to this study we are able to improve food processing and to extend the use of PSHE to the production of more complex, demanding and healthier foods.

Andrea Gabriele
Department of Chemical Engineering

## Chunk Learning and Move Prompting Making Moves in Chess

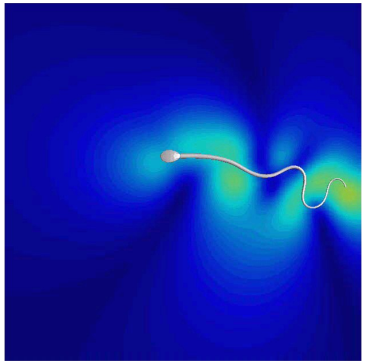
Can a computer be programmed to ‘think’ like a human? Consider the game of chess: computers work out a move by systematically examining every possible move and counter-move many ply ahead, evaluating millions of resulting chessboards; however, when observing human players it seems that expert players recognise groups of chess pieces and in doing so, focus their attention on a few possible moves. The process, known as ‘chunking’ is claimed to attribute the expert player with knowledge of chunk patters which direct attention to just a few salient moves. Is it possible to model human behaviour in a computer program, and if so, does the recognition of chunks in a computer chess program effectively reduce the search to the right moves?

A large number of transcripts from Grandmaster games were downloaded from the Internet to provide example chessboard configurations, and their resulting move. From each board all pieces were combined to make ‘chunks’, and the chunks were associated with the resulting move. When presented with a new chessboard the program also combines the chess pieces to build chunks and by comparing these with the reference chunks, a list of associations can be made. A list of moves can therefore be compiled and sorted into the number of chunk associations found.

The top four moves suggested by the chunking analysis included the best move on average 17% of the time. Although small, this is a significant result as the selection of moves is made without any knowledge of the rules of chess or properties of the pieces. Furthermore, applying the ‘chunk-ordered’ list of moves to an alpha-beta search gave on average a 50% decrease in the number of nodes searched, compared with a random ordered search.

Andrew Cook
Department of Computer Science

**Mechanics of sperm motility and fertilisation**
Clinical and Experimental Medicine



Fertility problems effect 1 in 6 couples, with male factors being present in over half of all cases. The most common problem is poor 'motility', the ability of sperm to swim to the egg and fertilise. Despite decades of research, the mechanics, forces and energy expenditures of normal and poor motility sperm are far from being fully understood. Central challenges are: 1) having the computing power to test large data sets of sperm tail beat waveforms and cell body shapes, and 2) taking into account the complex fluid properties of the reproductive tract mucus that sperm swim through, and the complex internal apparatus of the human sperm tail. For these challenges, supercomputing power is necessary.

Sperm tend to accumulate near microscope slides and coverslips, and people have worked on explaining this since the early 1960s. We developed the first long-timescale simulation method to explore this behaviour, and the mechanisms involved. Through using large numbers of parallel simulations on BlueBEAR we were able to explore the parameter space and show what tail beats result in this behaviour. The simulation capability of BlueBEAR also allowed us to discover a new symmetry-breaking phenomenon affecting the sperm tail beat, which could explain how sperm may become trapped as they migrate. These codes and methods are being used by researchers in Mathematics, in the Mathematical Institute at Oxford University, and also by researchers in the Medical School and Birmingham Women's Hospital to understand sperm swimming microscopy observations. Other problems being considered include the swimming of trypanosomes, which cause sleeping sickness, symmetry-breaking in embryo development, and drug delivery to the colon (jointly with chemical engineering).

