



NUI Galway
OÉ Gaillimh

School of Mathematical and Statistical Sciences

12th Annual Research Day

13th April 2022

Programme

	Talks take place in the Orbsen building seminar room Coffee, lunch, posters and reception take place in the Orbsen building atrium
9:20–9:30	Welcome by Aisling McCluskey , Head of School
9:30–9:40	Opening by Jim Livesey , Vice President Research
9:40–10:10	Hannah Conroy Broderick (NUI Galway) <i>Shear shocks in periodic elastic laminates</i>
10:10–10:40	Cathal Seoighe (NUI Galway) <i>The contribution of immunoediting to the profile of somatic mutations observed in human cancers</i>
10:40–11:00	Jared Gerlach (NUI Galway) <i>Research Office and SoMaSS</i>
11:00–11:30	Tea and coffee
11:30–12:00	Ed Curry (NUI Galway) <i>Data Spaces: A new opportunity for data science</i>
12:00–13:00	Lightning talks (Organiser: Mark Howard) Shane O’Connell • Kelvin Killeen • Donal O’Shea • Faiza Alssaedi • Victoria Sánchez Muñoz • Sarah Ennis
13:00–14:00	Lunch
14:00–14:45	Jane Coons (Oxford University) <i>Algebraic Approaches to Maximum Likelihood Estimation</i>
14:45–15:15	James Cruickshank (NUI Galway) <i>Rigid Structures, Topology and Combinatorics</i>
15:15–17:00	Poster session, reception and prizes

Contents

1	Introduction	2
2	Abstracts of invited talks	4
3	Abstracts of lightning talks	6
4	Abstracts of posters	9
5	Abstracts of PhD theses	26
6	Staff profiles	27
7	Visitors	45
8	Conferences, meetings, and workshops	46
9	School seminars	47
10	SIAM Student Chapter	48

1 Introduction

Fáilte chuig an ócáid speisialta seo, ceiliúradh cursaí taighde inár scoil, scoil le hainm nua: Scoil na nEolaíochtaí Matamaitice agus Staitistice.

Welcome to our 2022 annual School Research Day. Just as last year's celebration of our research marked an historic time in the world pandemic, this year's event is no less distinctive in reflecting the steady and powerful pulse of our research outputs and achievements against ongoing and considerable odds. It is also distinctive in reverting to a largely in-person format. This booklet demonstrates the continuing creativity, strength and resilience of our community in a year of uncertainty around public health, compounded by an impactful cyberattack in the autumn of 2021 and a stark and worsening severity of physical space limitations. Our capacity to not just endure but to excel in our research mission has surely been tested – and proved, and we wear our new School name, the *School of Mathematical and Statistical Sciences*, with pride as we look back over another year of research triumphing over tribulation. Our continuing excellence in research performance must be underpinned and supported by sustainability and we will continue to seek urgent action to address our critical physical space needs.

Today's programme of talks and poster exhibition highlight the quality, the breadth, and the international significance of the research activities in each of our disciplinary clusters: the de Brún Centre for Mathematics, the Stokes Cluster for Applied Mathematics and the new-look Sonraí Health Data Science Research Cluster.

Our research clusters encapsulate and extend from core blue skies research to very targeted and focussed applications. Our research covers a wide variety of subject areas including algebra and combinatorics, analysis, geometry and topology, mathematics education, quantum information theory, modelling of soft solids/tissues and drug delivery applications, and mathematical, statistical and genomics data science; our applications range from clinical research, sports and exercise science, traumatic brain injury, cancer, immunology to neuroscience.

Some highlights since last Research Day include:

- We welcomed to the School new members Davood Roshan Sangachin (academic), Anthony Walters (senior technical officer), Róisín Hill (postdoctoral researcher working with Niall) and Quan Zhang (postdoctoral researcher working with Stephan).
- The vibrancy of our PhD programmes continued unabated. We were proud to celebrate the successful PhD defence by Faiza Alssaedi and we extend a warm céad míle fáilte to our 17 new students who commenced their PhD studies with us in the same period.
- We continued to publish extensively in world-class journals, to be awarded distinguished visiting positions and other key research leadership roles, to undertake high-profile editorial positions, to host online seminar series and workshops with international participation and to participate and progress significantly (final outcomes not yet determined) in prestigious funding schemes.
- Indicative of the foregoing, we are proud to host in-person the 24th conference of the International Linear Algebra Society this June (delayed from 2020), a major event in the mathematical calendar with an expected in-person attendance in excess of 250.
- We lead NUI Galway's involvement in a €6.8M Disruptive Technologies Innovation Fund award on the development of cancer immunotherapies and a €4M North-South award on the use of liquid biopsies, virtual biobanks and the predictive modelling of disease progression and treatment response.
- Further research awards over the past year accrue in the region of €1.6M.

Today's event showcases the indefatigable spirit and impressive reach of our research community. Today we celebrate our collective research success whilst dreaming of where our research aspirations and insights will next bring us. The energy and ambition of our research success is aptly matched by the energetic and dedicated School Research and Graduate Studies team who have organised today – tá muid buíoch díobh (we are grateful to you). We also acknowledge the unstinting support of our administrative and technical staff year in year out.

Falling as it does just after the end of a busy second semester, let today mark the recharging and restoration of a newly productive and fulfilling research drive over the coming months.

Enjoy Research Day 2022 – it is a tribute to us all.

Aisling McCluskey
Head of School

2 Abstracts of invited talks

Hannah Conroy Broderick (NUI Galway): *Shear shock waves in periodic elastic laminates*

Abstract: Shear waves in solids have the potential to develop into shear shocks under the right conditions. In hard materials like metals the stress needed to achieve this is extremely high and the material fails before it can be achieved. However in soft solids, shear waves can develop into shocks at lower stress due to their high nonlinearity in shear. This has implications for many soft materials, for example, shear shocks may be a major contributor to traumatic brain injuries.

Elastic wave propagation in microstructured materials, such as layered or fibre-reinforced materials, can be controlled by applying a deformation. Periodic elastic laminates are one such layered material where changing the applied deformation, changes the wave properties e.g. the band gap structure (regions of frequency where waves can't propagate), so the lamination may have a significant effect on shock wave propagation.

In this talk, I will illustrate a model of shear waves developing into shear shocks in periodic elastic laminates. I will show that the orientation of the laminate imposes restrictions on when shocks can develop and highlight the effect of the difference in stiffness and volume ratio of the laminates on the wave propagation.

Jane Coons (Oxford University): *Algebraic Approaches to Maximum Likelihood Estimation*

Abstract: In the field of algebraic statistics, we use tools from algebra, geometry and combinatorics to answer questions about statistical model viewed as algebraic varieties. In this talk, we will discuss several ways in which this perspective can be used to approach problems related to maximum likelihood estimation. We will describe the maximum likelihood estimation problem in algebraic terms and then apply this formulation to specific models. First, we give a necessary and sufficient condition for a log-linear quasi-independence model to have rational maximum likelihood estimator. We also give a formula for the maximum likelihood estimate in these cases. Finally we discuss maximum likelihood estimation in linear Gaussian covariance models and compute the number of complex critical points of the log-likelihood function for general two-dimensional models.

James Cruickshank (NUI Galway): *Rigid Structures, Topology and Combinatorics*

Abstract: In 1776 Leonhard Euler made the following startling and somewhat provocative claim:

“A closed spatial figure allows not changes, as long as it is not ripped apart.”

This statement has inspired much investigation in the intervening centuries with many connections to various mathematical, scientific and engineering disciplines. I will survey some of the highlights in this story, focusing on the case of polyhedra and related structures, and on topics of current interest to the geometric rigidity community. I will also briefly report on recent joint work with Shinichi Tanigawa and Bill Jackson which resolves a conjecture of Bob Connelly and also extends the well known lower bound theorem for simplicial complexes. No prior background in the topic will be assumed on the part of the audience.

Ed Curry (NUI Galway): *Data Spaces: A new opportunity for data science*

Abstract: Forward-thinking societies must see the provision of digital infrastructure as a shared societal service, like that of water, sanitation, education, and healthcare. We desperately need new approaches to support the complex data ecosystems that our “smart” society is creating.

A data space can provide a clear framework to support sharing within a data ecosystem while addressing concerns including technical issues, governance, social interactions, and business processes.

Data spaces can enable individuals and organisations to share data in a trusted and controlled environment. With data science and AI, they offer the foundations for discovering solutions to global societal challenges.

The talk will outline the need for data commons, detail the dataspace paradigm, highlight future research challenges, and provide an overview of European efforts driving their realisation.

Cathal Seoighe (NUI Galway): *The contribution of immunoediting to the profile of somatic mutations observed in human cancers*

Abstract: The idea that the immune system plays a key role in preventing cancer through the recognition of non-self antigens expressed by tumours as they develop (referred to as the cancer immunosurveillance hypothesis) goes back to the middle of the last century. Initially receiving strong support through experiments on inbred mice, it was abruptly abandoned when key predictions concerning increased cancer risk in immune defective animals were not realized. More detailed animal experiments as well as observational data from humans revived the theory towards the turn of the century, lending relatively conclusive support and paving the way for the development of immune-based cancer therapies. A corollary of this theory is that cancers that develop successfully do so because they are capable of evading the immune response. This phenomenon, referred to as immunoediting, can be observed experimentally in the reduced proliferative potential of cancer cells that are transplanted from immune incompetent to immune competent mice and observationally in the frequency of cancer driver mutations that enable cells to evade the cellular adaptive immune response. Consistent with the immunoediting theory, two high-profile papers proposed that cancer driver mutations arise in HLA-dependent gaps in the capacity of the patient immune system to present the resulting neoantigens. We re-evaluated the evidence for this hypothesis and found that it is the result of incorrect statistical modelling assumptions. Furthermore, we show, through an analysis of data from the UK Biobank, that an important prediction of this hypothesis relating to increased cancer risk in individuals with lower capacity to present cancer driver mutations is not met. Our results indicate that the profile of immunogenic somatic mutations in cancer can be explained by mutation signature activity alone, without any contribution from immunoediting. Surprisingly, although tumour mutation burden is predictive of the success of immune checkpoint inhibitor therapies, there is no evidence that same is true for the success of immunosurveillance in cancer prevention.

3 Abstracts of lightning talks

Mathematical Models for Digital twins Based on Predictive Analysis in Industry 4.0

Faiza Alssaedi

Digital twin plays a pivotal role in the vision of Industry 4.0. The idea is that the real product and its virtual counterpart are twins that travel a parallel journey from design and development to production and service life. The intelligence that comes from digital twins' operational data supports the predictive analysis to pave the way for Industry 4.0. A unifying mathematical model is needed for formulating the digital twins for the implementation of Industry 4.0 applications. This talk will explain the opportunities for building mathematical models for digital twins based on predictive analysis in Industry 4.0.

This is joint work with Ou Ma (University of Cincinnati, Cincinnati, USA), Saeed Hamood Alsamhi, (SMART 4.0 FELLOW, AIT, TUS, Athlone, Ireland), N. S. Rajput (Indian Institute of Technology, Varanasi, UP, India) and Radhya Sahal (School of Computer Science and IT, University College Cork, Cork, Ireland).

References

- [1] Sahal, Radhya and Alsamhi, Saeed H. and Breslin, John G. and Brown, Kenneth N. and Ali, Muhammad Intizar "Digital Twins Collaboration for Automatic Erratic Operational Data Detection in Industry 4.0," *Applied Sciences*, vol. 11, <https://www.mdpi.com/2076-3417/11/7/3186>, 2021.

Single-cell characterisation of the hematopoietic bone marrow interactome in health and disease

Sarah Ennis

**Supervisors: Dr Eva Szegezdi, Dr Pilib
Ó Broin**

The bone marrow (BM) is a complex microenvironment and the primary site of hematopoiesis, coordinating the production of billions of blood cells every

day. This environment is tightly regulated by reciprocal interactions between hematopoietic cells and other cell types in the BM, which become dysregulated in the case of hematopoietic disease, such as leukemia. Here we present a high-resolution characterisation of the niche in health and disease by compiling a comprehensive single-cell gene expression atlas in BM aspirates obtained from healthy donors ($n = 32$), and patients with acute myeloid leukemia (AML, $n = 31$). We used this atlas to investigate changes in cell type proportions and cell type-specific gene expression that occur during the development of AML and show that the entire niche is disrupted by the disease. Given the importance of interactions between hematopoietic cells and their microenvironment in regulating their function and properties, we also predicted cell-cell interactions between hematopoietic cells and all other cell types in the BM. This analysis highlighted expansion of cell adhesion interactions and interactions associated with cytokine signalling in AML and revealed potential novel therapeutic targets.

Supported by Supported by Science Foundation Ireland.

Computing invariants of knotted manifolds

Kelvin Killeen

Supervisor: Graham Ellis

We show how the classical notions of homology with local coefficients, covering space, tubular neighbourhood and spinning can be encoded on a computer and used to calculate ambient isotopy invariants of continuous embeddings $N \hookrightarrow M$ of topological manifolds. More specifically, we are concerned with codimension-2 embeddings of links into S^3 and ribbon surface-links into S^4 . We have implemented algorithms for endowing these manifolds with an efficient regular CW-structure. Furthermore, we show how our implementation of Dehn surgery on link complements yields a regular CW-decomposition of any closed orientable 3-manifold. Supported by an Irish Research Council postgraduate scholarship, award number GOIPG/2018/2152.

Magnetic Resonance Imaging-based Deep Learning Predictive Models of Brain Disorders: A Systematic Review of Modelling Practices, Transparency, and Interpretability

Shane O’Connell

Supervisors: Pilib Ó Broin, Dara M
Cannon

The recent rise in the use of deep learning approaches on neuroimaging data has led to the reporting of impressive predictive performances as well as assertions of potential clinical utility [1]. Deep learning models however, have a number of properties that make their effective implementation, especially in clinical scenarios, challenging. These can include: 1) a variety of network architecture choices and stochastic initialisation of network weights leading to poorly defined convergence and sub-optimal solutions, 2) a large number of (hyper)parameters that require significant computational resources for weight optimisation and repeat experiments for robust performance evaluation, 3) interpretability issues, which make it difficult to understand what information is being used by the model, which thus limits its potential clinical utility [2]. Additionally, studies implementing these models can suffer from poor data separation practices during model training leading to information leakage and issues around reproducibility due to a lack of sufficiently detailed methodologies and code availability. In our work, we systematically review the: 1) modelling practices, 2) degree of transparency, and 3) interpretability of 60 studies that apply deep learning approaches to neuroimaging data, specifically brain MRI studies in the context of potential clinical utility. We evaluated 60 papers arising from a search of the Web of Science and Pubmed databases by applying a standardised questionnaire to each study. Our results show a lack of repeat experiments (26/60), code sharing (54/60), interpretability (40/60), and potential information leakage (28/60) across the selected articles. These findings suggest study reproducibility may be hampered by non-adherence to the outlined principles; furthermore, the clinical utility of models from studies not observing these principles may be limited. Our work demonstrated issues with modelling practices, transparency, and

interpretability across the studies examined. Careful consideration of these principles will inform a patient care framework that can effectively incorporate deep learning into diagnostic and prognostic systems, which could further our physiological understanding of these disorders and lead to improved patient care.

Supported by Science Foundation Ireland under Grant number 18/CRT/6214

References

- [1] Altug Yigit and Zerrin Işik. Applying deep learning models to structural MRI for stage prediction of Alzheimer’s disease. *Turkish J. Electr. Eng. Comput. Sci.*, 2020.
- [2] Zhongheng Zhang, Marcus W Beck, David A Winkler, Bin Huang, Wilbert Sibanda, Hemant Goyal, et al. Opening the black box of neural networks: methods for interpreting neural network models in clinical applications. *Annals of translational medicine*, 6(11), 2018.

Random-effects meta-analysis of effect sizes as a unified framework for gene set analysis

Dónal O’Shea

Supervisor: Cathal Seoighe

The role of gene set analysis is to identify groups of genes that are perturbed to an atypical extent in a genomics experiment. There are many software tools available for this task and they do not all test for the same types of differences between gene sets. We propose a new way to carry out gene set analysis that involves first working out the distribution of the group effect in the gene set and then comparing this distribution to the equivalent distribution in other genes. We show that the tests performed by existing tools for gene set analysis can all be related approximately to different types of comparisons in these distributions of group effects. This unified framework for gene set analysis provides for more explicit null hypotheses against which to test sets of genes for different types of atypical responses to the experimental conditions. The results are also more interpretable, because

the group effect distributions can be compared visually, providing an indication of how the experimental effect differs between the gene sets. We can also apply this method to identify sets of genes that behave atypically in subgroups of samples. This enabled us to identify differences in the expression of several gene sets in colon cancer samples between high and low-risk groups, consistent with clinical differences between these patient groups

Quantum Prisoner's Dilemma demystified

Victoria Sánchez Muñoz

Supervisor: Michael Mc Gettrick

The concept of a Quantum Game is relatively recent and rather unknown in general. It all started back in 1999 with an article by Eisert *et. al.* [1] in which the famous Prisoner's Dilemma was studied and reformulated within the framework of Quantum Mechanics. I will briefly explain how this was done in a lightweight manner in order to shed some light to the usual and fair question of "what on earth is a quantum game?".

Supported by College of Science and Engineering at NUI Galway.

