Loughborough University

SCIENCE MATTERS CREATING THE FUTURE

School of Science Annual Doctoral Research Conference

Friday 31 March 2023, 09:00-16:30
West Park Teaching Hub

PROFESSOR BAIHUA LI

LOUGHBOROUGH UNIVERSITY

Professor Li has an over 15-year research track record in AI, computer vision, machine learning, pattern recognition, and signal/image processing. Primary research topics include human motion analysis, activity, and behaviour recognition, HCI, motion tracking, object recognition, sensing, robot vision, medical image analysis, and data science.

Professor Li has more than 90 papers that have been published in high-impact journals and conferences. She also has a proven track record of attracting external funding. She contributed to several projects funded by EPSRC, Innovate UK, Newton, NHS, TSB, and industry. In the last three years, she has successfully secured over £1.4M external funding in total.

PROFESSOR SIR MARTYN POLIAKOFF

UNIVERSITY OF NOTTINGHAM

Professor Sir Martyn Poliakoff is a global leader in the field of green chemistry, where his most recent research interests involve the chemical applications of supercritical fluids. Since 2008, he has been a prominent presenter on the YouTube channel ‘Periodic Videos’, a popular sciences series with over 1.5 million subscribers and 700 videos dedicated to familiarising the public with all 118 elements on the periodic table. Owing to his research, ambassadorial services to the UK and outreach work, he has received numerous prestigious awards including a CBE in 2008, followed by a knighthood in 2015.

CONFERENCE SCHEDULE

TIME	ACTIVITIES
09:00-09:15	Registration & Refreshments
09:15-09:30	Welcome speech: the School Associate Dean for Research and Inoovation, **Professor Sergey Saveliv** and pre-recorded welcome speech: Pro Vice-Chancellor for Research and Innovation **Professor Daniel Parsons**
09:30-10:15	Keynote speaker: **Professor Baihua Li** Topic: **Machine Learning and AI for Industrial Automation**
10:15-12:00	PhD Student Research talks
12:00-13:00	Lunch & Poster Session
13:15-14:30	PhD Student Research talks
14:30-15:20	Poster Session & Break with Bom Bom cookies and coffee
15:20-16:05	Keynote speaker: **Professor Sir Martyn Poliakoff** Topic: **Making Chemistry More Sustainable**
16:05-16:30	Award and Prizes

RESEARCH TALKS SCHEDULE

MORNING SESSIONS

START	ACTIVITIES	DEPARTMENT	TITLE
10:15	Adam Essex	School of Mathematics	Bifurcation Mechanisms for Memory Formation in a Neural Network
10:30	Agnes Bokanyi-Toth	School of Mathematics	Liquid bridges suspended between horizontal cylinders
10:45	Bassey Oboho	School of Mathematics	Modelling Niobium-based Solid Electrolytes for Lithium-ion Batteries
11:00	Bobo Kai Yin Chan	Mathematics Education	The spacing effect and working memory resources depletion hypothesis – A cognitive load theory framework.
11:15	Charlie Huggins	Physics	A Method to Detect Quantum Coherent Transport in Lossy Devices
11:30	James Madeley	Computer Science	Internet-scale Testing: Large problems with Compact Solutions
11:45	Jan Cammann	School of Mathematics	Active Spaghetti: Collective Organization in Cyanobacteria

AFTERNOON SESSIONS

START	ACTIVITIES	DEPARTMENT	TITLE
13:15	Jonah Drake	School of Mathematics	Modelling human endurance: Power laws vs critical power
13:30	Megan Foulkes	Mathematics Education	Manipulatives with complex features play a role when teaching mathematics in the early years
13:45	Tom Mason	School of Mathematics	Active particles immersed in nematics
14:00	Xuetong Pei	Chemistry	Homogeneous and Single-site Heterogeneous Catalyst for Guerbet Reaction
14:15	Yangfan Jiang	Physics	Using AI methods to improve the performance of a gamma camera for medical imaging.