Dave Smith
School of Mathematics

## Parallel Computation of Braid Orbits with GAP and SCSCP

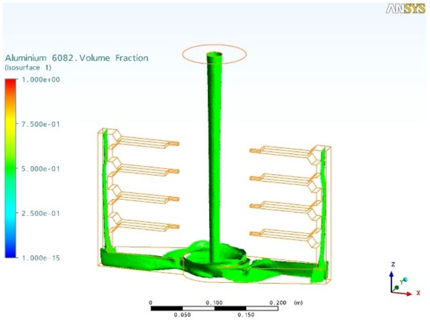
In algebra, the Inverse Galois Problem concerns whether or not every finite group G can be realized as a Galois group over the rational numbers. The case where G is soluble was resolved by Shafarevich in the 1950s, but the general case remains open. One approach to the realization of a group as a Galois group is via classification of Hurwitz loci of complex curves admitting G. These loci are indexed by the orbits of a suitable surface braid group acting on the generating tuples of G. When the genus of the curve is low, the braid orbits can be enumerated explicitly using GAP (Groups, Algorithm, Programming) computer algebra system and the BRAID package by Magaard, Shpectorov and Völklein. The length of the orbits dramatically increases with the size of G and genus of the curve. In order to handle larger orbits, we propose to use parallel computing in GAP via the package SCSCP (Konovalov and Linton).

Using parallel computation, we have successfully computed an orbit of size approximately 1.2 million using 15 processors in the server babbage2 in the School of Mathematics, where we set one master worker, eight applicator workers and six storage workers to do the parallel computation. We also repeated this computation in BlueBEAR.

The communication in the SCSCP package and queuing takes a lot of time. It turns out that almost two-thirds of the duration time are for waiting, encoding, decoding and so on. This needs to be improved. We want to use hundreds of processors at the same time for the cases of orbit length up to 10 million or more, and we want to use them for several hours. While we consider using more resources to handle the large orbits, we are also thinking about reducing the size of each computing task. This requires more work around the algorithm.

Gehao Wang
School of Mathematics

## Optimizing the Centrifugal Casting of Gamma Titanium Aluminides




The aim of the study is to investigate the effect of rotational velocity in the filling process of mould designs during the centrifugal casting process and also to investigate the effect of the centrifugal casting on the quality and reliability of TiAl-based alloy castings.

TiAl alloys have great potential as a substitute for heavier Ni superalloys for a range of high temperature components, including aerospace gas turbine blades.

Ti alloys are normally melted in an Induction Skull Melting furnace prior to casting into ceramic shell moulds but the low superheat makes it difficult to fill moulds completely using traditional gravity casting. Centrifugal casting is used to fill thin section castings in a variety of conventional alloys, but little research has been carried out to establish a scientific understanding which would allow the process to be applied to more difficult alloys such as TiAl. The high g-force assists in mould filling and may also help to feed the shrinkage during solidification, but these benefits may be partly offset by the surface turbulence during mould filling which may entrain various defects such as bubbles.

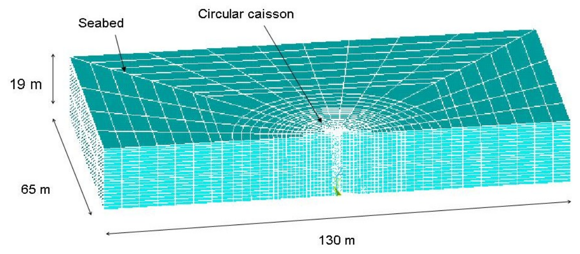
The aim is to establish means of controlling the flow in order to minimise entrainment defects. This will be subsequently complemented by a study of the effect of centrifugal casting on the quality and reliability of TiAl investment castings.

Using the indirect gating system offers a non turbulent and stable filling process. However, it is necessary to analyse the cast flat bars by X-ray test in order to determine their quality and reliability.

Eduardo Trejo
Department of Metallurgy and Materials

## Three-dimensional Numerical Modelling of Dynamic Saturated Soil and Pore Fluid Interaction

As is commonly known, soil is a multi-phase material that contains not only soil grains, but also air and pore fluid. When subjected to dynamic loading, these different phases inside the soil will interact with each other. These interactions can subsequently lead to various characteristic behaviours of soil such as liquefaction, cyclic mobility and dilation. These pore fluid-soil interaction induced phenomena are not only complicated in mechanism but also sometimes bring disastrous results i.e. building collapse during earthquakes, failure of offshore equipment under wave loading.