References

- [1] J. Eisert, M. Wilkens, and M. Lewenstein, "Quantum games and quantum strategies," *Phys. Rev. Lett.*, vol. 83, pp. 3077–3080, Oct 1999.

4 Abstracts of posters

Mathematically Modelling Solid Dispersions

Modhi Albaqami

Supervisor: Dr. Martin Meere

In this poster, we present some work describing the mathematical modelling of solid dispersions. Solid dispersions are used in the pharmaceutical industry to improve the solubility of poorly soluble drugs. The dispersion here is a ternary system containing the components - drug, polymer, and solvent. The purpose of the polymer is to maintain the drug in a molecularly dispersed state to improve its solubility.

The solid dispersion is modelled using the thermodynamics of polymer mixtures; specifically Flory-Huggins ternary theory. Ternary phase diagrams for solid dispersions are constructed using standard thermodynamic stability calculations. These diagrams identify the compositional regions where the mixture is stable, unstable, and metastable. The next step in the work is to confirm these predictions numerically by solving in detail for the evolution of the solid dispersion mixture using appropriate partial differential equations models.

Supported by (Saudi cultural bureau, Dublin).

References

- [1] Huang, Yanbin, and Wei-Guo Dai. "Fundamental aspects of solid dispersion technology for poorly soluble drugs." *Acta pharmaceutica Sinica B* 4.1 (2014): 18-25.

Considerations about Evaluation Tasks to Enhance Students' Statistical Literacy, Reasoning, and Communication-Skills

Malak Almutairi

**Supervisors: Dr. Rachel Quinlan,
Dr. Kirsten Pfeiffer**

This poster presents the work on the general theme of how students in the early stages of higher education work with statistical information. The focus here is on the ability and inclination of students

to interpret visual representations of data, and to connect the representation to context. After an extensive literature review, we found that statistical literacy and statistical reasoning have been defined and described by many statisticians and scholars. However, statistical educators have been unable to agree on definitions for these terms. As a result, in 2016 the **GAISE** revision committee avoided any attempt to define statistical literacy. They provide a list of goals for students which include statistical literacy as well as statistical reasoning and communication skills [3]. We have decided to focus on various aspects related to statistical reasoning. We selected some questions from the widely used **CAOS** test instrument [2], which has been developed with aim of identifying students' skills and challenges in the area of statistical reasoning [1]. To get a better idea of our students' performances in this area, we are planning to run a pilot study to identify students' difficulties using some of the **CAOS** questions which we adapted for our context. This poster reports on the development of this pilot, and discusses ideas for tasks design to support independent student learning.

References

- [1] Garfield J. *The challenge of developing statistical reasoning*. *Journal of statistics education*, 10(3),2002.
- [2] DelMas R., Garfield J. Ooms A., and Chance B. *Assessing Students' Conceptual Understanding After a First Course in Statistics*. *Statistics education research journal*, 6(2),2007.
- [3] Carver R., Everson M., Gabrosek J., Horton N., Lock R., Mocko M., and Wood B. *Guidelines for assessment and instruction in statistics education (GAISE) college report 2016*. 2016.

Results on Ask Zeta Functions

Sultan Alzahrani

Supervisor: Tobias Rossmann

This poster contributes to certain generating functions, averaging over sizes of kernels, known as

ask zeta functions $Z_M^{\text{ask}}(T)$ associated with modules M of matrices over compact discrete valuation rings [1], such as completions of rings of integers of number fields. We obtained the following results:

- We generalize a formula which converts a related zeta functions over Lie groups, so-called conjugacy class zeta functions, into ask zeta functions over the Lie algebras associated to these Lie groups.
- We provide a way of computing the local ask zeta functions for modules of anti-symmetric matrices using the set of all principal Pfaffians.
- We produce an explicit formula for the local ask functions of modules of anti-symmetric matrices with smooth Pfaffians hypersurfaces.
- We give an explicit formula for the local and global ask zeta functions of modules generated by a matrix.
- We write a formula for the generic local ask zeta functions of modules generated by a matrix pencil.
- We define weak equivalences between matrices of linear forms and introduce relation modules associated to a matrix of linear forms.
- We write formulas for the generic local ask zeta functions of relation modules associated to a matrix and a matrix pencil.

References

- [1] T. Rossmann. The average size of the kernel of a matrix and orbits of linear groups. *Proc. Lond. Math. Soc. (3)*, 117 (3): 574–616, 2018.

The Potential Role of Standing Genetic Variation in Cancer Therapy Resistance

Harrison Anthony

Supervisor: Prof. Cathal Seoighe

Despite the integration of ecology and systems biology into cancer research, there is still much population genetics theory not yet applied to the field. One notable gap of information surrounds the genetic origin of therapy resistance. When viewed from an evolutionary biology perspective, this is a clear example of rapid adaptation. Previous research has already established that most instances of rapid adaptation stem from mutations already present within the population, known as standing genetic variation [1]. It raises the question as to whether therapy resistance in populations of cancer cells would arise similarly. The scenario seems plausible as some researchers have previously discovered mutations related to therapy resistance in tumors prior to treatment [2]. We are interested in exploring whether there is a discernable relationship between standing genetic variation and therapy resistance. To investigate this, we downloaded whole exome sequencing patient data from The International Cancer Genome Consortium [3] which contains metadata on patients who relapsed after treatment (881) and those who did not (6,805). We now plan on estimating nucleotide diversity (π) to quantify standing genetic variation. Then, we will use a mixed effects model to see if standing variation can predict therapy resistance. This research has the potential to shed light on the genetic origin of therapy resistance by incorporating population genetics and an evolutionary perspective. It could also be impactful to work done by researchers and clinicians by revealing a relatively simple statistic that helps explain a clinically relevant, complex phenotype.

Supported in part by a research grant from Science Foundation Ireland (SFI) under Grant number 18/CRT/214.

References

- [1] Rowan D.H. Barrett and Dolph Schluter. Adaptation from standing genetic variation. *Trends in Ecology and Evolution*, 23(1):38–44, jan 2008.
- [2] Catherine Roche-Lestienne and Claude Preudhomme. Mutations in the ABL kinase domain pre-exist the onset of imatinib treatment. *Seminars in Hematology*, 40(2 SUPPL. 2):80–82, 2003.

- [3] Junjun Zhang, Rosita Bajari, Dusan Andric, Francois Gerthoffert, Alexandru Lepsa, Hardeep Nahal-Bose, Lincoln D. Stein, and Vincent Ferretti. The International Cancer Genome Consortium Data Portal. *Nature Biotechnology*, 37(4):367–369, 2019.

(SA)BIO: Self-Adaptive Bio-Inspired Optimised pipelines for kidney antibody mediated rejection prediction.

Mariel Barbachan e Silva
Supervisor: Pilib Ó Broin

Background

Antibody-mediated rejection (AMR) is one of the primary mechanisms of graft loss following organ transplantation, the diagnosis of which is complicated by late histopathological presentation and contradictory indications due to a lack of disease-specific lesions [1]. To predict AMR at an earlier stage, the application of machine learning methods in gene expression data has been a focus of research in transplant medicine [2]. The use of ensemble approaches for classification can improve the prediction performance of a classification system by combining the decision of a heterogeneous set of classifiers [3]. Additionally, feature selection techniques can improve the predictive capabilities of a classification system by removing non-important features.

Methods

In this work, we developed a feature selection and ensemble classification pipeline for AMR prediction. We implemented canonical bio-inspired optimisation approaches, particle swarm optimisation (PSO) and differential evolution (DE), as well as self-adaptive versions, fuzzy self-tuning PSO (FSTPSO) and success-history based adaptive DE (SHADE) using the JMetalPy framework [4], to select optimal sets of hyperparameters for the classification pipeline. Gene expression microarray data from three kidney transplant data sets were combined using reComBat, resulting in a 322 sample balanced data set that was divided into train, validation, and test sets (ratio of 50:25:25).

Results

Our results demonstrate that, by the end of the optimisation process, the algorithms have narrowly

distributed log-loss values among the 12 experimental replicates, particularly in the case of the DE and SHADE. The log-loss results using test data show a wider distribution in the DE and SHADE, with higher log-loss values, and narrower, significantly lower log-loss values when comparing the PSO and FSTPSO with the default pipeline (p-values of 8.19e-15 and 3.66e-16, respectively). This indicates that the DE and SHADE algorithms may have prioritised exploitation of the search space, highly tailoring the candidate solutions to the training data set, while the PSO and FSTPSO solutions were able to generalise their mapping to classify novel data. When comparing the canonical and self-adaptive implementations, FSTPSO led to significantly improved classification results (p= 0.0415), while log-loss results with SHADE have both the minimum and maximum log-loss values compared with any other approach. This points towards the need for a larger data set, enabling the self-adaptive approaches to learn more comprehensive mapping functions.

Supported by College of Science fellowship from NUI Galway.

References

- [1] Alexandre Loupy, Mark Haas, Candice Roufosse, Maarten Naesens, Benjamin Adam, Marjan Afrouzian, Enver Akalin, Nada Alachkar, Serena Bagnasco, Jan U Becker, et al. The banff 2019 kidney meeting report (i): Updates on and clarification of criteria for t cell- and antibody-mediated rejection, 2020.
- [2] Jeff Reeve, Georg A Böhmig, Farsad Eskandary, Gunilla Einecke, Carmen Lefaucheur, Alexandre Loupy, Philip F Halloran, MMDx-Kidney Study Group, et al. Assessing rejection-related disease in kidney transplant biopsies based on archetypal analysis of molecular phenotypes. *JCI insight*, 2(12), 2017.
- [3] Mariel Barbachan e Silva and Pilib Ó Broin. An optimised ensemble for antibody-mediated rejection status prediction in kidney transplant patients. In *2020 IEEE Congress on Evolutionary Computation (CEC)*, pages 1–8, 2020.

- [4] Antonio Benítez-Hidalgo, Antonio J. Nebro, José García-Nieto, Izaskun Oregi, and Javier Del Ser. jmetalpy: A python framework for multi-objective optimization with meta-heuristics. *Swarm and Evolutionary Computation*, page 100598, 2019.

inference of somatic mutation based phenotypes from population sequencing data

Declan Bennett

Supervisor: Prof. Cathal Seoighe

Mutational phenotypes can give insights into the evolutionary history of tissues and the processes that shape the mutational landscape, such as aberrant transcription-coupled nucleotide excision repair (TC-NER), transcription associated mutagenesis (TAM), replication associated errors and exogenous factors. Accurately defining somatic phenotypes from population scale data sets is inherently difficult due to low sequencing coverage of the sample and single tissue sequencing. This results in phenotypes with a large proportion of the variance across samples being explained by technical factors such as sequencing batch, sequencing error rate and mapping errors as well as intrinsic sequence properties such as the 5' and 3' nucleotide context in which the mutation arises. In order to detect the smaller contributing effects of somatic mutations large sample sizes are required when phenotype data is inherently noisy.

We have developed a pipeline to process 175 TB of data and extract information on somatic mutational processes from 200,000 individuals in the UK biobank. The resulting data, coupled with health phenotypes from the UK biobank, can be used in a wide variety of downstream analyses to give a novel and unprecedented insight into the role somatic mutational processes play in health-related outcomes of normal healthy ageing populations. These analyses include the investigation of genetic variation in 200,000 individuals and the age-related accumulation of somatic mutation and its impact on health.

This research has been conducted using the UK Biobank Resource under Application Number 23739. This publication has emanated from research conducted with the financial

support of Science Foundation Ireland under Grant number 16/IA/4612

Bayesian multiple imputation for missing functional data

Beatrice Charamba

Supervisor: Andrew Simpkin

Introduction

Functional data analysis (FDA) methods have recently been developed to analyse several variables measured repeatedly and concurrently over a domain such as time in a cohort of individuals. However, many FDA methods require data to be fully observed measured regularly, with data being collected at the same fixed times for all individuals. Often, with studies in humans, there tend to be missing data. One way of dealing with missing data is to impute missing observations and apply methods that require fully observed data. Multiple imputation in particular has been seen to be the best method for imputing data. In Bayesian FDA, multiple imputation was developed for either functional response with scalar covariates or scalar responses with functional covariates usually measured regularly. In this study, we developed a Bayesian multiple imputation method for missing functional responses and /or functional covariates measured on an irregular grid.

Methods

Multiple imputation datasets were generated based on the Bayesian functional concurrent regression model. Full data were obtained by taking a random sample of converged Markov Chain Monte Carlo (MCMC) chains. A simulation study was performed to compare the Bayesian multiple imputation with multiple imputation by chained equations (MICE) to determine which predict missing observation with less bias. Missing data were induced in four ways, 10%, 20% and 40% missing at random. Methods were compared using the root mean square error (RMSE).

Results

Bayesian multiple imputation was found to be superior to MICE with smaller RMSE regardless

of missingness percentage. The higher the missingness percentage, the higher the RMSE.

Conclusion

For missing functional data, either response or covariate the Bayesian multiple imputation method performs better than MICE which does not take into account the repeated nature of the data and evolution overtime. We recommend the use of Bayesian multiple imputation before fitting models that require full data.

Supported by Insight centre for data analytics.

References

- [1] Rubin DB. *Multiple imputation for nonresponse in surveys*. Vol 81. John Wiley & Sons; 2004.
- [2] He Y, Yucel R, Raghunathan TE. *A functional multiple imputation approach to incomplete longitudinal data*. *Statistics in Medicine*. 2011;30(10):1137-1156.
- [3] Petrovich J, Reimherr M, Daymont C. *Functional Regression Models with Highly Irregular Designs*. Published online 2018. <http://arxiv.org/abs/1805.08518>

nf-core/circrna: a portable workflow for the quantification, miRNA target prediction and differential expression analysis of circular RNAs

Barry Digby

Supervisors: Pilib Ó Broin,
Stephen Finn (TCD/SJH)

Background

Circular RNAs (circRNAs) have garnered increased attention from the research community due to their stability, tissue-specific expression and role as transcriptional modulators via sequestration of miRNAs [1, 2, 3]. Currently, multiple quantification tools capable of detecting circRNAs exist, yet none delineate circRNA - miRNA interactions, and only one employs differential expression analysis. Efforts have been made to bridge this gap by way

of circRNA workflows, however these workflows are limited by both the types of analyses available and computational skills required to run.

Results

We present nf-core/circrna, a multi-functional, automated high-throughput pipeline implemented in nextflow [4] that allows users to fully characterise the role of circRNAs in RNA Sequencing datasets via three analysis modules: (i) circRNA quantification, robust filtering and annotation (ii) miRNA target prediction of the mature spliced sequence and (iii) differential expression analysis. nf-core/circrna has been developed within the nf-core framework [5], ensuring robust portability across computing environments via containerisation, parallel deployment on cluster/cloud-based infrastructures, comprehensive documentation and maintenance support.

Conclusion

nf-core/circrna reduces the barrier of entry for researchers by providing an easy-to-use, comprehensive, platform-independent and scalable workflow for circRNA analyses. Source code, documentation and installation instructions are freely available at <https://github.com/nf-core/circrna> and <https://nf-co.re/circrna>.

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References

- [1] Memczak, S., Jens, M., Elefsinioti, A., et al. (2013) *Circular RNAs are a large class of animal RNAs with regulatory potency*. *Nature*, 495(7441), 333–338
- [2] Bahn, J. H., Zhang, Q., Li, F., et al. (2015) *The landscape of microRNA, Piwi-interacting RNA, and circular RNA in human saliva*. *Clinical chemistry*, 61(1), 221–230
- [3] Hansen, T. B., Jensen, T. I., Clausen, B. H., et al. (2015) *Natural RNA circles function as efficient microRNA sponges*. *Nature*, 495(7441), 384–388

- [4] Di Tommaso, P., Chatzou, M., Floden, E., et al. (2017) *Nextflow enables reproducible computational workflows*. Nature Biotechnol 35, 316–319
- [5] Ewels P. A., Peltzer A., Fillinger S., et al. (2020) *The nf-core framework for community-curated bioinformatics pipelines*. Nature Biotechnology 38:276-278

Comparing the XGBoost machine learning algorithm to polygenic scoring for the prediction of intelligence based on genotype data

Laura Fahey

Supervisors: Dr Pilib Ó Broin and Dr Derek Morris

Genome-wide association studies (GWAS) have revealed that the genetic component of many complex phenotypes is based on the cumulative contribution of a large number of small effects, this is referred to as a polygenic model. A polygenic score (PGS) is a linear combination of effects from a GWAS that represents and can be used to predict genetic predisposition to the phenotype in question. A key limitation of the PGS method is that it assumes additive and independent SNP effects, when it is known that epistasis (gene interactions) can contribute to complex traits. Machine learning methods can potentially overcome this limitation by virtue of their ability to capture nonlinear interactions in high dimensional data. Intelligence is a complex trait for which PGS prediction currently explains up to 5.2% of the variance, a relatively small proportion of the heritability estimate of 50% obtained from twin studies. Here, we use gradient boosting, a machine learning technique based on an ensemble of weak prediction models, to predict intelligence from genotype data. We found that gradient boosting did not outperform the PGS method in predicting intelligence based on SNP data, although it was capable of achieving similar predictive performance with less than a quarter of the SNPs.

