MATHEMATICS, PHYSICS & SPACE PGR CONFERENCE

Tuesday 28th January 2025

Time	Event
09:45	Welcome
09:50 - 10:50	Maths: Daniel Knott Physics: Matthew Freed
10:50 - 11:00	Break
11:00 - 12:00	Maths: Dan Catlin Physics: Astha Astha
12:00 - 13:25	Lunch
13:25 - 14:25	Maths: Elliott Farrall Physics: Kathleen Dunbar
14:25 - 14:35	Break
14:35 - 15:35	Maths: Esha Joshi Physics: Megan Eaton
15:35 - 15:45	Break
15:45 - 16:45	Maths: Lewis Napper Physics: Harry Addison
16:45 - 17:00	Closing and Prizes

Daniel Knott

Dynamic Mode Decomposition of Sleep EEG

Electroencephalography (EEG) recordings are commonly used for studying sleep, which can be nonlinear, nonstationary, and noisy. High density EEG improves the spatial resolution of the data; however, many traditional analysis methods like spectral analysis focus primarily on temporal or spatial properties in isolation, not capturing the full spatio-temporal dynamics of neural activity.

Dynamic mode decomposition (DMD) offers a data-driven approach to find a reduced-order model of the system, decomposing the data into dominant spatial modes with associated temporal dynamics. We show how this can be used to identify dominant patterns of neural activity, offering a new perspective on sleep-related brain dynamics. DMD is compared with existing EEG analysis methods, and preprocessing and parameter choices are discussed, including the use of time-delay embedding as a preprocessing step. We address the challenges of analysing nonstationary EEG data using DMD and propose approaches for systematic comparison of DMD modes across epochs, trials, participants, and conditions.

Matthew Freed

Creating Dark States with Permanent Dipoles

Dark states (states that don’t normally absorb or emit light) have been proposed as a mechanism that improves the efficiency of photosynthesis and light harvesting technologies.

Many organic molecules have strong permanent dipole moments, which can shift when the molecules are excited by light. We explored how these permanent dipoles affect optical properties in a paired, or "dimer," system of molecules. By calculating how different physical processes contribute to the light-absorption transitions, we can see how permanent dipoles influence the overall behaviour in different conditions.

Our study reveals two ways in which dark states can form in these systems. The first mechanism occurs when the transition dipoles of the two molecules interfere destructively, creating a dark state from a mixed or "superposition" state. In this scenario, permanent dipoles can cause the dark state to "leak," making it able to absorb light from either the ground or an excited (bright) state, depending on the orientation of the dipoles. The second dark-state formation mechanism is unique to systems with permanent dipoles and arises when the transition dipoles and permanent dipoles interfere destructively. These create accessible dark states that do not necessarily leak.

Dan Catlin

Dynamic Centrality and Clustering: Tools for Understanding Criminal Networks

This study examines methods for identifying key figures within dynamic criminal networks, addressing challenges of incomplete and obscured data. Using data from the Cicala investigation—a surveillance operation on the 'Ndrangheta —we apply the Katz centrality to measure information flow and K-means clustering to group nodes by influence in both static and dynamic network contexts. Our results reveal that Katz centrality uncovers critical nodes missed by traditional measures, and clustering exposes shifts in network control over time and identifies clusters of nodes directing the network. Simulating data gaps highlights the trade-offs in prediction accuracy, providing valuable insights into network resilience and aiding law enforcement in disrupting organized crime.

Astha Astha

The time-evolution of the mass-metallicity relation

The mass-metallicity relation is a tight correlation between V-band magnitude and [Fe/H] seen in galaxies over a wide range of masses, with a possible plateau or increased scatter below MV ~ -5 [1]. It has been shown to be particularly sensitive to feedback processes in dwarf galaxy formation models, with models that have too strong/weak feedback causing dwarfs to lie systematically below/above the redshift zero relation [2]. These same models also predict how galaxies move in MV-[Fe/H] over time. Here, we use resolved colour magnitude diagram data, combined with spectroscopic metallicity measurements, to determine how nearby dwarf spheroidal and irregular galaxies move through MV-[Fe/H] space over time. We compare this with similar tracks drawn from the EDGE simulations to determine what additional constraints the time-evolution of MV-[Fe/H] can provide on galaxy formation models, particularly feedback processes.