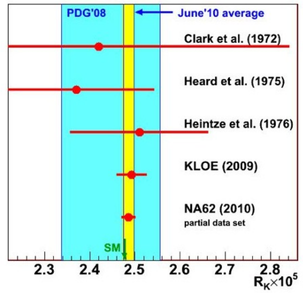



Aiming at a better understanding of the coupled interaction between saturated soil skeletons and pore fluid, as well as, more importantly, looking for a feasible way to predict and avoid the disastrous damage caused by these coupled interaction phenomena, a three-dimensional (3D) finite element methods program DYNE3WAC was developed, based on the same numerical scheme as the 2D version DYNE2WAC.

In order to verify and validate the program, a series of tests for both static and dynamic problems were conducted to verify the program. The numerical results were compared with the analytical solutions. In all of the tests the numerical results agree well with the analytical results. Additionally, to overcome the memory limit for global matrix storage, an out of core solution method was adopted for the Unix/Linux version by including the MA42 package into this program. The performed tests showed that, by adopting the out of core method, the memory required for the storage of the global matrix can be greatly reduced. The verified program was successfully applied to two types of analyses. The first type is concerned with the wave-induced response around the structures, a circular suction caisson and a breakwater; founded on the seabed; the other is concerned with the earthquake-induced liquefaction.

Jianhua Ou
Department of Civil Engineering

## Test of Lepton Flavour Universality at the CERN high-energy particle experiment NA62




The first phase of the NA62 experiment at CERN is dedicated to a very precise test of Lepton Flavour Universality (LFU), a cornerstone of the Standard Model of particle physics postulating that lepton coupling to gauge bosons is independent of lepton type ("flavour"), as opposed to the flavour-dependence of quark interactions. The origin of the observed LFU is a fundamental problem of modern physics. Precision tests of LFU with the aim of finding evidence for its violation can shed light on the question of whether the supersymmetry or any other Standard Model extensions are realized in nature. This is in turn closely related to the astrophysical problems of the composition of the Universe and Dark Matter. Using a data set collected in 2007, the ratio of the two leptonic decays of the charged kaon decays (Ke2/Km2), which is sensitive to possible manifestations of LFU violation, has been measured precisely to search for deviation from the Standard Model predictions. As is usual for precision measurements in particle physics, CPU-intensive Monte Carlo simulations are instrumental for achieving the proposed accuracy, extracting the signal out of the large background, and estimating all the background sources and all the experimental effects that could limit the precision.

All the Monte Carlo simulations required for the physics analysis have been carried out at the BlueBEAR cluster. A total of about 10 billion events have been simulated, using a custom programme based on the Geant toolkit that simulates kaon decays and traces the decay products in the detector. The simulation also takes care of the energy release of particles in the detector and their interaction with matter, and also of detection. All background sources and all relevant detector effects such as muon interactions in the liquid krypton calorimeter were simulated in detail. The simulation of muon interaction in lead has been crucial in order to achieve a precise background rejection. Overall, the various background components are reproduced extremely well. This makes us confident that the

Evgueni Goudzovski
School of Physics and Astronomy

## Micro- and Macromixing Studies in Two- and Three-Phase (Gas-Solid-Liquid) Stirred

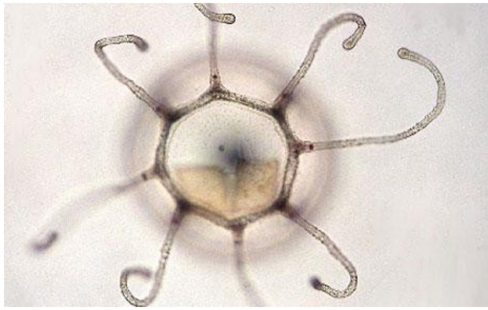
Mixing on a molecular scale (micromixing) has been studied extensively because of its potential importance in industrial chemical reactors, which are commonly used in pharmaceutical, chemical, biochemical and other industries. Better understanding of these phenomena would be beneficial for optimising product distributions, for instance to achieve required yield and quality of the product in polymerisation or precipitation. In this study, mixing in baffled and unbaffled stirred tanks is of particular interest and detailed information about the fluid flow in these two cases might help interpreting or even explaining results from experimental work.