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Genus g Partition Functions of Vertex Operator Algebras and Degree l Casimir Operators

Michael Flattery

Supervisor: Michael Tuite

This poster presents the partition functions of Vertex Operator Algebras (VOAs) on a genus g Riemann surface [1] as part of an investigation into a conjecture of Friedan and Shenker [2] that a VOA is determined by its partition functions of all genera. This genus g Riemann surface is constructed by sewing handles on a Riemann sphere through Schottky uniformisation. We focus on techniques using degree l Casimir operators of the Lie Algebra generated by the states of conformal weight 1 in order to deal with a broad class of VOAs [3]. There is an existing body of work on degree l Casimir operators to aid in this endeavour [4].

References

- [1] M. P. Tuite, M. Welby. *General Genus Zhu Recursion for Vertex Operator Algebras* arXiv:1911.06596, 2019.
- [2] D. Friedan, S. Shenker. *The analytic geometry of two-dimensional conformal field theory* Nuclear Physics, Section B, Vol.281 no. 3-4, pp. 509-545, 1987.
- [3] M. R. Gaberdiel, R. Volpato. *Higher genus partition functions of meromorphic conformal field theories* Journal of High Energy Physics, Vol. 2009, no. 6, pp. 48-92, 2009.
- [4] S. Okubu. *Casimir invariants and vector operators in simple and classical Lie algebras* Journal of Mathematical Physics, Vol. 18, 2382, 1977.

More accurate and unbiased associations in genetic association studies

Amanda Forde

Supervisor: Dr. John Ferguson

It has been observed that in general, the effect size of a single nucleotide polymorphism (SNP) tends to be lower in a replication study than in the genome-wide association study (GWAS) that discovered the

SNP-trait association. This observation is due to the phenomenon known as *Winner's Curse* [1]. In the context of a single discovery GWAS, the term *Winner's Curse* describes how the estimates of association strength for SNPs that have been deemed most significant are very likely to be exaggerated compared with their true underlying values. The focus of this project is on the evaluation and development of methods which attempt to reduce the effect of the bias induced by *Winner's Curse* using only GWAS summary statistics.

Eliminating this bias is known to be a difficult task. Several bias reduction approaches have been proposed in recent years, with one of the earliest being the Conditional Likelihood method [2]. In our work, we have made amendments to some existing *Winner's Curse* correction methods, namely the empirical Bayes method [3] and the bootstrap shrinkage estimator [4], in order to address certain weaknesses that these methods suffer from. By means of a thorough simulation study as well as engagement with two real data sets, we evaluate and compare *Winner's Curse* correction methods, including those which have adopted our modifications. Simulations allowed us to compare methods easily over a wide range of different possible genetic architectures, including scenarios in which a simple linkage disequilibrium (LD) structure has been considered. A UKBB body mass index (BMI) data set and a UKBB type 2 diabetes (T2D) data set were then used to see how these techniques would perform in realistic settings in which a large degree of LD exists. In both instances, assessment of methods was predominantly based on the computation of estimated mean squared error (MSE) over significant SNPs. A notable challenge that was encountered at the start of the work was the lack of available software to implement these various correction methods. Therefore, to complement our work, we have developed an R package, namely 'winnerscurse', which can be used to apply a number of *Winner's Curse* adjustment methods to GWAS summary statistics.

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References

- [1] Dudbridge, F. & Newcombe, P. *Handbook of Statistical Genomics*. 4th edn, 631–650 (Wiley Online Library, 2019)
- [2] Ghosh, A., Zou, F., & Wright, F. A. (2008). Estimating odds ratios in genome scans: an approximate conditional likelihood approach. *American journal of human genetics*, 82(5), 1064-1074.
- [3] Ferguson, J. P., Cho, J. H., Yang, C., & Zhao, H. (2013). Empirical Bayes correction for the Winner's Curse in genetic association studies. *Genetic epidemiology*, 37(1), 60–68.
- [4] Sun, L., Dimitromanolakis, A., Faye, L. L., Paterson, A. D., Waggott, D., DCCT/EDIC Research Group, & Bull, S. B. (2011). BR-squared: a practical solution to the winner's curse in genome-wide scans. *Human genetics*, 129(5), 545–552.

The selection and integration of datasets for the analysis of microRNAs as therapeutics in Sarcopenia

Karen Guerrero Vazquez
Supervisors: Dr. Katarzyna Whysall,
Dr. Pillib Ó Broin

Sarcopenia is characterized by the loss of skeletal muscle and contributes to the development of physical disabilities, various illnesses, and increasing mortality [4]. MicroRNAs (miRNAs) are small non-coding RNAs that inhibit translation of target messenger RNAs. Previous studies have shown that miRNAs play pivotal roles in the development of sarcopenia [4].

The use of miRNAs as therapeutics is highly appealing given the potential to target multiple genes/pathways as opposed to a single target as in the case of selective protein inhibitors [1].

As of 2018, 38,589 miRNA molecules in 271 species have been identified, including 1982 human precursor-miRNAs (pre-miRNAs) and 2694 human mature miRNAs [3]. These data are distributed across more than 106 miRNA databases

and datasets [2], complicating the analysis of the data for this study.

This poster will show a multi-objective approach for the selection of databases and their integration into a combined resource.

References

- [1] Badalian-Very, G., and Hydrin, P. *Clinical applications of mi- croRNAs*. F1000Research 2 (10 2013).
- [2] Paschoal, A. R., Maracaja-Coutinho, V., Setubal, J. C., Simoes, Z. L. P., Verjovski-Almeida, S., and Durham, A. M. *Non-coding transcription characterization and annotation: A guide and web resource for non-coding RNA databases*. RNA Biology 9, 3 (2012), 274–282.
- [3] Wu, K., He, J., Pu, W., and Peng, Y. *The Role of Exportin-5 in MicroRNA Biogenesis and Cancer*. Genomics, Proteomics & Bioinformatics 16, 2 (4 2018), 120–126.
- [4] Yanai, K., Kaneko, S., Ishii, H., Aomatsu, A., Ito, K., Hirai, K., Ookawara, S., Ishibashi, K., and Morishita, Y. *Micrnas in sarcopenia: A systematic review*. Frontiers in Medicine 7 (1 2020).

Predicting immunogenicity using mutational signatures and MHC-I genotype

Noor Kherreh

Supervisor: Cathal Seoighe

The presentation of intracellular antigens on the cell surface by Major Histocompatibility Complex class-I (MHC-I) molecules is one of the major determinants for CD8+ T-cell activation. Research has shown that patient MHC-I genotype influences immunotherapy responses; however, results are not consistent across cancer types. For example, the B44 HLA (Human Leukocyte Antigen) supertype is associated with a better response in Melanoma. Non-Small Lung Cancer (NSCLC) has a similar somatic mutation burden and immunotherapy response to melanoma but the B44 supertype has

not been found to influence immunotherapy response in NSCLC. This has been attributed to underlying differences in mutational processes active in Melanoma compared to NSCLC. For example, transition mutations, mainly C>T, caused by ultraviolet light exposure in melanoma cancer, tend to result in neoantigens that are more strongly bound by MHC molecules of the HLA B44 supertype than transversion mutations, particularly C>A associated with the tobacco smoking signature often found in NSCLC. Ultraviolet light exposure and tobacco smoking mutation signatures have been reported to have a positive influence in an ICB treated cohort, whereas the B44 study shows both signatures have different results for patients with B44 HLA supertype.

To generalize these findings, here we set out to perform an exhaustive characterization of the predicted immunogenicity of mutations arising from all cancer mutation signatures for the major HLA supertypes. We observed that mutations resulting from some mutation signatures were far more likely to be presented by certain HLA alleles than mutations from other signatures. The average number of mutations that were predicted to be immunogenic in a cancer type could be predicted with high accuracy ($R^2 = 0.87$) from the mean activity of the mutation signatures in that cancer. We use our method to predict expected immunogenicity in two ICB treated melanoma cohorts and observed that in one cohort higher expected immunogenicity was associated with improved immunotherapy response, whereas this effect was absent in the other cohort. It can be implied here that neither the presence of a certain HLA allele nor the activity of a certain mutation signature alone can be used to predict the immunotherapy efficacy. The association between the two is important but even that is not enough as the quality of neoantigen plays a key role in T-cell activation. The expected immunogenicity combines the effect of mutation signature activity and HLA genotype in ICB treatment response, but further investigation is required to study the prerequisite factors that are essential for inducing an HLA dependent immune response.

**The Role of Copy Number Alteration
and Gene Expression Data in Stratifying
Breast Cancer Patients within
Predictive Models for Survival Outcome**

Lydia King

**Supervisors: Simone Coughlan,
Róisín Dwyer, Emma Holian**

Breast cancer diagnosis, classification and treatment generally follows an integrative approach whereby both clinical features and tissue-based biomarkers are used. It is widely accepted that breast cancer is largely dominated by amplifications, deletions and chromosomal rearrangements and increasing evidence suggests that incorporating the genomic landscape of the tumour into treatment decisions is beneficial to the patient. This project focuses on assessing whether biomarkers derived from genomics data, in particular gene expression and copy number alteration (CNA) signatures, improve predictive models of overall survival and disease-specific survival for breast cancer patients in clinical settings.

We first define novel CNA metrics to measure GI in the METABRIC cohort requiring estimating the distribution of those metrics with missing value presentation. A further challenge is incorporating the CNA metrics into predictive models as this requires consideration to modelling the effect of the upper tail of those distributions, i.e. those with high GI rather than central tendency. To examine how CNA status influences gene expression, linear models are fitted, employing empirical bayes and multiple testing adjustments. Modelling survival with recursive partitioning survival trees enables us to investigate possible interactions between clinical variables and the CNA metrics, and the relationship with established molecular-based classifications such as PAM50 subtypes and Integrative Clusters.

Focus on the location of the CNA burden i.e. the chromosome arms and alteration status across genes at adjacent locations on chromosomes, indicates that higher levels of deletion burden on chromosome arm 3p is associated with poor disease-specific survival outcome.

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**Adaptive Evolution of Anti-Cancer
Mechanisms Could Offer an Explanation
of Peto's Paradox**

Sophie Matthews

**Supervisors: Simone Coughlan,
Cathal Seioighe**

Cancer is a ubiquitous disease observed across the mammalian tree of life. It can arise from mutations that allow cells to escape the cell cycle and proliferate uncontrollably. In principle, as every cell carries a risk of generating a mutation, and hence developing cancer, organisms with larger bodies (composed of more cells) and extended lifespan (more time to accumulate mutations) should be more at risk of developing cancer. However, Peto's paradox describes the evolutionary conundrum seen across taxa: cancer risk does not increase with body size or lifespan [1]. This phenomenon can be explained by the idea that large, long-lived organisms must have evolved effective anti-cancer mechanisms as an adaptation to increasing frequencies of cancer. We investigated this concept, hypothesising that as changes in body size and lifespan have occurred along branches of the phylogenetic tree, they are mirrored by changes in cancer risk. Using data from a recent study by Vincze et al. [2] we have inferred the rate of change in lifespan, body size and cancer risk across branches of the mammalian phylogeny. We found that changes in cancer risk across branches are significantly correlated with the relative rate of change in life expectancy. However significant correlation was not found between the relative rate of change in body size and change in cancer risk. Given these results, we are now investigating the evolution of one anti-cancer mechanism: the gain and loss of tumour suppressor genes. We hypothesise that tumour suppressor genes will be under selective constraint in long-lived organisms, and copy number of tumour suppressors will be maintained across phylogenetic branches in line with changes in cancer risk. If true, this further supports the argument that the evolution of long-lived organisms was accompanied by subsequent evolution of anti-cancer mechanisms, indicating that Peto's paradox is not

a paradox at all, but evidence of adaptive evolution.

Supported by (support source, if any); delete otherwise.

References

- [1] Peto R, Roe FJ, Lee PN, Levy L, Clack J. Cancer and ageing in mice and men. *British Journal of Cancer* 1975;32:411–26. <https://doi.org/10.1038/bjc.1975.242>. [2] Vincze O, Colchero F, Lemaître J-F, Conde DA, Pavard S, Bieuvre M, et al. Cancer risk across mammals. *Nature* 2021 2021:1–5. <https://doi.org/10.1038/s41586-021-04224-5>.

LncRNA based antigen load enables predictions of patient’s survival and immunotherapy outcomes in Melanoma

Sumaira Malik

Supervisor: Dr. Aaron Golden

ICB (immune checkpoint blockade therapy) is one of the promising treatments for melanoma. However, ICB response varies among patients, emphasizing the importance of identifying genomic biomarkers to predict likely responses in advance of treatment. LncRNAs are previously associated with cancer-specific epitopes. We aim to establish the association of lncRNA based immunogenicity scoring (lnc-IM) with tumor immune microenvironment (TIM), predicting ICB responses and prognostic value in melanoma. The data used includes TCGA-SKCM (n=101), and ICB treated melanoma cohorts UCLA (n=27) and MSKCC (n=21). Each patient was assigned a lnc-IM score based on the number of peptides it can present depending on its MHC-I genotype. A logistic regression-based classifier was used to predict ICB responses based on lnc-IM scores.

The survival analysis showed better survival of patients with low lnc-IM counts (HR=0.26, p=0.0012) in the TCGA-SKCM cohort. TIM is an indicator of tumor progression and immunotherapeutic responses. We compared immune cell scores (calculated using xCell algorithm) with lnc-IM scores. CD8-T cells showed a correlation of -0.33 (p=0.0008) with lnc-IM scores. Fur-

thermore, we divided immune cells into the anti-tumor (B cells, M1 macrophages, activated dendritic cells, CD4 -memory T cells, Th1 cells) and pro-tumor group (Th2 cells, T regulatory cells, M2 macrophages). Anti-tumor immune cells showed significant differences among low and high lnc-IM groups, while no such association was apparent among the pro-tumor group. The checkpoint proteins PD1 and CTLA4 also showed significant differences among the two groups. Based on these inferences, we further explored if such scoring can help improve the prediction of ICB efficacy. Lnc-IM count (derived in this study) and the neoantigen load (derived as a part of the trial) were used to assign each patient a combined antigen score in ICB treated cohorts. We hypothesized that such scoring could help predict ICB outcomes for tumors that are not hypermutated but can benefit from this therapy. We demonstrated that such a classifier improved the predictions, yielding an AUC of 0.8 with an accuracy of 0.83, precision 0.77 and recall 1. Survival analysis showed a significant association of combined antigen scoring with survival outcomes.

We concluded that Lnc-IM scores are associated with elevated anti-tumor immune responses and can be used as a potential biomarker to improve ICB efficacy predictions after validation in bigger cohorts.

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Modelling Chronic Heart Failure with Hidden Markov Models

Tyler Medina

Supervisor: Prof. Cathal Seoighe

Markov models are used to model stochastic processes over time, and have found use in modelling chronic disease. In typical applications for modelling patient disease progression, patients are assigned to defined disease stages at discrete time intervals during patient observation, forming a Markov chain with calculable transition rates. Markov models can additionally be used for economic evaluation by assigning healthcare costs and benefits to each disease stage.[1] As an alternative to simple Markov models, hidden Markov models assume an underlying “hidden” Markov chain

which is unobservable, but which outputs an observable state with a probability dependent only on the hidden state at each time step. In this work, we explore the utility of hidden Markov models (HMM) for modelling progressive heart failure in an Irish patient cohort.

HMM were constructed for 1276 Irish heart failure patients observed from 2004 until 2021, using underlying disease progression as hidden states and hospitalization status or death as observed states, per year. Transition, emission, and initial state probabilities were calculated using the Baum-Welch algorithm. To test model accuracy, test data was withheld and used to make truncated observation chains, for which the next most-likely observed state for each chain was predicted and compared against the true observed state.

Preliminary results indicate %85 prediction accuracy for 4 or 5 hidden states; however, this is no better than predicting subsequent observations based simply on the ratios of all observations. This is due to the sparsity of hospitalization and death observations in the dataset and generated Markov chains, which are thus nearly non-informative for training transition and emission probabilities, and makes the most likely prediction almost always the non-hospitalization state. Because of this, alternative methods are recommended, such as continuous-time HMM, which can account for sporadic events and have precedence for use in similar contexts.[2]

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References

- [1] A. Briggs and M. Sculpher. An introduction to markov modelling for economic evaluation. *Pharmacoeconomics*, 13(4):397–409, Apr 1998.
- [2] G. A. Powell, A. Verma, Y. Luo, D. Stephens, and D. Buckeridge. Modeling Chronic Obstructive Pulmonary Disease Progression Using

Continuous-Time Hidden Markov Models. *Stud Health Technol Inform*, 264:920–924, Aug 2019.

Movement pattern discovery with application in sport science

Pouyan Nejadi

Supervisors: Prof. John Newell,

Dr. Davood Roshan

The objectives of sports analytics are varied and are differentiated according to interest group. Professional sport uses the data for game analysis, training load management, injury prevention and to support player transfers. Sports scientists can use the enormous data pool to analyse performance structures, to investigate academic claims and to develop new paradigms in the development of theory.

In recent years, the advances of sensor technologies allowed enormous data to be collected within the sport industry. This is particularly true for group sports (e.g. football, basketball, American football), where all players' movement data can be recorded via installed motion capture sensors around a playing field. However, these vast amounts of data have little value in themselves. Rather, the challenge is to develop new methods of data analysis to enhance our knowledge about sport. To date, such motion tracking spatiotemporal position data is typically used to learn about the tactical strategies (i.e. formation, players' role) in a game.