BIFURCATION MECHANISMS FOR MEMORY

ADAM ESSEX

NN are abundant in applications across a range of fields and their importance in advanced technology is becoming ever clearer. However, there is a fundamental lack of transparency in the mechanisms underpinning their intelligent behaviour even in the simplest systems, namely, those responsible for memory formation and decision making. Many attempts to combat this issue have been so far unsuccessful and hence we propose a different approach to the NN by considering it as a non-autonomous dynamical system and analysing its velocity vector field which we believe may hold the key to unlocking its transparency. Here we study an 81-dimensional version of the Hopfield network, one of the simplest neural models available, using several visualisation methods to view both the formation of attracting fixed points which code the memories of a network but also their 81-dimensional basins of attraction which dictate the neural networks decisions

LIQUID BRIDGES SUSPENDED BETWEEN HORIZONTAL CYLINDERS

AGNES BOKANYI-TOTH

DMITRI TSELUIKO, ANDREW ARCHER AND HEMAKA BANDULASENA

Liquid bridges suspended between two horizontal cylinders are studied using (i) experiments, (ii) direct numerical simulations and (iii) reduced-order model equations. The reduced-order model is based on Onsager's variational principle, which is equivalent to the minimum energy dissipation principle in Stokesian hydrodynamics. The model equations are implemented in MATLAB, and liquid bridges are investigated both in the presence and absence of gravity. We show both analytically and numerically that the equilibrium contact angle minimises the free energy and the minimum of the Rayleighian function gives the dynamics. The results from the solution of the simplified model are corroborated by direct numerical simulations in COMSOL.

Additionally, we analyse the influence of the electric field resulting from an imposed potential difference between the cylinders on the dynamics of liquid bridges, using a boundary-element method to solve the electric-field equations. We find that electrified bridges move up and develop stable, flatter interfaces.

We also developed an experimental setup and filmed the dynamics of both electrified and non-electrified liquid bridges. Silicone oil droplets were suspended between parallel cylindrical electrodes and observed under high electric fields. We find that the experimental observations are well described by the model equations for a wide range of parameter values.

MODELLING NIOBIUM-BASED SOLID ELECTROLYTES FOR LITHIUM-ION BATTERIES

BASSEY OBOHO

ROGER SMITH AND POOJA GODDARD

In an effort to create an all solid state lithium-ion battery, a Niobium based garnet material ($Li_5La_3Nb_2O_{12}$, LLNO) is a promising alternative to the common Zirconium based solid electrolyte. Niobium normally exhibits oxidation states ranging from +3 to +5. This virtue alone makes Niobium a challenging element to model theoretically as a main component element or as a main doping element. There are a few papers that experimentally introduce LLNO as a viable solid electrolyte and shows that the addition of external defects improves the energy density and electrochemical performance of the battery. However, it is shown that the unit cell of LLNO varies depending the preparation technique and the type of external defect used; making this a controversial material. To this day there are no modelling papers on a pure LLNO material.

In this talk, I will show theoretically that pure LLNO adopts a cubic crystal system of around 12.75 Å supported by Bo et al. I will also show that using Zinc as a dopant is more favourable on the Niobium site than on the Lanthanum site but still maintains its cubic crystal system as well as the Lithium diffusion pathways in pure and Zn doped LLNO.