In addition to well established experimental techniques, computer simulations, i.e. Computational Fluid Dynamics (CFD), can be helpful for studying fluid flow phenomena using numerical methods. Models of baffled and unbaffled stirred vessels are being simulated using the commercial software package CFX. The region around the feed pipe is of particular importance for micromixing and is resolved with fine structured meshing.

The results from CFD simulations are being validated with experimental findings, for instance the impeller power number, and should lead to a better understanding of the studied cases. In the long run, established models might be solely used to look at various potential scenarios applied to stirred reactors for achieving better results without the need for expensive and cumbersome experiments.

Julia Hofinger
Department of Chemical Engineering

## Co-evolutionary body-brain couplings in models of simple undulatory animals



I am interested in how evolution has led to an emergence of primitive animals having very specific couplings between their body plan morphologies and nervous systems. I attempt to examine how constraints such as energy consumption and behavioural fitness can affect such couplings on both physical and dynamical levels. Understanding such processes is important from both biological and computer science perspectives. From a biological perspective, we can attempt to shed light on how nature has come to organise information so efficiently; we can try to identify precisely why evolution has honed in on particular structures. From a computer science perspective, we can aim to build more efficient information systems.

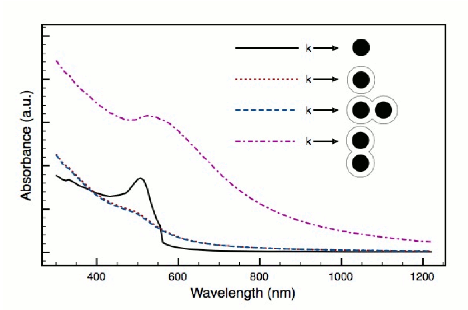
In both cases, results have demonstrated that the model nervous system will typically emerge with minimal complexity with much of the body plan morphology providing passive actuation. The model nervous system is further observed to become architecturally coupled in such a way that allows for maximum survivability and minimal energy consumption.

Ongoing work consists of complexifying the simulated environment and exploring how a variety of behaviours can emerge to meet the demands of several situations. This is computationally intensive and via a utilisation of the message passing interface, is continuing to benefit from a parallel distribution over tens of cores.

Ben Jones
Department of Computer Science

## Theoretical Studies of the Optical Properties of Gold and Palladium Nanoparticles

The excitation of surface-plasmons by light on planar surfaces is called surface-plasmon resonance (SPR), or localised surface plasmon resonance (LSPR) for metal clusters in the nanometre size range. Nanoplasmonics has received considerable attention in recent times due to technological advances which now allow us to manipulate and structurally characterise clusters on the nanometre scale, and the resulting important applications of these features e.g. sensors. The optical properties of nanoparticles are size and shape dependent, allowing for tunability; in the case of heterogeneous nanoclusters composition also contributes. Nanorod shapes are of particular current interest due to their display of two axis-dependent SPRs.




Research focuses on calculations using the discrete dipole approximation (DDA) to model the interaction of light with homo- and hetero-geneous metallic nanoparticles of varied shapes and sizes. Typically, calculations consist of over 100,000 dipolar points (N), and with 3N linear equations to be solved the process can become very computationally intensive. The BlueBEAR cluster allows high-class computational facilities to perform these calculations. From our results we can then draw up simulated UV-Vis absorption spectra for these nanoparticles, and compare them with experimental data to identify distinct contributing features, thus aiding the experimentalists' work towards nanoparticles which are very wavelength specific in their responses.

In the graph above, DDSCAT calculations for isolated Au and Au(core)Pd(shell) spheres compared to Au(core)Pd(shell) particles oriented with conjoining axis parallel and perpendicular to light (k). Au and Pd are represented in the schematics by black and white, respectively.