The main goal of our research is to use motion tracking data to generate player specific motion signatures in a way that can be used to inform training intensity and drill selection. Techniques for such pattern discovery are mainly done using clustering via extracted features using a Von Mises mixture distribution in domains such herd movement and in understanding how people move in busy streets. We propose the use of a bivariate Generalised Linear Model (GLM) to model movement angles and distance from the origin (i.e. (θ, D)). In particular, our proposed bivariate model is an extension of the Von mises and Rayleigh joint probability distribution functions, where the XY coordinates can be translated to the form of (θ, D) . This model allows us to identify the most common trajectories and

personalised movement patterns for a particular player by clustering the model parameters. Identifying personalised movement patterns can benefit players in terms of quantifying the physiological demands and movement profiles conditional on playing position. Furthermore, sports scientists can use this information to customise drill selection, duration and intensity and to design an injured player's rehabilitation program.

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Comprehensive synthetic ground truth simulation for NGS tumour data.

Brian O'Sullivan

Supervisor: Cathal Seoighe

Contemporary tumour NGS simulation has a number of issues.

- Simulation is based on read fractions. NGS is a stochastic process.
- The bulk of somatic burden resides at low allele frequencies where it is impossible to tell somatic variant from sequencing error.
- Biases in the calling process mean the true variant frequency is not recovered.

We address these with a novel NGS framework enabling true NGS simulation of somatic allele spectra from a personalised, diploid tumour genome. Variant read fractions are determined by ground truth allele frequency and stochastic modelling of the sequencing process. Resulting NGS output is fully synthetic and compatible with all somatic variant callers. The complete ground truth of every non-reference allele (ie., germline, somatic, sequencing / mapping artefact etc.) is known. Phased tumour and normal synthetic NGS output is derived from the personalised diploid genome of any 1000 Genomes donor [1].

References

- [1] Auton et al. A global reference for human genetic variation. *Nature*, 526(7571):68–74, 2015.

Towards Joint Models for binary and longitudinal response outcomes, with application in Breast Cancer Biomarker data

Maxwell Paganga

Supervisors: Dr. Emma Holian,

Prof. John Newell & Dr. Nicola Miller

Prediction models based on all available information are useful in identifying high-risk patients at the right time in order to tailor their treatment in personalised medicine. Unlike survival time outcomes, few studies have demonstrated how to predict binary outcomes using repeatedly measured biomarkers. In this multicentre trial, Cancer Trials Ireland - Irish Clinical Oncology Research Group (ICORG), provides clinicopathological variables, candidate miRNA biomarkers and observed treatment outcome, recorded for a cohort of 125 breast cancer patients undergoing neoadjuvant chemotherapy treatment (NACT). MiRNAs are small, noncoding RNA molecules that modulates gene expression, and are believed to influence response to NACT. Expression levels of a pre-determined miRNA panel (i.e. Let-7a, miR-21, miR-145, miR-155 and miR-195) were relatively quantified from blood samples using RQ-PCR at five predetermined time-points, before, during and after NACT.

Classical models like the logistic regression are not suitable for predicting a binary outcome using longitudinal measurements, as they are not suited to jointly model changes of the biomarkers over time. Generally, longitudinal biomarkers are measured with error, which tends to under/over-estimate their association with outcome risk; therefore, we consider including subject-specific random effects that capture the evolution of the biomarkers over time through a mixed effects model. We explore implementation of likelihood based shared random effect 2-stage models, joint models and the pattern mixture modelling approach. [[1] [2]].

References

- [1] Horrocks, Julie, and Marianne J. van Den Heuvel. *Prediction of pregnancy: A joint model for longitudinal and binary data*. Bayesian Analysis 4.3 (2009): 523-538.

- [2] Liu, Danping, and Paul S. Albert. *Combination of longitudinal biomarkers in predicting binary events*. Biostatistics 15.4 (2014): 706-718.

Construction of Specht Modules for Finite Type - B_n Coxeter Groups

Koushik Paul

Supervisor: Prof. Götz Pfeiffer

Let $n, p, q \in \mathbb{N}$ and $n = p + q$. Let λ is a bipartition of n , denoted $\lambda \models n$, such that $\lambda = (\lambda_p, \lambda_q)$ where $\lambda_p \vdash p$ and $\lambda_q \vdash q$. We call a pair of *Young tableaux* having shapes λ_p and λ_q to be standard if the labels inside the boxes are $\{1, 2, \dots, n\}$ arranged in such way that every row and every column is increasing. To study type- B_n group representations we need to study about a pair of Young tableaux as they give a nice combinatorial understanding of the topic.

Previously with the help of the novel concepts of *Specht matrices* introduced in [2], we have constructed a new understanding of the basis for the Specht modules for type- A_n Coxeter groups which also points towards its irreducible representations. This construction of the new method is analogous to the theory of *polytabloids* present in [1].

In [3], we find some ideas on character theory side of the Coxeter group representations along with few combinatorial approaches. By studying these concepts and using the notions of Specht matrices we have constructed a new way to represent finite type- B_n groups.

These methods are extremely computational and could take immense amount of time if tried by hand, and therefore [4] is used as the primary computational tool to support all the computations required to execute the tasks. Needless to say that this novel way of constructing the Specht modules for type- B_n groups are more complicated computationally but easier to understand and rather more fascinating than the existing literature.

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References

- [1] Bruce E. Sagan. *The Symmetric Group: Representations, Combinatorial Algorithms,*

and Symmetric Functions. Wadsworth & Brooks/Cole mathematical series, Belmont, CA, 1991.

- [2] John D Wiltshire-Gordon, Alexander Woo, Magdalena Zajaczkowska. *Specht Polytopes and Specht Matroids*. Combinatorial Algebraic Geometry, Fields Inst. Communicat., Springer, New York, NY, 2017

- [3] Meinolf Geck and Götz Pfeiffer. *Character of Finite Coxeter Groups and Iwahori-Hecke Algebras*. Oxford University Press, Oxford, UK, 2000.

- [4] The GAP Group, GAP – Groups, Algorithms, and Programming, Version 4.11.1; 2021. (<https://www.gap-system.org>)

DGA Structures on minimal free resolutions of binomial edge ideals

Peter Phelan

Supervisor: Emil Sköldbberg

Definition. A differential graded algebra (DGA) is a graded algebra A equipped with a differential $d: A \rightarrow A$ of degree -1 that satisfies the following conditions.

- [1] $d^2 = 0$, so (A, d) has the structure of a chain complex.

- [2] $d(a \cdot b) = d(a) \cdot b + (-1)^{\deg(a)} a \cdot d(b)$, where \deg is the degree of the homogeneous elements.

We are interested in studying the classes of binomial edge ideals whose minimal free resolutions admit a DGA structure. Much work has already been carried out in the study of DGA resolutions; for example, we know that a DGA structure is admitted in the case of complete intersection ideals, Gorenstein ideals of codimension 3 [1], almost complete intersection ideals of codimension 4 [2], stable monomial ideals [3], squarefree monomial ideals [4], cointerval edge ideals [5] and squarefree matroidal ideals [6]. We have also seen an investigation into homological obstructions to the existence of multiplicative structures on resolutions [7].

Currently, our attention is focused on the binomial edge ideals of complete graphs. If we let \mathbb{K} be a field and G be a simple graph, we present the following definition:

Definition. The binomial edge ideal of a graph G is given by

$$J_G = (x_i y_j - x_j y_i \mid \{i, j\} \in E(G)) \subseteq \mathbb{K}[x_i, y_i \mid i \in V(G)]$$

In this poster, we outline some current approaches which may be used to tackle this problem. In particular, we will describe how algebraic Morse theory, or homological perturbation theory might allow us construct multiplicative structures on the minimal free resolutions of these binomial edge ideals.

References

- [1] D. A. Buchsbaum, D. Eisenbud, *Algebra structures for finite free resolutions, and some structure theorems for ideals of codimension 3*, Amer. J. Math., 99.3, 447-485 (1977)
- [2] A. Kustin, *The minimal resolution of a Codimension Four Almost Complete Intersection Is a DG-Algebra*, J.Algebra, 168.2, 371-399 (1994)
- [3] I. Peeva, *0-Borel fixed ideals*, J.Algebra, 184.3, 945-984 (1996)
- [4] L.Katthän, *The structure of DGA resolutions of monomial ideals*, Journal of Pure and Applied Algebra, Volume 223, Issue 3, 1227-1245 (2019)
- [5] E. Sköldberg, *The minimal resolution of a cointerval edge ideal is multiplicative*, Preprint, arXiv: 1609.07356 (2016)
- [6] E. Sköldberg, *Resolutions of modules with initially linear syzygies*, Preprint, arXiv: 1106.1913 (2011)
- [7] L. L. Amarov, *Obstructions to the existence of multiplicative structures on minimal free resolutions*, Amer. J. Math., 103.1, 1-31 (1981)
- [8] M. Miller, *Multiplicative structures on finite free resolutions*, Free resolutions in commutative algebra and algebraic geometry, Sundance, UT (1990)

Modelling Linear Wave Propagation using Physics Informed Neural Networks (PINNs)

Vikrant Pratap

**Supervisors: Dr. Bharat Tripathi &
Prof. Michel Destrade**

Background, Motivation & Objective: Millions of people suffer from traumatic brain injury every year. Recently, shear shock waves were observed in brain tissue which may be the primary cause of injury [1]. Shear shock waves simulation in complex geometry like human head can be computationally exhaustive. To mitigate this, recently formulated physics informed artificial neural networks [2] could be a viable alternative. We intend to develop a artificial neural network based numerical method for propagation of shear shock waves in brain. In this work, we have developed PINNs for linear wave equation formulated as a system of first order PDEs [3].

Statement of Contribution: Non-dimensionalized physical system of equations were formulated to facilitate efficient training of PINN [4]. Data-driven PINN was constrained by 1) initial and boundary conditions, 2) uniformly distributed internal collocation points, and 3) the non-

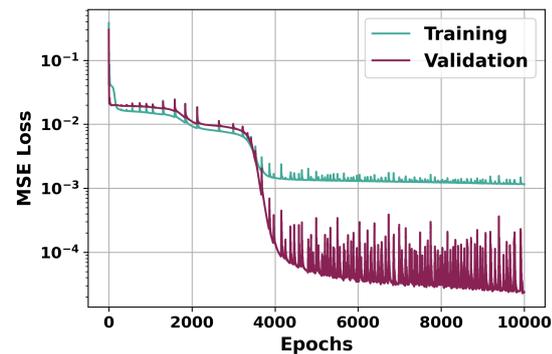


Figure 1: MSE Losses

dimensionalized system of PDEs. PINNs with two input neurons containing spatial and temporal variables were used to approximate PDE solutions. The weights and biases of the neural network were initialized using Glorot normal method. The optimal set of hyperparameters (activation function, optimizer etc.) and the network architecture was

chosen through multiple iterations performed systematically.

Results & Conclusions: The MSE loss for the training and validation dataset are 1.15×10^{-3} and 2.37×10^{-5} respectively as shown in Figure 1. The PINNs solution for wave equation has relative error of 3% as compared with the analytical solution. This result motivates the natural extension of the PINN to a nonlinear system of first order PDEs as formulated for shear waves in soft solids [1].

Supported by *College of Science and Engineering, NUI Galway*

References

- [1] B. B. Tripathi et al. *Int J Numer Mech Biomed Engg.* 2019.
- [2] M. Raissi et al. *Journal of Computational Physics*, 2019.
- [3] R. J. Leveque *Cambridge University Press*, 8 2002.
- [4] G. Kissas et al. *Computer Methods in Applied Mech and Engg*, 2020.

Exploring the therapeutic potential of patient-derived tumour stromal cells as a source of neoantigens.

Kevin Ryan

**Supervisors: Dr Pilib Ó Broin,
Dr Laura Barkley (Lambe Institute for
Translational Research)**

Cancer-associated fibroblasts (CAFs) are a heterogeneous cell type found in the tumour microenvironment. They are involved in a complex interplay with tumour cells and the immune system. CAFs have traditionally been thought to play a tumour promoting role, by supporting angiogenesis and tumour growth, and by inducing therapeutic resistance through the production of extracellular matrix. This has made them the subject of great interest as a potential therapeutic target. However, treatments targeting CAFs can cause off-target effects such as anaemia and cachexia [1], and recent work suggests that they can have tumour inhibitory roles [2]. These issues raise the question of whether a personalised medicine approach is necessary to determine the likely outcome of ablating CAFs in a particular patient. The goal of this

project is to investigate the presence of neoantigens, (non-self peptides which can induce an immune response) specific to CAFs and not found in normal resident tissue stromal cells, and to deepen our understanding of the transcriptomic landscape of CAFs. Neoantigens have the potential for use as cancer vaccines, priming the immune system to remove cells harbouring somatic mutations. NeoFuse [3], a fusion neoantigen prediction pipeline which takes tumour RNA-sequencing data as input and performs HLA typing, identification of gene fusion peptides and prediction of binding between the peptide and the patient's HLA alleles, was implemented using matched CAF/tumour-associated normal (TAN) stromal cell samples from 12 breast cancer patients. 4 of the 12 patients were predicted to have at least one fusion neoantigen specific to their CAF sample. Some genes involved in fusions are thought to be involved in the pathogenesis of cancer, including *PI4KA*, which has been proposed as a target for anti-cancer treatment [4]. These preliminary findings suggest a potential role of neoantigen prediction in the identification of strategies for targeting CAFs in breast cancer.

Supported by The SFI Centre for Research Training in Genomics Data Science.

References

- [1] E. W. Roberts, A. Deonaraine, J. O. Jones, A. E. Denton, C. Feig, S. K. Lyons, R. Larder, A. P. Coll, S. O'Rahilly, K. M. Brindle, S. A. Teichmann, D. A. Tuveson, and D. T. Fearon. Depletion of stromal cells expressing fibroblast activation protein- α from skeletal muscle and bone marrow results in cachexia and anemia. *The Journal of Experimental Medicine*, 210(6):1137, Jun 2013.
- [2] T. Simon and B. Salhia. Cancer-Associated Fibroblast Subpopulations With Diverse and Dynamic Roles in the Tumor Microenvironment. *Molecular Cancer Research*, 20(2):183–192, Feb 2022.
- [3] G. Fotakis, D. Rieder, M. Haider, Z. Trajanoski, and F. Finotello. NeoFuse: predicting fusion neoantigens from RNA sequencing data. *Bioinformatics*, 36(7):2260–2261, Apr 2020.

[4] Y. Park, J. M. Park, D. H. Kim, J. Kwon, and I. A. Kim. Inhibition of PI4K III α radiosensitizes in human tumor xenograft and immune-competent syngeneic murine tumor model. *Oncotarget*, 8(66):110392, 2017.

Quantum CHSH game played with 3 players in a triangle

Victoria Sánchez Muñoz

Supervisor: Michael Mc Gettrick

Today's widely-accepted theory of Quantum Mechanics was severely challenged when it was formulated back in the early 20th century, due to its ground-breaking implications to the physics and framework known at the moment. In that context, John Bell was crucial in deciding the validity of Quantum Mechanics. He proposed in 1964 what are known today as Bell's inequalities [1]. A Bell inequality is an inequality (or a bound) between a combination of certain quantities in a given system, whose violation cannot be explained by any classical theory using local realism (*see [2] for more on local realism and Quantum Mechanics*). In contrast, the violation of a Bell's inequality can be perfectly explained using Quantum Mechanics, which is a non-local theory. One of the most famous Bell's-type inequality is the Clauser-Horne-Shimony-Holt (CHSH) inequality [3]. As it was mentioned, the CHSH inequality emerged in the context of testing the validity of Quantum Mechanics, which helped to its experimental validation [4]. However, the CHSH inequality can also be illustrated using a simple game of 2 players with binary inputs and outputs. This is known as the **CHSH game**. In the present poster, the CHSH game is explained as well as the proposed extension to 3 players playing pairwise the CHSH game in a triangle configuration.

Supported by College of Science and Engineering at NUI Galway.

References

[1] J. S. Bell, "On the einstein podolsky rosen paradox," *Physics Physique Fizika*, vol. 1, pp. 195–200, Nov 1964.

[2] A. Einstein, B. Podolsky, and N. Rosen, "Can quantum-mechanical description of physical reality be considered complete?," *Phys. Rev.*, vol. 47, pp. 777–780, May 1935.

[3] J. F. Clauser, M. A. Horne, A. Shimony, and R. A. Holt, "Proposed experiment to test local hidden-variable theories," *Phys. Rev. Lett.*, vol. 23, pp. 880–884, Oct 1969.

[4] A. Aspect, P. Grangier, and G. Roger, "Experimental tests of realistic local theories via Bell's theorem," *Phys. Rev. Lett.*, vol. 47, pp. 460–463, Aug 1981.

Modelling and Predicting New Drug ADRs via Integrating Heterogeneous Data

Yezhao Zhong

Supervisor: Dr. Haixuan Yang,
Prof. Cathal Seoighe

Adverse drug reactions (ADRs) affect human health and even lead to death in severe case. However, ADRs are not considered as major threat until cases were reported unexpectedly and drugs were recalled even though they were approved by Food and Drug Administration (FDA). These post-marketing drug reaction is at the cost of patients' health. At the same time, research on ADRs is time consuming and costly especially when drugs, developed with high cost, were recalled due to ADRs. Drug-side effect interaction prediction and ADRs prediction approaches are well studied, but methods for new drugs still have great potential for development.