THE SPACING EFFECT AND WORKING MEMORY RESOURCES DEPLETION HYPOTHESIS – A COGNITIVE LOAD THEORY FRAMEWORK

BOBO KAI YIN CHAN

OUHAO CHEN AND TIM JAY

The spacing effect refers to the improvements of learning performance when comparing to massed practice after the insertion of temporal gaps between learning sessions (Ebbinghaus, 1885). The effect has been widely investigated and many theoretical frameworks have been developed to explain the effect. However, none of these frameworks can fully explain the spacing effect. Therefore, a new alternative named working memory resources depletion hypothesis is developed under the cognitive load theory to explain the spacing effect. In the experiments, materials high in element interactivity were used as learning materials. Element interactivity refers to the interconnectedness of elements in a piece of learning material, which is also an indicator of the complexity of tasks. Level of element interactivity is determined by the number of interactive elements in a piece of material (Sweller et al., 2010). Materials that are low in element interactivity consist of a low number of interactive elements and those elements can be processed in the working memory in isolation. Conversely, materials that are high in element interactivity consist of a huge number of interacting elements that have to be processed in the working memory simultaneously which overloads the working memory as working memory is limited in capacity. The experiments compared spaced and massed practice and aimed at explaining the spacing effect induced by the working memory resources depletion hypothesis. Working memory resources depletion hypothesis suggested that limited working memory resources are depleted when extensive cognitive effort has been put to learning and replenished after deliberate-resting-from-learning (Chen et al., 2018).

A METHOD TO DETECT QUANTUM COHERENT TRANSPORT IN LOSSY DEVICES

CHARLIE HUGGINS

A ZAGOSKIN, S SAVEL'EV AND A BALANOV

Advances in electronics are being limited by the approaching end of Moore's law. As we attempt to fit more and more components into smaller chips, we need to take into account quantum effects in circuits. Quantum analogues for lossless elements in circuits (Inductors, Capacitors) already have quantum analogues, our work is focusing on describing/testing lossy elements (Resistors, Memristors). In this talk, we discuss our paper on testing for quantum correlations in such lossy circuit components. We look at a general form for a qubit-controlled quantum memristor and look for ways to distinguish classical and quantum transport.

We do this by taking regular measurements to collapse the state of the qubit, using Fourier methods to look for a spectral fingerprint of state switching at the measurement frequency, indicative of the state collapse that we would expect from a quantum device, not a classical one. We simulate the system and indeed find the evidence of the signal mixing that we were looking for, in a variety of testing circuits. We see relevant spectral components particularly when the projective measurements switch frequently, and find evidence of the switching events in dissipative and noisy systems.

INTERNET-SCALE TESTING: LARGE PROBLEMS WITH COMPACT SOLUTIONS

JAMES MADELEY

IAN PHILLIPS, POSCO TSO

In the last 30 years the Internet has grown rapidly. There are now billions of connected devices all capable of sending and receiving massive amounts of data every second. To allow information transfer on this scale, the Internet has been built with robust and reliable protocols in place to make sure that every cat video and passive-aggressive email gets where it needs to go almost every time. Moving all this traffic around comes with some challenges beyond the logistics of just working out where to send each packet.

With so much relying on the Internet's expected operation, testing new technology on the live network is a dangerous idea. To get around this, developers of such technologies opt to use methods like simulation, emulation, or physical testing environments. Each of these come with their own pros and cons, however they often share one drawback – large setup costs. Whether that comes in the form of monetary costs paying for equipment, or time costs to configure virtual test environments, a lot of investment is usually required to get large-scale testing started.

We have created a software system that takes minimal user input and generates high numbers of configuration files for emulating large networks. The goal is to give the user as much control as possible, whilst having very few requirements to get started. Users can configure a network with nothing more than a name and number of devices. However, every amount of detail can also be specified, and our system will fill in the blanks.

The system is built using Python and a template-based approach, so it can be configured for different emulation platforms. Large emulation testbeds can be created and edited in a reproducible fashion, which provides a solid middle ground between simulations and physical testing. Templating brings flexibility in emulated software and emulated environments. The former are technologies such as Quagga, Bird, and FRRouting, and the latter are environments such as Kathara, Minimega, etc.

The Internet is divided into Autonomous Systems (ASes). Each AS needs to know about all the others to route traffic across them. There are over 800k ASes in the routing table, which uses a lot of storage and is slow to search. Routers have been built with ever-increasing resources to deal with this problem, but that solution is unsustainable.