Andrew Logsdail
School of Chemistry

## Cross-Correlation Nanoparticle Tracking for 2D Spatial Drift Correction in Post-

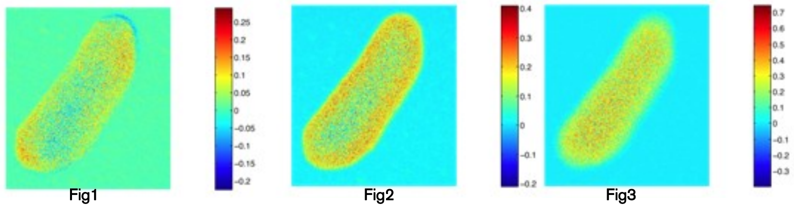


Fig1 Fig2 Fig3

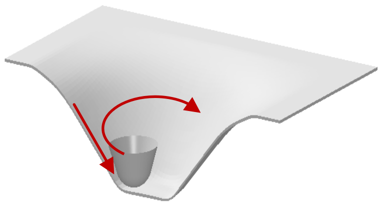
Scanning Transmission Electron Microscopy (STEM) with aberration correction is a powerful tool for nanostructures. However, like many other microscopy techniques, lateral spatial drift due to the relative movement of the probe and the sample often hinders quantitative analysis of images taken under varying experimental conditions. Fig. 1 shows the relative position of Au nanorod in the images and Fig. 2 is the normalized uncorrected image subtraction, in which blue and red parts comes from nonalignment of the sample. Due to the large dataset involved, manual alignment of the images is not feasible.

In this study, we have developed a semi-automatic routine based on the cross-correlation algorithm for post-acquisition image analysis to improve the efficiency of alignment. Correlation coefficient was employed as the criterion, taking advantage of its linear invariability. The maximum of correlation coefficient indicates the relative drift distance. These images can then be re-aligned through matrix manipulation.

We applied this method to the images we had taken of Au nanorod structures. With comparison of the centroids of successive images (512x512pixels), the standard deviation is within 2 pixels and subtracted images are much more uniform (Fig. 3). This demonstrates the validity of this approach and improves greatly the efficiency of post quantitative information extraction.

Dongsheng He
School of Physics and Astronomy

## Evaluation of deformation mechanisms in single point incremental forming SPIF (Single



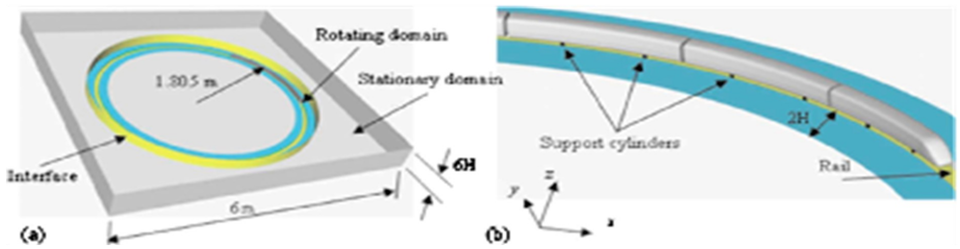
Many of the previous investigations have focused on an analysis of deformation mechanics of SPIF through experimental investigations or by using the finite element (FE) method. The work, however, is contradictory with different views on the detailed deformation modes. From a review of the literature, it was suggested that stretching and thinning are the dominant modes of deformation. Conversely, experimental measurements from some investigations indicated that high values of transverse shear are present through the thickness. Numerical methods, for example FE modelling, permit a detailed study of complex deformation behaviour and as experimental observations of through -thickness phenomena are extremely difficult, modelling of the SPIF processes becomes an essential tool.

The aim is to evaluate the presence of through-thickness shear deformation through a multi-level FE approach and to investigate how it is affected by the process parameters. Additionally, improve the geometrical accuracy without affecting the process flexibility.

Using a dual-level FE modelling approach, a significant value of through-thickness shear in two planes is predicted. One of these planes is perpendicular to the tool movement and the other is parallel to the tool direction. This suggests that this shear strain could be a major contribution to the increase in the forming limit of the material in this process. Simple strategies such as adding a backing plate, using a  kinematic supporting tool and tool path optimization result in considerable improvement in the geometrical accuracy of the final product.