In this poster, we introduce an adaptive Graph regularized Non-negative Matrix Factorization (GRNMF) method [1]. In case of new drug ADRs prediction, all ADRs remain unknown, represented by zero columns or rows in a drug-ADRs matrix. For this reason, most NMF based methods cannot make prediction for the new drugs. Our idea is to utilize not only the drug-ADRs data, but also some additional drug-drug similarity information to predict side-effects. As similar drugs might have close ADRs, drug-drug similarity graphs were adopted to regularize NMF, propagating the known information to zero rows and columns. These information

are from different sources, including chemical structure fingerprints from PubChem, drug-gene interaction from DGIdb.

By using addition similarity information, we can predict ADRs for new drugs, but one single similarity graph might not be able to cover all of them. We also considered integrating different similarity graphs to improve coverage, because different graphs might cover distinct group of drugs. We adopted linear regression model to fit coefficients of the graphs [2]. The explanatory variables are similarity graphs, and the response variable was constructed from the drug-ADRs matrix, in the same way as the GeneMania [3]. Through this coefficients we can construct a integrated graph that has higher coverage.

Supported by H202 MSAC, SFI [18/CRT/6214].

References

- [1] Cai, D., He, X., Han, J., & Huang, T. S. *Graph regularized nonnegative matrix factorization for data representation..* IEEE Transactions on Pattern Analysis and Machine Intelligence, vol. 33, no. 8, pp. 1548-1560, Aug. 2011, doi: 10.1109/TPAMI.2010.231.
- [2] Torres, M., Yang, H., Romero, A.E. et al. *Protein function prediction for newly sequenced organisms..* Nat Mach Intell 3, 1050-1060, (2021). <https://doi.org/10.1038/s42256-021-00419-7>
- [3] David Warde-Farley, Sylva L. Donaldson, Ovi Comes, Khalid Zuberi, Rashad Badrawi, Pauline Chao, Max Franz, Chris Grouios, Farzana Kazi, Christian Tannus Lopes, Anson Maitland, Sara Mostafavi, Jason Montojo, Quentin Shao, George Wright, Gary D. Bader, Quaid Morris. *The GeneMANIA prediction server: biological network integration for gene prioritization and predicting gene function..* Nucleic Acids Research, Volume 38, Issue suppl_2, 1 July 2010, Pages W214-W220, <https://doi.org/10.1093/nar/gkq537>

5 Abstracts of PhD theses

Algorithms for the accurate and efficient solution of fourth-order boundary-layer problems

Faiza Alssaedi

Supervisor: Niall Madden

In this thesis, we study the analysis and numerical solution of second-order complex-valued reaction-diffusion equations, and two families of fourth-order singularly perturbed problems. The problems are all *singularly perturbed*, meaning that each has a parameter, ϵ , multiplying the highest derivative. This parameter is positive but maybe arbitrarily small. However, as $\epsilon \rightarrow 0$, the differential equations become ill-posed, hence the singular nature of the perturbation.

The choice of problems we study are motivated by models based on the Rayleigh equation (see, e.g., [1]) and the Orr-Sommerfeld equation for hydrodynamic stability, (see, e.g., [1, 2]). The physical meaning of these models is not important to this thesis. What is important is that they are challenging to solve using standard numerical schemes. Therefore, novel methods are required.

References

- [1] P. G. Drazin and W. H. Reid. Hydrodynamic stability. Cambridge University Press, 2nd edition, 2004. (*Cited on pages 1, 128, and 129.*)
- [2] N. Madden, M. Stynes, and G.P. Thomas. On the application of robust numerical methods to a complete-flow wave-current model. *In Proc. Bail, Toulouse, 2004.* (*Cited on pages 1, 6, and 128.*)

Exploiting individual agent properties for analysis and control of collective network evolution

Roberto Galizia

Supervisor: Dr Petri Piironen

In this thesis, we investigate linearly coupled dynamic networks made up of identical oscillators. We study the principles in which the dynamical features of the underlying constituent agents transfer to the collective dynamics of the entire network.

This is carried out from two points of view: analysis and control. In the former case, the objective is to predict the dynamical behaviour of the entire network, by studying the structural properties and the asymptotic dynamical behaviour of the uncoupled agents. However, due to the high complexity that arises when many agents are connected with each other, it is not always possible to determine all the asymptotic solutions of a network. Therefore, we focus on analysing under what conditions we can guarantee a 1-to-1 correspondence between the limit sets of the uncoupled agents and the network. In other words, we investigate the scenario where all network agents behave like a single uncoupled agent. This behaviour, which we refer to as reduced dynamics, extends the subject of network synchronization to a global scale. In some cases, we are able to prove analytically that a region of reduced dynamics exists if the network parameters satisfy certain conditions. In the more general case, we conjecture the conditions for existence of this region and support the conjecture with numerical experimental evidence. In the latter case, we define a control strategy to obtain a desired global dynamical behaviour while only acting on a small subset of the network nodes, without using any global information. In other words, we design a decentralised control algorithm that drives the entire network towards a desired state, based only on local information of a small subset of nodes and their neighbours. In order to validate the control algorithm we test it via simulations for networks with different properties and topologies. First, these numerical experiments are conducted on networks of bistable agents with vector field given by a cubic function. We compare the decentralised strategy with three centralised algorithms in order to evaluate its performance. Finally, we extend our experiments to a network of agents where the uncoupled dynamics presents a discontinuity. In particular, we consider the model of a ball or a particle impacting on an oscillating floor. The strong nonlinearity introduced by impacts makes the network dynamics very unpredictable and we show some numerical examples of the complexity that can arise in such systems. Despite the complexity, we also show that with a proper control action we can use the decentralised control algorithm to control the network and thus synchronizing all the agents.

6 Staff profiles

Balbi, Valentina

Current research interests

My research field is in soft tissues mechanics, I am interested in both experimental and theoretical aspects. Due to their complexity, soft tissues are difficult to test. From the experimental viewpoint, I am interested in developing robust and reliable testing protocols suitable for different tissues. Theoretically, I develop new mathematical models to capture the non-linear mechanical behaviour of soft tissues. Continuum mechanics, non-linear elasticity and visco-elasticity are my everyday tools.

Research outputs

- **Balbi V** & Righi M (2022). *Foundations of viscoelasticity and application to soft tissues mechanics*, Chapter in “Modelling of Biomaterials”. Publisher: Birkhauser. Editors: Josef Málek and Endre Suli. Here we review the foundations of the theory of Quasi-Linear Viscoelasticity and show how to apply this theory to model the viscoelastic response of soft tissues.
- **Balbi V**, Destrade M & Goriely A (2020). *Mechanics of human brain organoids*. *Physical Review E*, 101(2), 022403. In this work, we proposed a morphoelastic model to predict lissencephaly, a brain malformation occurring at the early stages of human brain organoids development.

Research activities

- I recently gave a seminar at Excellence Seminar Series in the Department of Mathematics at the Politecnico di Torino (here is the link to the talk)
- I am organising the mini-symposium “Instabilities of soft materials” at the ESMC 2022 in NUI Galway (4th-8th July) (link to the mini-symposium)

Berjamin, Harold

Current research interests

My current research deals with the mechanical modelling of soft biological tissues within the frameworks of nonlinear elasticity, viscoelasticity and poro-elasticity. These research activities are mainly motivated by the study of shock wave formation in brain tissue, a topic which arises in the context of Traumatic Brain Injury (TBI). Recent results and ongoing developments are mostly of theoretical and computational nature. Parallel research works concern the acoustoelasticity theory and phase transitions.

Recent publications

- [1] H. Berjamin, M. Destrade, A hyperbolic framework for shear sound beams in nonlinear solids, *Commun. Nonlinear Sci. Numer. Simul.* 103 (2021), 106036. doi:10.1016/j.cnsns.2021.106036
- [2] H. Berjamin, Nonlinear plane waves in saturated porous media with incompressible constituents, *Proc. R. Soc. Lond. Ser. A Math. Phys. Eng. Sci.* 477 (2021), 20210086. doi:10.1098/rspa.2021.0086
- [3] H. Berjamin, S. Chockalingam, Shear shock formation in incompressible viscoelastic solids, *Wave Motion* 110 (2022), 102899. doi:10.1016/j.wavemoti.2022.102899
- [4] H. Berjamin, R. De Pascalis, Acoustoelastic analysis of soft viscoelastic solids with application to pre-stressed phononic crystals, *Int. J. Solids. Struct.* 241 (2022), 111529. doi:10.1016/j.ijsolstr.2022.111529

Research activities

- *Grants*: This research has received funding from the European Commission under the Marie Skłodowska Curie Fellowship programme.
- *Conferences*: 2. 5th SofTMech Soft Tissue Modelling workshop, St. Andrews (UK, virtual); 15^{es} Journées d’Étude des Milieux Poreux, Strasbourg (France, hybrid).

- *Invited talks*: 3. School of Mathematics, NUI Galway (Ireland); LabTAU Inserm, Lyon (France); Institut de Recherche en Génie Civil et Mécanique, Nantes (France).
- *Papers refereed*: 9.
- *Memberships*: SIAM, AFM-Euromech.

Burns, John

Current research interests

My research interests are Algebra (Lie algebras, Lie groups, Weyl groups) and Differential Geometry (Homogeneous manifolds, Symmetric spaces). One current topic of interest is discrete (Weyl group) analogues of maximal tori in compact Lie groups and their application to classical (and new) configurations of lines on del Pezzo surfaces.

Recent publications

- [1] Burns, John M.; Pfeiffer, Goetz Maximal order Abelian subgroups of Coxeter groups. *Glasg. Math. J.* (to appear).
- [2] Burns, J. M.; Makrooni, M. A. Coxeter exponents and orthogonal complements of highest roots. *Comm. Algebra* 48 (2020), no. 7, 2833-2843.
- [3] Burns, John M.; Makrooni, Mohammad A. Parabolic subroot systems and their applications. *Glasg. Math. J.* 62 (2020), no. 2, 355-366.
Burns, John M.; Makrooni, Mohammad A.

Carnevale, Angela

Current research interests

My research is mostly in the fields of algebraic and enumerative combinatorics. These days, I am especially interested in posets and permutation statistics related to Coxeter groups. I also like to apply combinatorial tools and techniques to problems related to zeta functions in algebra.

Recent publications

- [1] F. Brenti, A. Carnevale and B. E. Tenner, *Odd diagrams, Bruhat order, and pattern avoidance*, *Combinatorial Theory* (2022), 2(1), Paper 13, 19 pp.
- [2] A. Carnevale and T. Rossmann, *Linear relations with disjoint supports and average sizes of kernels*, *J. Lond. Math. Soc.*, to appear (2022), 51 pp.
- [3] A. Carnevale and E. Tielker, *On Denert's statistic*, arXiv:2108.04700, 16 pp.
- [4] A. Carnevale, M. Dyer and P. Sentinelli, *The intermediate orders of a Coxeter group*, arXiv:2203.00405, 14 pp.

Research activities

- Invited talk: “Matrices, board games, and orbits”, *Lincoln-Lund Algebra Seminar*, November 2021.
- Conference organised: *Groups in Galway 2021* (with Tobias Rossmann), December 2021.
- Conference organised: *Workshop on Enumerative Combinatorics 2022* (with Mark Dukes and Götz Pfeiffer), April 2022.
- Invited speaker of the (upcoming) *Fifth International Workshop on Zeta Functions in Algebra and Geometry*, Nice, France, May 2022.
- Invited speaker of the (upcoming) *Geometry meets Combinatorics in Bielefeld*, September 2022.

Conroy Broderick, Hannah

Current research interests

My current research interests lie in modelling soft active materials (dielectric & magnetoactive elastomers) and microstructured materials (laminates & composites). In particular, I am interested in modelling instability, pattern formation and wave propagation in these materials so to understand

and predict their behaviour. Current ongoing work includes modelling shear shock waves in microstructured materials and wave propagation in various magnetoactive materials.

Recent publications

- [1] H. Conroy Broderick, L. Dorfmann, M. Destrade. Electro-elastic Lamb waves in dielectric plates. *Extreme Mech. Lett.*, 39:100782, 2020.
- [2] H. Conroy Broderick, M. Righi, M. Destrade, R.W. Ogden. Stability analysis of charge-controlled soft dielectric plates. *Int. J. Eng. Sci.*, 151:103280, 2020.

Research activities

- Began work as a postdoctoral researcher working on wave mechanics and magnetoactive materials in April 2021.
- Talk accepted for minisymposium on Electro- and Magneto-Elasticity and its Applications at the European Solid Mechanics Conference (Galway, July 2022).

Coughlan, Simone

Current research interests

My current research interests are in pathogen genomics, metagenomic analysis of bacteria and viruses in the human gut and wider environment (wastewater and soil), cancer genomics, and structural variation discovery and analysis.

Recent publications

- [1] Heenan-Daly, D., Coughlan, S., Dillane, E., Prestwich, B.D. Volatile Compounds From Bacillus, Serratia, and Pseudomonas Promote Growth and Alter the Transcriptional Landscape of Solanum tuberosum in a Passively Ventilated Growth System doi:10.3389/fmicb.2021.628437 *Front Microbiol.*, 12:628437, 2021.
- [2] King, Lydia., Flaus, Andrew., Coughlan, S., Holian, E., Golden, A. GNOSIS:

an R Shiny app supporting cancer genomics survival analysis with cBioPortal. doi:https://doi.org/10.12688/hrbopenres.13476.1 *HRB Open Research*, 5:8, 2022

Research activities

- Students: 2 PhD students from the Genomics Data Science CRT: Sophie Matthews and Mark Maguire
- Co-supervising 3 PhD students: Lydia King, Stephen Smith and Micheál Ó Dálaigh
- 2 summer interns in summer of 2021: Adam Dunne and Michelle Maher
- Processed SARS-Cov-2 genomes sequenced using nanopore by Dr Kate Reddington and PhD student Grainne Mc Andrew on ICHEC as part of the SFI funded Irish Coronavirus Sequencing Consortium
- Current research activity includes research into approaches to preoccupy a baby for more than 5 minutes so that I can write this list

Cruickshank, James

Current research interests

My current research interests include

- Geometric rigidity theory. This is the mathematical theory of structural rigidity. I am particularly interested in the combinatorial theory e.g. which graphs arise from rigid bar-joint frameworks.
- Face numbers of simplicial complexes. In particular lower bound theorems for face numbers.
- Multilinear algebra over local rings. In particular combinatorial objects associated to various hermitian or skew-hermitian forms.

Recent publications

- [1] James Cruickshank, Bill Jackson, and Shin-ichi Tanigawa. Global rigidity of triangulated manifolds, 2022. URL: <https://arxiv.org/abs/2204.02503>

- [2] James Cruickshank, Eleftherios Kastis, Derek Kitson, and Bernd Schulze. Braced triangulations and rigidity, 2021. URL: <https://doi.org/10.48550/arxiv.2107.03829>
- [3] J. Cruickshank, L. Gutiérrez Frez, and F. Szechtman. Weil representations via abstract data and Heisenberg groups: a comparison. *J. Algebra*, 547:129–161, 2020.
- [4] James Cruickshank, Bill Jackson, and Shin-ichi Tanigawa. Vertex splitting, coincident realisations and global rigidity of braced triangulations, 2020. URL: <https://doi.org/10.48550/arxiv.2002.06860>
- [5] James Cruickshank and Bernd Schulze. Symmetric contact systems of segments, pseudo-triangulations and inductive constructions for corresponding surface graphs, 2020. URL: <https://doi.org/10.48550/arxiv.2006.10519>
- [2] A. Anssari-Benam, M. Destrade, G. Saccomandi. Modelling brain tissue elasticity with the Ogden model and an alternative family of constitutive models. *Philosophical Transactions of the Royal Society A* (2022) to appear.
- [3] J. Blackwell, M.J. Krasny, A. O'Brien, K. Ashkan, J. Galligan, M. Destrade, N. Colgan. Proton resonance frequency shift thermometry: A review of modern clinical practices. *Journal of Magnetic Resonance Imaging*, 55 (2022) 389-403.
- [4] H. Berjamine, M. Destrade. A hyperbolic framework for shear sound beams in nonlinear solids. *Communications in Nonlinear Science and Numerical Simulation*, 103 (2021) 106036.
- [5] J.-P. Remenieras, M. Bulot, J.-L. Gennisson, F. Patat, M. Destrade, G. Bacle. Acousto-elasticity of transversely isotropic incompressible soft tissues: Characterization of skeletal striated muscle. *Physics in Medicine and Biology*, 66 (2021) 145009.

Research activities

- 2 journal submissions in the last year, 5 submissions currently under review.
- Participation in the Fields Institute Thematic Program on Geometric Constraint Systems, Framework Rigidity, and Distance Geometry, January-June 2021.
- Conference presentation at Southeastern International Conference on Combinatorics, Graph Theory and Computing, March 2022.

Destrade, Michel

Current research interests

I work on the modelling of dielectric and magneto-elastic elastomers, on acoustic waves travelling in soft tissues and in stressed solids, and on the imaging of soft solids.

Recent publications

- [1] G.-Y. Li, A.L. Gower, M. Destrade, S.-H. Yun. The sound of cling film: Non-destructive mapping of stress and strain in soft thin films. *Communications Physics* (2022) to appear.