[1] https://ui.adsabs.harvard.edu/abs/2013ApJ...779..102K/abstract
[2] Agertz, O. et al. EDGE: the mass-metallicity relation as a critical test of galaxy formation physics. Mon. Not. R. Astron. Soc. 491, 1656–1672 (2020)

Elliott Farrall

Minimisation of the Dirichlet Energy amongst a class of constrained maps

A common approach to modelling physical phenomena in modern physics is through variational methods, which involves minimising a functional that is associated with the system. If one wishes to model the deformation of an elastic material, the associated functional is the Dirichlet Energy functional:

$$E[u] = \int_\Omega |\nabla u(x)|^2 \, dx$$

However, one find that the minimiser (in the standard space H^1) of this functional are a-physical in the sense that they do not represent (in general) mass-conserving deformations. This is in stark contrast to other problems modelled through variational methods, where minimisers satisfy necessary conservation laws and these laws can often be derived from the functional using symmetries. The only way to rectify this approach and recover physical minimisers is to adjust the space in which we minimise, constraining it to a subspace of maps representing physical deformations. The most obvious space would be

$$A = \{u \in H^1(\Omega) : \det \nabla u = 1 \text{ a.e.} \}$$

This is a non-linear space which leads to several complications in showing the existence/uniqueness of minimisers which we will discuss in this talk. My research focuses mainly on the existence of minimisers amongst a generalised class of maps given by

$$A = \{u \in H_{u_0}^1 (\Omega) : \det \nabla u = \det \nabla u_0 \text{ a.e.} \}$$

Time allowing, we shall discuss some sufficient conditions for the existence of minimisers in this class and techniques for constructing constrained optimisation problems that have a minimiser.

Kathleen Dunbar

Increased hydrogen production from genetically modified Escherichia coli and their use within biocoatings

Hydrogen offers a source of energy that does not produce any greenhouse gas when combusted, and hence the global demand for hydrogen fuel is growing. The production of hydrogen by bacteria is an attractive alternative because it does not require fossil fuel feedstocks, however, the yield needs to be increased for biohydrogen to be commercially competitive.

In this work, hydrogen was produced using genetically modified Escherichia coli in liquid cultures via dark fermentation. Bacteria were cultured anaerobically (in a hydrogen free environment) in Balch tubes for 24 hours, and the headspace gas was measured using a residual gas analyser. Single knockouts of genes from the mixed acid fermentation pathway were initially investigated with the best performing single gene knockouts being combined to produce double knockouts. The best performing double knockout produced significantly more hydrogen than the single gene knockouts and produced four times more hydrogen than the wildtype strain. Interestingly, this double knockout also produced two times less carbon dioxide compared to the wildtype strain, making biohydrogen an attractive alternative to brown and grey hydrogen production methods.

Confining E. coli in a waterborne polymeric coating (to make a biocoating) was found to keep the bacilli metabolically active, but non-dividing. The genetically modified strains were confined in a biocoating to contain them in bioreactors and to protect them from external contaminants that can affect hydrogen production. Hydrogen production was measured over five days using hydrogen microsensors. This is the first time that E. coli biocoatings have been used to produce hydrogen.

Lewis Napper

<u>Synthetic Geometry, Curvature, and Comparison – A Primer</u>

Rather than invoking the dark magic of differential geometry, it is possible to study Riemannian manifolds in a synthetic manner, using only distances and angles between curves. Indeed, by defining properties such as length in this way, they can be extended to lower regularity, non-smooth structures, namely metric spaces. Furthermore, although curvature is usually defined via differentiation, by comparing our metric spaces to Riemannian manifolds of known constant curvature, it is even possible to bound the curvature of a metric space. These tools have been essential in the development of optimal transport, Gromov–Hausdorff convergence, and crystallographic group theory.