Khamis Essa
School of Mechanical Engineering

## CFD (Computational Fluid Dynamics) Simulations of Train Slipstreams on a Rotating Rail




The highly turbulent non stationary nature of the slipstreams make their measurement difficult and time consuming. Moreover, several passes of the train have to be made in order to identify the trends of behaviour and the statistics of the slipstream. A new technique has been developed in order to minimise considerably the measuring time. It consists of a rotating rail rig to which a 1/50th scale model of a four coach train is attached. Although this technique allows the tests to be carried out more rapidly, it also introduces a curvature that affects the velocity results on either side of the train. CFD calculations, with different turbulence models, are carried out and results are validated using the experimental data. Further CFD calculations for different rig curvatures should enable a judgment to be made on recommendations for the design of a larger more representative rig that retains the utility of being able to simulate many train passes rapidly whilst being more representative of reality

Ansys ICEM-CFD was used to create the computational domain. The transient behaviour of the slipstream around the train is investigated using LES with the standard Smagorinsky model. To investigate the reliability of using RANS to predict the slipstream velocity, a RANS simulation has been performed using the SST- KOmega model at the same Reynolds number as the LES simulation.

The LES results are in close agreement with the experimental results. Although RANS didn't predict the slipstream velocity accurately, results are good enough to capture the differences in slipstream velocities between the inner concave side of the train and its outer convex side. Therefore, in the simulations to come, RANS will be used to find the maximum curvature the rig can present to be repre-

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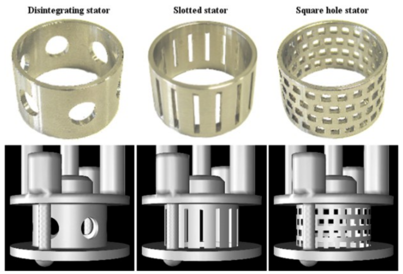
## High shear rotor-stator mixers




A rotor-stator mixer consists of a rotor closely surrounded by a stator with a small gap between the rotor and stator, typically of the order of 0.1 mm. High speed jets emerge from stator openings as the rotor rotates at a few thousand rpm. Rotor-stator mixers have been used extensively in industry to make products containing dispersed solid and/or liquid such as shampoo, body lotion, mayonnaise, lipstick, toothpaste, printing ink, etc. However, the interaction between the rotor and stator, the effect of rotor and stator geometries on the mixing performance and the scale-up procedure for rotor-stator mixers are still not well understood. CFD simulation (Computational Fluid Dynamics) was used to investigate the hydrodynamics in the rotor-stator mixer. The presence of a small gap between the rotor and the stator and high speed of the rotor make the simulation of rotor-stator mixers a very challenging task. The rotor diameter is 2.82 mm and the gap between the rotor and stator is 0.175 mm. The CFD model uses full 3-D with more than one million computational cells. Due to periodic nature of rotor-stator interaction, a transient sliding mesh model with a time step of 0.0005 s was used to simulate rotor rotation making this simulation very time consuming. The flow patterns in the stator holes are characterised by emerging jets in the proximity of the leading edge which induce circulation flows behind them. Jets emerging from disintegrating stators (wide holes) move in the same direction as the rotor, while those emerging from slotted and square hole stators (narrow holes) move against the rotor. Laser Doppler anemometry was also used to measure time-averaged velocity profiles of emerging jets and good agreements with CFD predictions were obtained. In all investigated stators the high energy dissipation rates occur in the proximity of the leading and trailing edges due to stagnations on those regions. Stators with narrow holes generate a more uniform energy dissipation rate in the holes than stators with wide holes, suggesting that they can produce dispersion with narrow drop size distribution. Two papers have been published from this work. Currently, the CFD simulation is used to simulate larger scale rotor-stator mixers to investigate the effect of scale-up procedures, i.e. constant tip speed and con-

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