Research activities

- *Current research grants*: 2 IRC postgraduate scholarships; 1 Marie Skłodowska Curie Doctoral Fellowship; 2 Marie Skłodowska Curie Postdoctoral Fellowships; 111 Project Visiting Grant from Zhejiang University; Ulysses Grant.
- *Conferences/Seminars*: Modena, Moscow, Hangzhou, Dresden, Glasgow, Keele.
- *Graduate Course*: Nonlinear Elasticity, Zhejiang University, Hangzhou.
- *Appointments*: External Examiner at TUD; Reviews Editor at Proceedings of the Royal Society A; Associate Editor at International Journal of Non-Linear Mechanics, Mechanics of Soft Solids, Journal of the Acoustical Society of America, SIAM Journal on Applied Mathematics; Adjunct Professor of Mechanical Engineering at University College Dublin and Zhejiang University; Directeur de Recherche at Institut d'Alembert, CNRS,

Paris, France (on leave); Member of the International Brain Mechanics and Trauma Lab (Oxford).

Ellis, Graham

Current research interests

I am interested in computational topology with a view to applications in group theory, number theory, data analysis.

Recent publications

- [1] G. Ellis. Introductory computations in the cohomology of arithmetic groups. *Advanced Studies: Euro-Tbilisi Mathematical Journal*, Special Issue (9 - 2021), pp. 1–31.
- [2] G. Ellis & K. Killeen. Cohomology with local coefficients and knotted manifolds. *Journal Symbolic Computation*, 107, 299–321 (2021).

Research activities

- Khaled Alzobydi started his PhD studies in March 2022. Kelvin Killeen plans to complete his PhD studies by August 2022.
 - Co-edited a special volume of ASETMJ on *Cohomology, Geometry, Explicit Number Theory*.
 - In June 2022 will deliver a series of lectures with Bettina Eick (Braunschweig) and Alexander Hulpke (Colorado State) on *computational cohomology of groups* at the 2022 COGENT Summer School in Grenoble, France.
 - Continued to co-organize the fortnightly online COGENT Seminar.
 - Continued editorial work for: Homology, Homotopy & Applications; Journal Homotopy and Related Structures; Applicable Algebra in Engineering, Communication & Computing; Advanced Studies: Euro-Tbilisi Mathematical Journal; GAP Council.
-

Flannery, Dane

Current research interests

Computation with linear groups; algebraic design theory.

Recent publications

- [1] Z. Bácskai, D. L. Flannery, and E. A. O'Brien. *Classifying finite monomial linear groups of prime degree in characteristic zero*, International Journal of Algebra and Computation **31**, no. 8, 1547–1585, 2021.
- [2] D. L. Flannery, and E. A. O'Brien. Monomial: MAGMA-based classification of finite irreducible monomial groups in characteristic zero and prime degree.

Research activities

- Invited conference talk, Computational Aspects of Discrete Subgroups of Lie Groups, The Institute for Computational and Experimental Research in Mathematics, USA, June 14–18, 2021.
 - Oberwolfach Research Fellows, Mathematisches Forschungsinstitut Oberwolfach, Germany, 1–14 August, 2021.
 - Research in Pairs, Centre International de Rencontres Mathématiques, Luminy, France, 23 August–3 September, 2021.
-

Golden, Aaron

Current research interests

Electromagnetic processes in brown dwarf and exoplanetary atmospheres & magnetospheres.

Spin-orbit alignment in the very low mass binary regime.

Astronomical instrumentation.

Recent publications

- [1] King, Lydia and Flaus, Andrew and Coughlan, Simone and Holian, Emma and Golden, Aaron GNOSIS: an R Shiny app supporting cancer genomics survival analysis with cBioPortal. *HRB Open Research*, 5 (8):1-11, 2022.

- [2] Ó Fionnagáin et al. Coronal Mass Ejections and Type II Radio Emission Variability during a Magnetic Cycle on the Solar-type Star ϵ Eridani. *Astrophysical Journal*, 924 (2):115-132, 2022.
- [3] Murphy et al. First results from the REAL-time Transient Acquisition backend (REALTA) at the Irish LOFAR station. *Astronomy & Astrophysics* 655:A16-A38, 2021.
- [4] Geever et al. Research 387: GRACE Monitoring of Groundwater over Ireland - A Feasibility Study. Environmental Protection Agency, Dublin, 2021.
- [5] Golden, A et al. Host and intestinal microbiota derived metabolomic blood plasma signature for prior radiation injury. Alexandria, Virginia: US Patent and Trademark Office No. 11092591, 2021.

Research activities

- Telescope Time Awards
James Clerk Maxwell Telescope, USA - *Circumpulsar debris disks* (8.9 hrs); I-LOFAR, Birr - *Giant radio pulses from PSR B0656+14* (ongoing); NenuFAR, France - *Studying Uranian Lightning* (5 hrs); European VLBI Network - *Stellar wind environment of λ And.* (18 hrs); Vatican Advanced Technology Telescope, USA - *A JWST ephemeris for the exoplanetary analogue VHS 1256-1257 b* (13 nights).
- New Funding Awards
Science Foundation Ireland Future Innovator Prize 2019
- Existing Research Grants
Environmental Protection Agency STRIVE award 2018-W-MS-35 - *The Diversity and Resilience of kelp ecosystems in Ireland*; Environmental Protection Agency STRIVE award 2017-W-MS-30 - *Remote Sensing of Irish Surface Waters*; Health Research Board (COVID-19 Rapid Response Research & Innovation Programme)
- Research Meetings
Session C1.04 AI4EO applications for Land

and Water, European Space Agency Living Planet Symposium 2022, Bonn, Germany, 23–27 May 2022 - Convenors: Sita Karki (Irish Centre for High End Computing), Aaron Golden (National University of Ireland), Ricardo Bermejo (Universidad de Cádiz).

- Research Supervision Postdoctoral Fellows: 1. Current PhD Students: 5. Current MSc(Res) Students: 2. Research Assistant: 1

Hill, Róisín

Current research interests

My research interest is in scientific computing, particularly in finite element methods for partial differential equations. I work over a range of software platforms and am specifically proficient in programming in FEniCS. At present, I am working on the design and implementation of adaptive-meshing algorithms for boundary and interior layer problems.

Recent publications

- [1] Róisín Hill and Niall Madden, Generating layer-adapted meshes using mesh partial differential equations. *Numer. Math. Theory Methods Appl.*, 14(3):559–588, 2021.

Research activities

- I submitted my PhD thesis entitled “Moving mesh methods for problems with layer phenomena” in March 2022. I am currently preparing for my viva and preparing additional articles for publication.
- In March 2022, I gave a presentation at the 18th Workshop on Numerical Methods for Problems with Layer Phenomena in Hagen, Germany.
- I was invited and presented my research (online) at a SIM (Short Informal Mathematics) talk to academics and postgraduate students at UL in 2021.

- I was a panellist at the PhD Panel Discussion: The Life of a PhD Student. The event was organised by the SIAM-IMA Dublin Area Student Chapter and was aimed at students interested in doing a PhD in Mathematics. It took place online in 2021.
- I gave a presentation at FEniCS 2021, Cambridge (online). This has been published as part of their conference proceedings, at <https://doi.org/10.6084/m9.figshare.14495376.v1>.
- I started a research assistant position on 1st April 2022, with Niall Madden, on advanced finite element methods for applied problems.

Holian, Emma

Current research interests

Prognostic models in Breast Cancer, in particular; variable selection in survival models for data with various missingness mechanisms, modelling treatment outcome on longitudinal biomarkers. Statistical methods in Genomics Data Science; hypothesis testing in Microarray analysis, Next-Generation Sequencing (NGS), genome Copy Number Alterations, with focus on the error structure, improved standard error estimators, distribution estimation and multiple testing adjustment techniques. Statistical challenges in environmental impact studies and climate data; challenges of left-censored distributions in groundwater data. Classification and cluster analysis of longitudinal data profiles via Regression Cluster Model (RCM), mixture modelling using generalized linear mixed models and penalized smoothing models. Modelling Composition Response data, e.g. influencing factors in blood clot composition, via Dirichlet Regression.

Recent publications

- [1] L. King, A. Flaus, S. Coughlan, E. Holian, A. Golden. GNOSIS: an R Shiny app supporting cancer genomics survival analysis with cBioPortal *HRB Open Research*, 2022.
- [2] L. King, A. Flaus, E. Holian, A. Golden. Survival Outcomes are Associated with Genomic Instability in Luminal Breast Cancers. *Plos One*, 2021.
- [3] R. Waldron, B. Moloney, K. Gilligan, A. Lowery, M. Joyce, E. Holian, M.J. Kerin, N. Miller. MicroRNAs as biomarkers of multimodal treatment for rectal cancer *British Journal of Surgery*, 2021, 108 (8).
- [4] E. McGrory, E. Holian, L. Morrison. Assessment of groundwater processes using censored data analysis incorporating non-detect chemical, physical, and biological data. *Journal Of Contaminant Hydrology*, 235, 2020.
- [5] A. McGuire, et.al. Prospective Assessment of Systemic MicroRNAs as Markers of Response to Neoadjuvant Chemotherapy in Breast Cancer. *Cancers*, 12(7), 2020.

Research activities

Ph.D Student Supervision (3): Maxwell Paganga - NBCRI, Lydia King - SFI CRT Genomics Data Science, Olga Kalinina - NBCRI.

Affiliations: Biostatistics and Bioinformatics Research Cluster, Biostatistics Unit HRB CRFG, INSIGHT NUIG, ISA, International Biometric Society.

Howard, Mark

Current research interests

I'm primarily interested in quantum information theory, specifically:

- Stabilizer formalism (generalization to d-level systems, quantum error-correcting codes, Gottesman-Knill theorem)
- Clifford group and classical simulability of restricted quantum circuits
- Discrete Wigner functions (negative quasiprobabilities, relationship with GK theorem)
- Magic state distillation and Quantum Fault tolerance more generally
- Nonlocality & Contextuality, Mutually unbiased bases, SIC-POVMs, foundations of quantum theory

Research outputs

- 1 Pierre-Emmanuel Emeriau, Mark Howard, Shane Mansfield
Quantum Advantage in Information Retrieval
PRX Quantum (In press) 2022.
- 2 Michael Beverland, Earl Campbell, Mark Howard, Vadym Kliuchnikov
Lower bounds on the non-Clifford resources for quantum computations
Quantum Sci. Technol. 5 035009 (2020).
- 3 S. Bravyi, D. Browne, P. Calpin, E. Campbell, D. Gosset and M. Howard,
Simulation of quantum circuits by low-rank stabilizer decompositions.
Quantum 3, 181 (2019).
- 4 M. Howard, and E. T. Campbell,
Application of a resource theory for magic states to fault-tolerant quantum computing
Physical review letters 118 9 090501 (2017).
- 5 M. Howard, J. Wallman, V. Veitch, and J. Emerson,
Contextuality supplies the “magic” for quantum computation.
Nature, 510, 351 (2014).

Research activities

- Invited Talk “A Resource Theory for Quantum Computation”, Irish Mathematical Society September Meeting MTU/UCC.
- Invited Seminar “Topics in Stabilizer Quantum Computation”, Oxford ZX-calculus seminar Online.
- Awarded Royal Society Enhanced Research Expenses for PhD & Summer Studentships
- PhD student Mark Ryder won a IRC Postgraduate Scholarship (for Sept 2022)
- PhD student Billy Ray won a IRC Postgraduate Scholarship (declined)
- Acted as External Examiner, Ph.D. Candidate, University College London, (Sept. 2021).
- Acted as External Expert, Ph.D. Midterm Discussion, Chalmers University, Sweden

(Aug. 2021).

Kerin, Martin

Current research interests

My research is primarily aimed at understanding Riemannian manifolds with either positive or non-negative sectional curvature. This often leads to the use of techniques from, and to deep questions emerging in, areas such as Lie Groups, Representation Theory, Algebraic and Differential Topology, and Rational Homotopy Theory. Recently, much of my research has involved manifolds which can be decomposed as the union of two disk-bundles.

Recent publications

- [1] J. DeVito, F. Galaz-García and M. Kerin, *Manifolds that admit a double disk-bundle decomposition*, to appear in Indiana Univ. Math. J.

Research activities

- *Conferences organised*: 1 (Groups in Galway meets the Irish Geometry Seminar (NUIG))
- *Seminars organised*: 1 (Irish Geometry Seminar)
- *Conferences attended*: 2 (Münster; Irish Maths Society)
- *Referee reports*: 3
- *Reviews for Mathematical Reviews*: 2
- *PhD students*: 1 (Badriah Safarji)
- *External examiner*: 1 (Transfer from Masters to PhD register at MTU)

Madden, Niall

Current research interests

My research relates to the numerical analysis of partial differential equations, especially those with boundary and interior layers in their solutions. My work covers novel discretizations (such as weighted finite elements), meshing techniques (such as r -refinement), and solvers for resulting linear systems (such as multigrid methods).

Recent publications

- [1] R. Hill and **N. Madden**. Generating layer-adapted meshes using mesh partial differential equations. *Numer. Math. Theory Methods Appl.*, 14(3):559–588, 2021.
- [2] **N. Madden** and M. Stynes. A weighted and balanced FEM for singularly perturbed reaction-diffusion problems. *Calcolo*, 58(2): 28, 2021.
- [3] T.A. Nhan and **N. Madden**. An analysis of diagonal and incomplete Cholesky preconditioners for singularly perturbed problems on layer-adapted meshes. *J. Appl. Math. Comput.*, 65(1-2):245–272, 2021.
- [4] N. Poddar, K.K. Mondal, and **N. Madden**. Layer-adapted meshes for solute dispersion in a steady flow through an annulus with wall absorption: Application to a catheterized artery. *Korea-Aust. Rheol. J.*, 33(1):11–24, 2021.
- [5] H. Jahandari, S. MacLachlan, R.D. Haynes, and **N. Madden**. Finite element modelling of geophysical electromagnetic data with goal-oriented *hr*-adaptivity. *Comput. Geosci.*, 24(3):1257–1283, 2020.

Research activities

- Faiza Alssaedi and Róisín Hill both submitted their PhD theses, completed under my supervision, this year.
- In recent times, I have refereed manuscripts for various journals, including *Calcolo*, *IMA J. Numer. Anal.*, *SIAM J. Sci Comput.*, and *Irish Math. Soc. Bulletin*.
- I am an associate editor of *Numerical Algorithms* (Springer).
- I was an invited speaker at a conference on *Numerical Methods and Scientific Computing*, Centre International de Rencontres Mathématiques, in November 2021. And I presented at the 18th Workshop on Numerical Methods for Problems with Layer Phenomena, Hagen, Germany, March 2022.

McCluskey, Aisling

Current research interests

My current research interests revolve around generalising the classic notions of betweenness, equidistance and relativeness closeness in Euclidean geometry to the natural context of metric spaces. Such notions can be viewed from an axiomatic perspective which then can be interpreted in a metric space, especially one where the metric is induced by a vector space norm. Betweenness intervals naturally give rise to a notion of convexity and so convexity has been a particular focus for my research. For normed vector spaces, it turns out that betweenness intervals are always convex when the dimension is at most two, but the convexity property easily fails in higher dimensions. Relative closeness regions in a normed vector space are convex precisely when the norm arises from an inner product. Providing a characterisation of normed vector space properties purely in terms of abstract betweenness and relative closeness is a motivation for further research on the topic.

Recent publications

- [1] D. Anderson, P. Bankston, A. McCluskey Convexity in topological betweenness structures. *Topology and its Applications*, 304, 2021, paper no. 107783 (20pp)
- [2] A. McCluskey, B. McMaster Integration with complex numbers - a primer on complex analysis *Oxford University Press*, April 2022

Research activities

- Member of Steering committee for 22nd Galway Topology Colloquium, June 2022 at the University of Portsmouth, UK

Mc Gettrick, Michael

Current research interests

I am actively doing research in the theory of quantum computing and quantum information, mathematical aspects of transport networks (trams etc.) and algorithmic composition (how to write music using mathematical rules).

Research activities

- In September 2021, Ian Craig began his PhD research under my supervision, working in quantum walks.
- In 2021, I was active in the initial establishment of QIreland as part of QWorld (see <https://qworld.net/qireland/>)
- In January 2022, I visited Stefan Siegmund at TU Dresden (Germany) for two weeks to initiate a collaboration. Our work is on iterated quantum games played on a graph, viewed as a dynamical system.
- In March 2022, a two week research visit was made to the group of Sergio Gomez at Universitat Rovira i Virgili (Tarragona, Spain). Our work together looks at interacting quantum agents on networks.
- I am an active participant in the COST actions on “European Network for Game Theory” and “Mathematical models for interacting dynamics on networks”.
- As a member of the National Advisory Forum for Quantum Technologies, I have contributed to the recently published “Ireland’s National Strategy for Quantum Technologies” (2021).
- I am a member of the EPSRC (Engineering and Physical Sciences Research Council, UK) Peer Review College.

Meere, Martin

Current research interests

Modelling enzymatic processes; modelling diffusion in strained crystals; modelling drug delivery applications.

Research outputs

One peer reviewed publication in 2021.

- [1] Vinh Q. Mai & Martin Meere, Modelling the phosphorylation of glucose by human hexokinase I, *MDPI Mathematics*, 9(18), 2315; <https://doi.org/10.3390/math9182315>, 2021.