One proposed method to reduce the table size in routers is Compact Routing. This is a hierarchical routing approach based on Cowen's Landmark Routing. We are creating a simulator to test the feasibility of this approach. The simulator is written in Golang, allowing concurrent execution and a closer approximation to real router-based execution than other methods.

After the simulations are complete, we aim to test in an emulated environment (where our previously mentioned work will be useful) with a view to eventually implement Compact Routing in BGP.

ACTIVE SPAGHETTI: COLLECTIVE ORGANIZATION IN CYANOBACTERIA

JAN CAMMANN

MIXON FALUWEKI, LUCAS GOEHRING AND MARCO MAZZA

Collective organisation is a defining feature of living matter. It has received vivid attention for its applications in the life sciences, and as an example of how nonequilibrium forces can drive flows of matter and energy. As an important example of active matter, cyanobacteria are among the most abundant organisms on Earth. They evolved the photosynthetic mechanisms that led to our oxygenrich atmosphere and perform nearly all nitrogen fixation in marine environments. Filamentous cyanobacteria also straddle the boundary between single and multicellular organisms; they can grow into chains of cells several millimetres long through ‘filamentation’, perhaps the oldest form of multicellularity. They can show fascinating patterns of self-organisation, which however are not well-understood from a physical perspective. We investigate the motility and collective organisation of colonies of these simple multicellular lifeforms. As their area density increases, linear chains of cells gliding on a substrate show a transition from an isotropic distribution to bundles of filaments arranged in a reticulate pattern. Based on our experimental observations of individual behavior and pairwise interactions, we introduce a model accounting for the filaments’ large aspect ratio, fluctuations in curvature, motility, and nematic interactions. This minimal model of active filaments recapitulates the observations, and rationalises the appearance of a characteristic lengthscale in the system, based on the Péclet number of the filaments. We note that the parameters governing their self-organisation identified in our work are evolutionarily selectable traits, which can inform the study of the fossil record.

MODELLING HUMAN ENDURANCE: POWER LAWS VS CRITICAL POWER

JONAH DRAKE

In endurance sports like cycling, running, or rowing, athletes (from recreational to elite level) and their coaches are typically interested in answering questions like the following:

What finish time can a particular runner achieve in a marathon?
How long can a particular cyclist sustain a given power output?
Is the athlete's fitness improving under the current training regime?

Answering these questions requires modelling and estimating the intensity--duration relationship, i.e. the relationship between exercise intensity (e.g. power output in cycling/rowing or velocity in running) and the time to exhaustion.

The dominant paradigm in Exercise Physiology and Sports Science asserts that this intensity—duration relationship is hyperbolic. Indeed, this hyperbolic shape is thought to be a "fundamental bioenergetic property of living systems". Consequently, the so-called hyperbolic (a.k.a. "critical power") model, which formalises this hyperbolic shape, is the basis for (a) fitness metrics used by millions of athletes worldwide; (b) a vast number of studies on the effectiveness of training-regime or nutritional interventions.

We investigate the adequacy of the hyperbolic model and compare it with an alternative power-law model.

Methods
Empirical studies of thousands of athletes from running, cycling and rowing, as well as some simple algebra.

Results
The intensity—duration relationship is not hyperbolic. In fact, it is much more adequately represented by a power-law model.

Conclusion
Our findings call into question one of the dominant paradigms in Exercise Physiology and Sports Science. Our results show that athletes and coaches can improve fitness assessment and performance prediction by discarding the hyperbolic ("critical power") paradigm in favour of simple power-law modelling. Further results and discussion can be found in our pre-print.

MANIPULATIVES WITH COMPLEX FEATURES PLAY A ROLE WHEN TEACHING MATHEMATICS IN THE EARLY YEARS

MEGAN FOULKES

FRANCESCO SELLA AND CAMILLA GILMORE

Early mathematics achievement has been strongly associated with later academic success and occupational outcomes, making it fundamental when thinking about 'creating the future'. Physical objects, often referred to as manipulatives, play a key role for children when engaging in early mathematical learning. This is because physical manipulation and exploration can help make abstract mathematical ideas more accessible for younger learners. Despite a relative consensus on the benefits of their use, there is a dispute as to which kinds of manipulatives are best to use with children when teaching mathematics.