This talk is intended as a primer to the ideas behind synthetic geometry and curvature comparison. We begin by defining a metric space and describing what it means for such a space to be geodesic. The technique of triangle comparison for bounding the curvature of a metric space is then introduced and we establish criteria for when a metric space has local vs global curvature bounds. This is accompanied by some natural examples. Furthermore, we show that a space with curvature bounded below by some $k>0$ has an upper bound on its diameter. If time permits, we shall compare and contrast these techniques with their comparably new Lorentzian analogues — the Lorentzian pre-length spaces.

Megan Eaton

Use of a Convolutional Neural Network as a Breast Density Estimation Tool

Breast density is the proportion of glandular tissue within the breast compared to the fat (or adipose) content. Dense breasts are a significant risk factor for breast cancer, but measuring density is challenging. To address this, AI models have been developed to estimate breast density from mammograms. These have been deployed clinically in the United States but not in the UK due to a lack of consistency and overall higher density estimations. This work combines AI analysis with spectral imaging using a spectroscopic photon-counting detector as a novel way to estimate breast density. A blended spectral training set consisting of simulated and experimental data has been built using simplistic slabs of breast-equivalent tissue as phantoms. A convolutional neural network was developed with the simulated and experimental spectral data and breast thicknesses as inputs. The model was trained on these to estimate breast density and was tested on a random selection of unseen spectra. This was effective, with a very low mean squared error in the model’s predictions. Future work will focus on constructing more realistic breast phantoms as experimental test objects and simulated models. By developing a reliable breast density estimation method, it would be possible for early detection of breast cancer by tailoring the screening interval based on risk.

Esha Joshi

Mechanistic modelling for pre-clinical drug trials using spatially resolved tumour cells: A dive into some initial insights

How to reduce the translation gap between results of pre-clinical and clinical drug trials is an important question in the pharmacology. By establishing a better mathematical understanding of the results of pre-clinical trials our aim is to improve translation and reduce the need for animal models.

As a first step, we use data from patient derived xenografts (PDX) from Novartis that includes tumour growth and pre-clinical trial drug response. This data constitutes tumour volume measurements for 6 different types of cancer: Pancreatic ductal adenocarcinoma (PDAC), breast cancer adenocarcinoma (BRCA), carcinomatous meningitis (CM), gastric cancer (GC), non-small cell lung cancer (NSCLC), colorectal carcinoma (CRC) captured at approximately every three to four days post tumour implantation, with and without treatments of drugs.

In this talk, I will show some initial results from fitting empirical growth laws which tend to capture the longitudinal tumour growth. Our analysis includes mixed-effects modelling to account for differences between cancer types.

Longer term, our aim is to understand pre-clinical tumour growth data using mathematical models that, unlike empirical tumour growth models currently used in industry, are based on mechanistic principles. Using a mechanistic framework will enable us to incorporate spatial and pharmacokinetic and pharmacodynamic (PKPD) effects, with a focus on developing models which are fit-for-use in industries.

Harry Addison

<u>Commissioning the 4MOST Telescope: Enabling Next-Generation Spectroscopic Surveys</u>

The 4-metre Multi-Object Spectroscopic Telescope (4MOST) is a state-of-the-art survey instrument designed to transform our understanding of the cosmos through wide-field spectroscopic observations. Installed on the VISTA telescope at the European Southern Observatory (ESO) in Chile, 4MOST is equipped with 2,400 fibers and three spectrographs, capable of gathering high-quality spectra for thousands of celestial objects simultaneously. The 4MOST survey is poised to advance a broad range of astrophysical research, from mapping the structure and dynamics of the Milky Way to probing the large-scale distribution of galaxies and dark matter. In this talk, I will discuss the inner workings of 4MOST and my involvement in the telescope's commissioning phase, a critical period where hardware, software, and optical systems are tested and optimized to meet stringent scientific requirements. I will outline the challenges of calibrating and fine-tuning 4MOST's intricate fiber positioning and spectroscopic systems, as well as the collaborative efforts required to ensure successful integration with ESO’s infrastructure. My role in commissioning has involved hands-on work in system verification and data validation, providing insights into both the technical demands and rewarding outcomes of preparing this next-generation telescope for operational readiness. This experience has underscored the importance of teamwork, innovation, and adaptability in bringing ambitious astronomical instrumentation to life.

Organiser: Jessica Furber

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