Research activities

I have one PhD student, Modhi Albaqami. Modhi is working on modelling ternary solid dispersions. One PhD student graduated in 2020 - Dr Vinh Q. Mai. I have a number of active collaborations.

Newell, John

Current research interests

My current research interests are in the development and application of statistical methods in clinical research, health data science, sports science and Translational Statistics.

Recent publications

- [1] Morrissey, E.C., Byrne, M., Casey, B. Newell, J. et al. Improving outcomes among young adults with type 1 diabetes: the D1 Now pilot cluster randomised controlled trial. *Pilot Feasibility Study*, 8, 56 (2022).
- [2] Pedlar CR, Myrissa K, Barry M, Newell, J., Scarrott, C., et al. Medical encounters at community-based physical activity events (parkrun) in the UK. *British Journal of Sports Medicine*, 2021;55:1420-1426.
- [3] Moghaddam, S.; Newell, J.; Hinde, J. A Bayesian Approach for Imputation of Censored Survival Data. *Stats.*, 2022, 5, 89–107.
- [4] Finucane, E., O’Brien, A., Treweek, S., Newell, J., et al. Does reading a book in bed make a difference to sleep in comparison to not reading a book in bed? The People’s Trial—an online, pragmatic, randomised trial. *Trials*, 22, 873 (2021).
- [5] de Paula Oliveira, T., Bruinvels, G., Pedlar, C.R., Newell, J. Modelling menstrual cycle length in athletes using state-space models. *Nature Scientific Reports* 11, 16972 (2021).

Research activities

- Grants:
UniCov Trial (Biostatistician), CURAM (funded PI with one 1 Postdoctoral Researcher), Insight (funded PI), HRB Primary

Care Clinical Trials Network Ireland (Biostatistician), HRB D2 Now Trial (Biostatistician), HRB CREST Trial (Biostatistician).

- Postgraduates:

Diarmuid Daniels (graduated 2021). Blood Biomarker Monitoring in Professional Soccer: Longitudinal Analysis of Inflammation in English Premier League Players. Insight/Orrco Project.

Lara Coyne (graduated 2021). Evaluation of a Markerless Motion Capture System in a Premier League Football Academy. Insight/Arsenal Project.

Current Postgraduates: 3 PhD students.

- External examiner:

UCC (2019-2022): MSc in Data Science and Analytics TCD Postgraduate Certificate in Statistics.

- Software:

R package ‘DynNom’ for generating Dynamic Nomograms, 45,000+ downloads to date.

The ELIXIR Machine Learning focus group, Jennifer Harrow, Fotis E. Psomopoulos & Silvio C.E. Tosatto. *Nature methods* 18(10), 1122-1127, 2021.

[3] Deep Learning of Histopathological Features for the Prediction of Tumour Molecular Genetics. Pierre Murchan, Cathal Ó’Brien, Shane O’Connell, Ciara S McNevin, Anne-Marie Baird, Orla Sheils, Pilib Ó Broin, Stephen P Finn. *Diagnostics* 11(8), 1406, 2021.

[4] Computational identification of variables in neonatal social communication predictive for post-pubertal social behaviors in a mouse model of 16p11.2 deletion. Mitsuteru Nakamura*, Kenny Ye*, Mariel Barbachan e Silva*, [...], Pilib Ó Broin, Mitsuyuki Matsumoto, Noboru Hiroi. *Molecular psychiatry* 26(11), 6578-6588, 2021.

[5] US Patent 11,092,591: Host and intestinal microbiota derived metabolomic blood plasma signature for prior radiation injury, AAJ Golden, P Ó Broin, C Guha, I Kurland.

Ó Broin, Pilib

Current research interests

My research interests lie primarily in clinical/translational bioinformatics with a particular focus on the development and application of machine learning methods for genomic data in the cancer, immunology, and neuroscience domains.

Research outputs

[1] ‘Thirteen Independent Genetic Loci Associated with Preserved Processing Speed in a Study of Cognitive Resilience in 330,097 Individuals in the UK Biobank’. Joan Fitzgerald, Laura Fahey, Laurena Holleran, Pilib Ó Broin, Gary Donohoe, Derek W Morris. *Genes*, 13(1), 122, 2022.

[2] DOME: Recommendations for supervised machine learning validation in biology’. Ian Walsh, Dmytro Fishman, Dario Garcia-Gasulla, Tiina Titma, Gianluca Pollastri,

Research activities

- My research group this year included: 8 PhD students, 2 MSc in Biomedical Genomics students, and 1 MSc in Chemoinformatics and Toxicology student.

- Research funded by: SFI (CRT in Genomics Data Science, €400k), NUIG Library and Student Project Fund (OER Development Scheme, €3k), DBEI (Disruptive Technologies Innovation Fund, €654k), IRC (Ulysses, €2.5k), Shared Island Fund (North-South Research Programme, €428k).

- External activities: Invited reviewer, Journal of Psychiatric Research, Irish Centre for High-End Computing; Executive Board Member, Irish Translational Medicine Network; Committee Chair, Alexandre Pelettier (PhD candidate, Bioinformatics and Systems Biology, Insitut Pasteur de Lille)

- Memberships: European Association for Cancer Research (EACR), International So-

ciety for Computational Biology (ISCB), Irish Society for Human Genetics (ISHG), European Society for Human Genetics (ESHG), Marie Curie Alumni Association (MCAA), ELIXIR Machine Learning Focus Group

Ó Fionnagáin, Dúalta

Current research interests

My primary research interest is in radio astronomy of low-mass stars and (exo)planets. I am currently working on detecting lightning in the atmosphere of Uranus using ground-based radio telescopes such as LOFAR, NenuFAR, and the OVRO-LWA. I am interested in low-mass stars (similar to our Sun), their winds, coronae, and magnetic fields. I research these phenomena using a combination of 3D magnetohydrodynamic simulations on parallel superclusters (incl. the national computing facility Kay, ICHEC) and radio observations. Utilising synergy between simulations and observations (using telescopes such as the EVN and LBA) we can achieve a better understanding of stellar atmospheres and their effects on their environments including exoplanets. Finally, I have a keen interest in exoplanets and star-planet interactions. As exoplanets orbit their host stars they can excite stellar atmospheres producing radio emission. I research the ways in which these interactions can happen to help us understand the star-planet environment and how we can advance observations to measure this phenomena.

Recent publications

- [1] Ó Fionnagáin D., et al., 2022, "Coronal Mass Ejections and Type II Radio Emission Variability during a Magnetic Cycle on the Solar-type Star ϵ Eridani", *The Astrophysical Journal*, 924, 115. doi:10.3847/1538-4357/ac35de
- [2] Ó Fionnagáin, D., et al. 2021, " λ And: a post-main-sequence wind from a solar-mass star", *Monthly Notices of the Royal Astronomical Society*, 500, 3438. doi:10.1093/mnras/staa3468

Research activities

- Observing campaign over six weeks with I-LOFAR and NenuFAR in the search for electrostatic discharges on Uranus.
- Awarded 18 hours to observe the binary star λ Andromedae with the European VLBI Network to study its stellar atmosphere.
- Member of the I-LOFAR and OVRO-LWA telescopes working groups.
- BCool consortium member, investigating the magnetic fields of low-mass and solar-type stars.

Pfeiffer, Götz

Current research interests

Complex hyperplane arrangements and their symmetry groups, various algebras related to these arrangements and their roles as modules for the group and as cohomology rings, Hecke algebras of complex reflection groups and their centers.

Recent publications

- [1] John M. Burns and Götz Pfeiffer. Maximal Order Abelian Subgroups of Coxeter Groups. *Glasgow Math. J.*, to appear.
- [2] J. Matthew Douglass, Götz Pfeiffer and Gerhard Röhrle. Invariants and semi-invariants in the cohomology of the complement of a reflection arrangement. arXiv:2009.12847.
- [3] L. Hellebrandt and G. Pfeiffer On the Left Connected Subalgebra of the Descent Algebra of a Coxeter Group of Classical Type. arXiv:2109.01473.
- [4] E. Chavli and G. Pfeiffer. Centers of Hecke Algebras of Complex Reflection Groups. arXiv:2112.10853.

Research activities

- Graduate Students: 1
- Papers refereed: 3.

- Conferences: Groups in Galway 2021, 2–3 December 2021, online; Dartellungstheorielage and Nikolaus Conference 2021, Aachen, Germany, 9–11 December 2021;
- Invited Talks: *Falling Powers and the Algebra of Descents* (March 2022, Algebra Number Theory Seminar at University of Arizona, Tucson, USA);
- Editorial Board Member: Journal of Symbolic Computation; Mathematical Proceedings of the Royal Irish Academy.
- Member: Irish Mathematical Society; American Mathematical Society.

Quinlan, Rachel

Current research interests

Combinatorial matrix theory, including affine and linear spaces of matrices with special rank properties, alternating sign matrices, and linear algebra over rings. I am also interested in mathematics education at tertiary level. I have a recreational interest in geometric origami, which is related to my “serious” mathematical activity.

Research outputs

- [1] Cian O’Brien and Rachel Quinlan. *Alternating sign matrices of finite multiplicative order*, to appear in Linear Algebra and its Applications.
- [2] Rachel Quinlan, Moumita Shau and Fernando Szechtman. *Linear diophantine equations in several variables*, Linear Algebra and its Applications, Vol. 630, 67–90, 2022.
- [3] C. O’Brien, K. Jennings and R. Quinlan. *Alternating signed bipartite graphs and difference-1 colourings*, Linear Algebra and its Applications, Vol. 604, 370–398, 2020.
- [4] O. O’Mahony and R. Quinlan. *Exponent-critical primitive graphs and the Kronecker product*, Electronic Journal of Graph Theory and its Applications, Vol. 7, no. 2, 329–347, 2019.

- [5] Hieu Ha Van and Rachel Quinlan. *Almost-nonsingular entry pattern matrices*, Linear Algebra and its Applications, Vol. 578, 334–355, 2019.

Research activities

- I am the co-chair of the local and scientific organising committees of the 24th Conference of the International Linear Algebra Society, will take place in NUI Galway in June 2022, having been deferred from 2020. About 250 participants are expected at this conference.
- In 2021 I gave (online) research presentations at the Western Canadian Linear Algebra Meeting (on matrix theory) and at the meeting of the German and Austrian Mathematical Societies, the Gathering for Gardner Celebration of Mind event, and the Groups in Galway Conference (on geometric origami).
- I am currently supervising the research of two PhD students at NUI Galway, Dana Saleh and (with Kirsten Pfeiffer) Malak Almutairi.
- In 2021 I supervised the summer research projects of Michael McGloin and Anton Sohn.

Roshan, Davood

Current research interests

My primary research interest is in the longitudinal analysis of clinical biomarkers. In particular, I am interested in developing statistical models and algorithms to generate adaptive reference regions from high dimensional streaming data from medical devices. The development of early-warning systems in real-time will be a key enabler for enhanced patient monitoring and care. I also have special interest in Translational Statistics, Data Visualisations and Data Science with a focus on developing predictive tools.

Research outputs

- V. Fay-Watt, S. O’Connor, D. Roshan, AC. Romeo, VD. Longo, F. Sullivan (2022). *The*

impact of a Fasting Mimicking Diet on patients with Prostate Cancer and features of Metabolic Syndrome: a Pilot Feasibility Study. Journal of Prostate Cancer and Prostatic Diseases.

- Eimear C Morrissey, ..., John Newell, Davood Roshan, Sean F Dinneen, et al. (2022). *Improving outcomes among young adults with type 1 diabetes: the D1 Now pilot cluster randomised controlled trial.* Pilot and feasibility studies 8, no. 1: 1-20. doi: <https://doi.org/10.1111/dme.14337>.
- Moloney, S., McGrath, B. M., Roshan, D., & Gethin, G. (2021). *The Personal Impact of Daily Wound Care for Hidradenitis Suppurativa.* Dermatology, 1-10. doi: <https://doi.org/10.1159/000520262>.
- Kilmartin, Darren, ..., Newell, John, Roshan, Davood, Grace Callagy, et al (2021). *Intra-tumour heterogeneity is one of the main sources of inter-observer variation in scoring stromal tumour infiltrating lymphocytes in triple negative breast cancer.* Cancers, 13.17. doi: <https://doi.org/10.3390/cancers13174410>

Research activities

- Provision of bio-statistical training and support for CÚRAM researchers in research design, analysis and reporting.
- Collaborating in UniCoV (<https://unicov.org/>) project as one of the statisticians to analyse the relevant data as well as to develop and maintain an interactive online data visualisation tool for displaying relevant statistical summaries of the streamed data from four different sites (NUIG, UCC, UCD and TCD).
- I continue to serve as the executive member of Young Irish Statistical Association where we organise the Inaugural Young-ISA meeting; twitter poster conference; and Young-ISA monthly webinar series.
- Memberships: Young-ISA, Irish Statistical Association, International Society for Clinical

Biostatistics, International Biometric Society, Statistical Modelling Society.

- Graduate students: Pouyan Nejadi, Modelling Motion Tracking Data in Elite Soccer to Design Personalised Training Sessions for Post Injury Rehabilitation

Rossmann, Tobias

Current research interests

I am interested in asymptotic, computational, and enumerative aspects of algebra and neighbouring fields.

Recent publications

- [1] T. Rossmann and C. Voll, *Groups, graphs, and hypergraphs: average sizes of kernels of generic matrices with support constraints.* To appear in Mem. Amer. Math. Soc., arXiv:1908.09589, 114 pp.
- [2] A. Carnevale and T. Rossmann, *Linear relations with disjoint supports and average sizes of kernels.* To appear in J. Lond. Math. Soc., arXiv:2009.00937, 51 pp.
- [3] T. Rossmann, *Enumerating conjugacy classes of graphical groups over finite fields.* Bull. Lond. Math. Soc., doi:10.1112/blms.12665, 21 pp.
- [4] T. Rossmann, *Zeta, a SageMath package for computing local and topological zeta functions, version 0.4.2, 2022.* See <https://github.com/torossmann/Zeta>

Research activities

- Invited talk “Towards a symbolic enumeration of orbits” at the workshop *Computational Group Theory*, MFO, August 2021.
- Invited seminar talk “Enumerating linear orbits and conjugacy classes”, *Lincoln-Lund algebra research seminar*, December 2021.
- (Upcoming:) Invited talk at the *Fifth International Workshop on Zeta Functions in Algebra and Geometry*, Nice, May 2022.

- Conference organised: Groups in Galway 2021 (with Angela Carnevale), 2–3 December 2021.
- PhD student: Sultan Alzahrani (since 2018).

Rudykh, Stephan

The research group focuses on non-linear elasticity of couple problems with application to design of new materials. The group employs a combination of theoretical development, multiscale numerical modeling, 3D-printing and experiments to gain the understanding about the nonlinear material behavior.

Ryan, Raymond A.

Current research interests

Functional Analysis; Tensor Products of Banach Spaces and Banach lattices; Polynomials and Holomorphic Mappings on Banach Spaces and Riesz Spaces.

Recent publications

- [1] C. Boyd, R.A. Ryan, S. Snigereva, Synnatzschke's theorem for polynomials *Positivity*, 25(1):144, 2021.
- [2] C. Boyd, R.A. Ryan, S. Snigereva, Orthogonally additive sums of powers of linear functionals *Archiv der Mathematik*, 118, 283–290 (2022)

Seoighe, Cathal

Current research interests

Research interests are mainly in genomics (especially cancer genomics) and molecular evolution; in particular, variation in germline and somatic mutation rates and their relationship with cancer risk, development and application of models and computational methods to analyze molecular sequence evolution and gene expression data and the analysis of genomic data in order to generate insights into the links between genomic and phenotypic variation.

Research outputs

- Controlling for background genetic effects using polygenic scores improves the power of genome-wide association studies [1]
- Perspectives on Allele-Specific Expression [2]
- No evidence that HLA genotype influences the driver mutations that occur in cancer patients [3]

Recent publications

- [1] D. Bennett, D. O'Shea, J. Ferguson, D. Morris, and C. Seoighe. Controlling for background genetic effects using polygenic scores improves the power of genome-wide association studies. *Scientific reports*, 11(1):1–10, 2021.
- [2] S. Cleary and C. Seoighe. Perspectives on allele-specific expression. *Annual Review of Biomedical Data Science*, 4:101–122, 2021.
- [3] N. Kherreh, S. Cleary, and C. Seoighe. No evidence that hla genotype influences the driver mutations that occur in cancer patients. *Cancer Immunology, Immunotherapy*, pages 1–9, 2021.

Research activities

- Scientific Director of the SFI Centre for Research Training in Genomics Data Science
- SFI Principal Investigator award to study variation in germline and somatic mutation rates
- Research group consisting of two postdoctoral researchers, seven PhD students (principal supervisor) and three co-supervised PhD students

Simpkin, Andrew J.

Current research interests

My research focusses on longitudinal data analysis, functional data analysis, genomics and data science. In particular I'm interested in modelling high-throughput data such as those arising from sensor technologies.