A key point of contention concerns whether different manipulative features help or hinder learning. Researchers frequently argue that more complex features (e.g., bright colours, interesting textures), or features associated with real life objects that often activate prior knowledge (e.g., toy animals or natural world objects like conkers) can distract children. Their irrelevant surface features are said to take up valuable cognitive resources, and can divert children's attention away from the idea the manipulative is intended to represent. Therefore, researchers tend to recommend the use of more perceptually basic manipulatives to provide transparent links between the manipulative and the mathematical concept being taught.

However, the extent to which research contexts represent learning in more naturalistic settings is questionable, with practitioners potentially prioritising factors beyond optimal cognition when selecting manipulatives. In this presentation, I will discuss results from interview and online survey data collected from Early Years and Year 1 teachers, which revealed that manipulatives with interesting features play an important role in early mathematics teaching in UK classrooms. Features that are often perceived as 'irrelevant' by researchers were said to help engage children's attention, boost positive affect towards mathematics, and facilitate the creation of additional learning opportunities. Additionally, teachers described managing the potential for distraction through the use of various instructional strategies and tactical introduction of manipulatives at different stages in children's learning.

In light of these findings, I will highlight the complexity of manipulative use with young children when learning mathematics, particularly in relation to different manipulative features and the context in which they are presented. Relatedly, I will consider the extent to which research designs reflect varying factors associated with manipulative use in naturalistic contexts, and emphasise the value of collaborating with practitioners to best determine future research directions.

ACTIVE PARTICLES IMMERSED IN NEMATICS

TOM MASON

Microswimmers are natural or artificial self-propelled objects that can convert some source of energy into directed motion and thus move through fluid environments. Artificial or biohybrid swimmers have the potential to be used for highly targeted drug delivery, microsurgery, and disease monitoring. To achieve these technological goals, control over microswimmers' trajectory and orientation is needed in complex fluid environments. While the dynamics of swimmers immersed in Newtonian fluids have attracted considerable attention and their basic principles are rather well understood, complex fluid environments featuring anisotropy and elasticity, such as nematic liquid crystals are relatively less understood.

Recently, new computational methods have been developed to study the dynamics of spherical microswimmers in a nematic fluid. The multi-particle collision dynamics method (MPCD) is a particle-based, mesoscale fluid simulation technique well known for its simplicity as well as its ability to fully incorporate thermal fluctuations and complex hydrodynamic interactions. Recent work has successfully modified the MPCD method to replicate a nematic liquid crystal environment, and also investigated the presence of a spherical microswimmer model, known as squirmer, in the nematic MPCD simulations. Their behavior within these models matches current experimental results.

In this presentation we report on the hydrodynamic interaction forces between two squirmers in a variety of mutual configurations and distances. We have found strong attractive forces between squirmers when placed head-to-tail, and a weaker repulsive force when placed side-by-side. Future work will include the squirmers' dynamical behavior and effects of confinement.

HOMOGENEOUS AND SINGLE-SITE HETEROGENEOUS CATALYST FOR GUERBET REACTION

XUETONG PEI

Owing to the increasing rate of CO_2 emission associated with environmental problems, the application of biofuels seems to be the desired solution for solving the rising energy demand as they shared similar energy density with fossil fuel. The catalytic Guerbet reaction is used for ethanol to n-butanol transformation, which can be catalysed by employing either homogeneous or heterogeneous catalysts, under mild conditions. Ruthenium catalysts are known to be highly stable and active for the rate limiting dehydrogenation step for n-butanol formation from ethanol.

Experimental

Homogeneous catalyst: Dichloro(p-cymene)ruthenium(II) dimer was synthesis referring to literature. The [RuCl(p-cymene)(dppm)]Cl was synthesis during the catalysis. Single-site heterogeneous catalyst: PPhen-bipy and PPhen-[bipy-RuIIICl4]H (Ru PPhenbipy) was prepared by the method from literature. Both fresh catalysts were characterised by XRD, BET, IR, XRF, STEM, EXAFS. Catalysis: Catalytic activity for both homogeneous and single site catalysts was tested using Parr reactor with ethanol. Same conditions were applied for homogeneous and heterogeneous catalysts. 30% H_2O was added to the reaction. The solution was analysed by GC-FID and MP-AES. The syngas was analysed by GC-TIC.

Results and conclusion

4 wt% Ru was found in Ru PPhenbipy framework via XRF, providing 25.3% ethanol conversion after 16 h. The [bipy-RuIIICl4]- site enable to transform ethanol to n-butanol with a turnover number of 3495 Ru^{-1}, offering much higher catalytic activity comparing with that of Ru homogeneous catalyst with dppm ligand. H_2, CO and CH_4 were found as syngas. No leaching for Ru and Pd in reaction solution proved the high stability for Ru PPhenbipy comparing with other homogenous and heterogeneous catalysts. Similar XRD diffraction spectrum and FTIR spectra were observed for fresh and post reaction polymer framework catalysts, whereas n-butanol was found trapped into the framework after post reaction. The decrease in ethanol conversion after water addition indicated catalyst deactivated by water. The post reaction with addition of molecular sieves showed a dramatic increase in catalytic activity, proving that water deactivates polymer framework catalyst. The time online reaction showed the catalyst deactivated after 48 h. EXAFS data showed the changed of structure after reaction. 0.34 wt% Pd was found in PPhenbipy, showing high activity on n-butanol production (15919 Pd^{-1} for TON).

USING AI METHODS TO IMPROVE THE PERFORMANCE OF A GAMMA CAMERA FOR MEDICAL IMAGING.

YANGFAN JIANG

SARAH BUGBY AND GEORGINA COSMA

Gamma imaging is essential in the field of nuclear medicine and is widely applied for cancer diagnosis. The traditional gamma cameras used in hospitals are bulky (they take up a whole room) and so cannot be used for intra-operative imaging. Real-time imaging information during surgery can aid surgeons in identifying tissue of interest and is particularly important for complex surgeries in areas such as the brain or neck. There is therefore clinical interest in using portable gamma cameras to localise lesions during surgery.

A hybrid Gamma Camera (HGC) was developed by the University of Leicester in 2014 [Lees et al., 2014, Bugby, 2015, Lees et al.,2017], which provides the potential for real-time gamma imaging during surgery. This is a portable system, which provides both gamma and optical images of a 2D field of view however the surgical area of interest is 3-dimensional and depth, as well as 2D position, is important.

Creating 3D images from portable gamma cameras is possible but existing techniques either require additional optical tracking systems [Matthies et al., 2014], time-consuming calculations of triangulation and/or human input to match sources across different views [Bugby et al., 2021].

Deep learning (DL) Artificial Intelligence techniques have employed in a wide range of applications in medical imaging processing and for visual depth estimation in computer vision. Examples include small biomarker detection in medical images [Xu et al., 2019] and autonomous driving [Grigorescu et al., 2020].
The fundamental techniques behind these applications are object detection and recognition.

During my PhD I have applied these techniques to data outputted by the HGC creating a new DL object recognition model (DeepSplashSpotter [Jiang et al., 2022]) which can improve the HGC's detection performance. I am now extending DL methods from visual object estimation to obtain source depth information from 2D HGC images. However, DL methods require large datasets to train the models and so I have first implemented and validated a Monte Carlo (MC) for simulating stereoscopic gamma images. The overall goal of this section of work is to develop a model that will provide surgeons with real-time 3D information from the HGC.

This talk will include an introduction to deep learning and Monte Carlo simulation and show how these can be applied to the HGC for medical imaging.