Recent publications

- [1] Connolly NP, Simpkin AJ, Mylotte D, Rosseel L Impact on percutaneous coronary intervention for acute coronary syndromes during the COVID-19 outbreak in a non-overwhelmed European healthcare system. *BMJ Open*, 11, 2022.
- [2] Lussier AA, Zhu Y, Smith BJ, Simpkin AJ, Smith AD, Suderman MJ, Walton E, Ressler KJ, Dunn EC Updates to data versions and analytic methods influence the reproducibility of results from epigenome-wide association studies. *Epigenetics*, 1, 2022
- [3] Zhu Y, Simpkin AJ, Suderman MJ, Lussier AA, Walton E, Dunn EC, Smith AD A Structured Approach to Evaluating Life-Course Hypotheses: Moving Beyond Analyses of Exposed Versus Unexposed in the-Omics Context. *American Journal of Epidemiology*, 190(6), 2021

Research activities

- Current research grants: Simpkin AJ (PI), Moran K, Bargary N. Modelling sensor data in recreational runners. Insight Platform Research Budget. September 2021 to August 2025; €110,000; Simpkin AJ, Laffey J (co-PIs). Joint modelling of survival and longitudinal data in the WEAN SAFE study. €110,000. January 2021 to December 2024; Simpkin AJ, Bargary N (co-PIs). Functional data Analysis for Sensor Technology. SFI Frontiers for the Future project. December 2020 to November 2024; €467,569;
- Graduate students: Beatrice Charamba, *Modelling continuous longitudinal glucose and heart rate data*; Anna Grossbach *The epigenetics of early life adversity*; John Andrew *Modelling joint functional and time-to-event data*; Daniel Gordon, *Developing specific training modalities to reduce injury incidence and optimise performance in football*, Massey University, NZ; Joe Gwatsvaira, *Functional data analysis for multivariate sensor data*, University of Limerick

- External service: Secretary of the Irish Statistical Association; Statistical Editor: Euro intervention; Honorary Research Fellow, Bristol Medical School

Tripathi, Bharat B.

Current research interests

My current research interest is in modeling and simulation of shear shock waves in brain in context of traumatic brain injury. This involves development of novel nonlinear continuum mechanics models, construction of state-of-the-art numerical algorithms like discontinuous Galerkin method, development of machine learning tools for optimization, prediction, calibration etc. In general, I am motivated to research in the field of computational mechanics to bring together the aspects of physics and mathematical/scientific computing with the theory of statistics. The amalgamation of the three for modeling propagation of information/material in biomedical applications, remains the overarching theme of his research.

Recent publications

- [1] Sandhya Chandrasekaran, Francisco Santibanez, Bharat B. Tripathi, Ryan DeRuiter, Ruth Vorder Bruegge, and Gianmarco Pinton. In situ ultrasound imaging of shear shock waves in the porcine brain. *Journal of Biomechanics*, 110913, 2022.
- [2] Bharat B. Tripathi, Sandhya Chandrasekaran, and Gianmarco Pinton. Super-resolved shear shock focusing in the human head. *Brain Multiphysics*, **2**, 100033, 2021.
- [3] Sandhya Chandrasekaran, Bharat B. Tripathi, David Espindola, and Gianmarco Pinton. Modeling ultrasound propagation in the moving brain: applications to shear shock waves and traumatic brain injury. *IEEE Trans. Ultras., Ferr. Freq. Cont.*, **68**(1), 201-212, 2021.
- [4] Bharat B. Tripathi, David Espindola, and Gianmarco F. Pinton. Modeling and Simulations of Two Dimensional Propagation of Shear Shock Waves in Relaxing Soft Solids, *J. Comput. Phys.*, **395**: 205-222, 2019.

- [5] Bharat B. Tripathi, David Espindola, and Gianmarco F. Pinton. Piecewise parabolic method for propagation of shear shock waves in relaxing soft solids: one dimensional case, *Int. J. Numer. Meth. Biomed. Engg.* **35**(5):e3187, 2019.

Research activities

- Oral presentation in *6th Oxford International Neuron and Brain Mechanics Workshop* (April 19-20, 2021), Oxford, UK.
- Oral presentation in *2020 IEEE International Ultrasonics Symposium* (September 7-11, 2020), Las Vegas, USA.

Tuite, Michael

Current research interests

My main area of interest is in vertex algebras. In particular, I'm working on the deep relationships between vertex algebras and Riemann surface theory. This includes recent work with Michael Flattey on the Freidan-Shenker conjecture concerning the reconstruction of a vertex operator algebra from its genus g partition function. I'm also working on partial differential equations, involving the Bers function, satisfied by genus g partition functions with Mike Welby and Tom Gilroy. I've also been involved in a very detailed study of the possible holomorphic super vertex algebras of central charge ≤ 24 in collaboration with Geoff Mason, Gail Yamskulna and Matt Krauel. This work is related to Mathieu Moonshine which relates the Mathieu group M_{24} to elliptic Jacobi and mock modular forms.

Recent publications

- [1] Tuite, M. The Heisenberg generalized vertex operator algebra on a Riemann surface. *Contemp.Math.* **768** 321–342 (2021)
- [2] Krauel, M., Mason, G., Tuite, M. and Yamskulna, G. Decompositions of index one Jacobi forms into $N = 4$ characters and formulas for mock modular forms. To appear

- [3] Bringmann, K., Krauel, M. and Tuite, M. Zhu reduction for Jacobi n -point functions and applications. *Trans.AMS* **373** 3261—3293 (2020)
- [4] Krauel, M., Tuite, M. and Yamskulna, G. (Editors). *Vertex Operator Algebras, Number Theory and Related Topics* Contemporary Mathematics, Vol 753 (AMS 2020).

Research activities

- American Institute of Mathematics Square online meeting on "Vertex operator superalgebras, Jacobi functions and Mathieu moonshine" July 2021.

Yang, Haixuan

Current research interests

My focus is in Bioinformatics & Statistical Modelling, especially of network data such as protein-protein interactions, co-expression, and functional similarity. A bio-molecular network can be viewed as a collection of nodes, representing the bio-molecules, connected by links, representing relations between the bio-molecules. I am working on inferring valuable information from bio-molecular networks.

Recent publications

- [1] M. Torres, H. Yang, A.E. Romero, A. Paccanaro. Protein function prediction for newly sequenced organisms. *Nature Machine Intelligence*, 3(12):1050-1060, 2021.
- [2] M. Timilsina, A. Figueroa, M. d'Aquin, H. Yang. Semi-supervised regression using diffusion on graphs. *Applied Soft Computing*, 104:107188, 2021.
- [3] M. Timilsina, D. Kernan, H. Yang, M. D'Aquin. Synergy Between Embedding and Protein Functional Association Networks for Drug Label Prediction using Harmonic Function. *EEE/ACM Transactions on Computational Biology and Bioinformatics*, doi: 10.1109/TCBB.2020.3031696, 2020.

- [4] C. Seoighe, SJ Kiniry, A. Peters, PV Baranov, H. Yang. Selection shapes synonymous stop codon use in mammals. *Journal of Molecular Evolution*, 88(7):549-561, 2020.
- [5] N. Zhou et al. The CAFA challenge reports improved protein function prediction and new functional annotations for hundreds of genes through experimental screens. *Genome Biology*, 20:244, 2019.
- [3] Dolega M., Zurlo G., Le Goff M., Greda M., Verdier C., Joanny J.-F., Cappello G., Recho P., Mechanical behavior of multi-cellular spheroids under osmotic compression, *J. Mech. Phys. Solids* 147, 104205 (2021).
- [4] Zaza D., Ciavarella M., Zurlo G., Strain incompatibility as a source of residual stress in welding and additive manufacturing, *Europ. J. Mechanics A/Solids* 85, 104147 (2021).
- [5] Zurlo G., Blackwell J., Colgan N., Destrade M., The Poynting effect, *American J. Phys.* 88, 1036 (2020).

Research activities

- Supervising 1 PHD student and 1 MSc student.

Zurlo, Giuseppe

Current research interests

I am interested at how elasticity can be employed to describe the behavior of solids in a broad range of scales, from the sub-cellular level, to the macroscopic level of the material. I have worked on the modelling of damage of rubber, and on the non-linear elastic response of rubbers and silicones under the action of pressure or electromagnetic fields. Recent collaborations in these fields include joint works with M.Joglekar from IIT Roorkee, India, and with G.Puglisi from Politecnico di Bari, Italy. More recently I have developed a special interest into the emergence of inelastic effects during additive manufacturing and in biological growth. In these fields I have intense collaborations with L.Truskinovsky (Paris, France), A.Elrach (Marseille, France), G.Tomassetti and S.Marfia (Roma, Italy), M.Ciavarella, S.Campanelli (Bari, Italy).

Recent publications

- [1] Khurana A., Joglekar M.M., Zurlo G., Electromechanical stability of wrinkled dielectric elastomers, *International Journal of Solids and Structures* (accepted, April 2022).
- [2] Saccomandi G., Speranzini E., Zurlo G., Piezoelectric machines: achieving non-standard actuation and sensing properties in poled ceramics, *Q. Jl Mech. Appl. Math.*, 74(2) (2021).

Research Activities

- Supervisor of a Joint PhD Degree (Cotutelle) Pisa-Galway (2022).
- Sabbatical leave in Roma-Sapienza, Italy (June 2021).
- Delivered a 20h PhD Course in Roma-Sapienza, Italy (June 2021).
- Research visit to ESPCI ParisTech (Nov 2021).
- Reviewer Editor - *Frontiers in Mechanical Engineering* (since Sep 2021).
- 3 invited webinars 2021/2022.
- Organisation of a ESMC mini-symposium, Galway (July 2022).

7 Visitors

Tielker, Elena (Bielefeld University)
Visiting: Angela Carnevale

Dates of visit: 6 September 2021 – 24 September 2021

Research activity

We discussed follow-up work to our preprint *On Denert's statistic*. We focussed on other statistics on (multiset) permutations and their applications to counting integer points in polytopes. Elena gave an informal seminar on her work on q -Ehrhart polynomials. Elena's visit was supported by Bielefeld University through a BGTS Mobility Grant.

8 Conferences, meetings, and workshops

- **Irish Geometry Seminar**

Dates: September 2021 – April 2022

Speakers: Lee Kennard (Syracuse University, USA), Jason DeVito (University of Tennessee, USA), Brendan Guilfoyle (Munster Technical University), Marco Radeschi (University of Notre Dame, USA), Patrick Heslin (Florida State University, USA), Ramiro Lafuente (University of Queensland, Australia), Emilio Lauret (Universidad Nacional del Sur, Argentina), Romina Arroyo (Universidad Nacional de Córdoba, Argentina), Anusha Mangala Krishnan (WWU Münster, Germany), Aaron Tyrell (University of Texas, USA), Thomas Huettemann (Queen’s University Belfast), Nadine Große (Universität Freiburg, Germany), Matthias Wink (WWU Münster, Germany), David González Álvaro (Universidad Politécnica de Madrid, Spain), Philipp Reiser (Karlsruhe IT, Germany), Bernhard Hanke (Universität Augsburg, Germany), Michael Magee (Durham University, UK), Stefan Bechtluft-Sachs (Maynooth), Emily Dryden (Bucknell University, USA), Andrea Mondino (University of Oxford, UK), Asma Hassannezhad (University of Bristol, UK), Kevin Poljsak (WWU Münster, Germany), Nikos Georgiou (Waterford IT)

Organisers: Martin Kerin (NUIG), David Wraith (Maynooth), Mark Walsh (Maynooth)

Web page: <https://sites.google.com/view/irishgeomseminar/home>

- **Groups in Galway 2021**

Dates: 2–3 December 2021

Speakers: Cristina Acciarri (University of Brasilia), Jesús Hernández Hernández (Universidad Nacional Autónoma de México), Caroline Lassueur (RWTH Aachen University/TU Kaiserslautern), Paula Lins (KU Leuven), Alastair Litterick (University of Essex), Rachel Quinlan (NUI Galway), Bernardo Rodrigues (University of Pretoria)

Organisers: Angela Carnevale, Tobias Rossmann

Web page: <https://torossmann.github.io/gig21/>

9 School seminars

School Seminars

- [1] Giuseppe Zurlo, NUIG. *Growing, melting, twisting: three stories from mechanics*, 16/09/2021. (Contact: Michael Mc Gettrick)
- [2] Harold Berjamine, NUIG. *Recent developments on the propagation of mechanical waves in soft solids*, 22/10/2021. (Contact: Michael Mc Gettrick)
- [3] Quan Zhang, NUIG. *Low-Frequency Elastic Wave Manipulation and Vibration Isolation with Metamaterials*, 28/10/2021. (Contact: Michael Mc Gettrick)
- [4] Pawel Dlotko, Polish Academy of Sciences. *Mild introduction to Topological Data Analysis*, 04/11/2021. (Contact: Graham Ellis)
- [5] Dessislava Kochloukova, University of Campinas, Brazil. *On the weak commutative construction in group theory*, 10/02/2022. (Contact: Graham Ellis)
- [6] Máire Ní Leathlobhair, Trinity College Dublin. *To be Determined*, 21/04/2022. (Contact: Cathal Seoighe)
- [3] Peter Phelan, *Computing the Hilbert Series of Monomial Ideals*, 02/12/2021
- [4] Aoife Hill, *Computational modelling of biodegradable polymers for biomedical applications*, 16/12/2021
- [5] Harold Berjamine, *Computational modelling of volume preserving motion*, 24/02/2022
- [6] Róisín Hill, *Generating layer-adapted meshes using mesh PDEs*, 31/03/2022

Postgraduate Seminar Group

The Postgraduate Seminar Group is a student-run, hybrid seminar group in The School of Mathematical & Statistical Sciences, NUI Galway. Each week, members will have the opportunity to deliver a short presentation (15-30 minutes) and answer questions on any topic in mathematics of their choosing. Seminars will be held both online and in person, and are intended to be accessible to a general maths postgraduate audience. If you would like to join the group, ask some questions or contribute a talk, please contact one of the organisers: Victoria Sánchez Muñoz or Peter Phelan.

- [1] Koushik Paul, *Specht Modules of type- A_n groups*, 18/11/2021
- [2] Victoria Sánchez Muñoz, *Nash Equilibria in certain two-choice multi-player games played on the ladder graph*, 25/11/2021

10 SIAM Student Chapter

The NUI Galway Student Chapter of SIAM, the Society for Industrial and Applied Mathematics, aims to bring together students and researchers from across campus to generate interest in applied mathematics, share ideas, and develop leadership skills. Members are drawn from a range of disciplines, including pure and applied mathematics, computer science, physics and engineering. The current officers and committee (2021/2022) are:

President: Victoria Sánchez Muñoz

Vice-president: James Blackwell

Treasurer: Michael Flattery

Secretary: Sophie Plunket

Faculty Advisor: Niall Madden

Committee members: Róisín Hill, Aoife Hill, Thomas Hayes, Koushik Paul, Sairam Pamulaparthi Venkata, Vikrant Pratap, and Badriah Safarji.

Since the last booklet, the Chapter activities included:

- *25/05/2021* Annual General Meeting.
- *21-24/06/2021* Some of the Chapter members **assisted** in organising and running the Seventh Annual **Stokes Modelling Workshop** for undergraduates.
- *08/07/2021* Four chapter members attended the online **social** event hosted by **SIAM-IMA Dublin Student Chapter**.
- *27-28/07/2021* Victoria Sánchez Muñoz gave a presentation and a poster contribution at the **Sheffield SIAM-IMA Conference 2021**, and won the 3rd poster prize in the postgraduate category.
- *25/11/2021* Organisation of a **Maths quiz** with Math Soc. The chapter members provided some questions for the quiz and 4 SIAM mugs and 3 One for All vouchers for the prizes. One member of SIAM was in the winning team.
- *07/01/2022* **Annual Meeting of SIAM UKIE 2022**. The conference was going to be in-person in Dublin with a poster session for

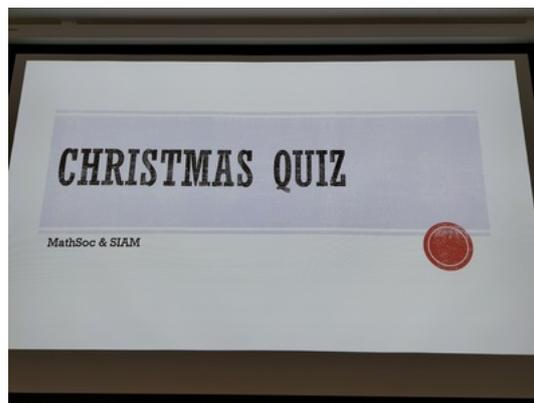


Figure 1: Maths quiz with Maths Soc.

postgraduates. However, it was moved online and some of the contributing postgraduates were randomly picked to give a short talk online. Victoria Sánchez Muñoz was one of the contributing postgraduates that was randomly picked to give a short talk.

- *21/01/2022* **8th Annual Irish SIAM Student Chapter** hosted by the University of Limerick. Victoria Sánchez Muñoz gave a talk in person and Róisín Hill attended the conference online.



Figure 2: 8th Annual Irish SIAM Student Chapter in UL running hybrid.

- *14/03/2022* Two talks for the **International Day of Mathematics**. The even run in a hybrid format. The first speaker Niamh Cahill, from Maynooth University, gave a talk online about “Monitoring Country-Level Changes in Family-Planning Indicators Over Time”. The second speaker Faiza Alsaedi, from NUI Galway, gave a talk in person about “Parameter robust methods for fourth-order real-valued singularly perturbed problems”.

The attendance was around 12 people, mixed between joining online and in person.

14th March 2022

INTERNATIONAL DAY OF MATHEMATICS
MARCH 14

- **2pm: Niamh Cahill** (Maynooth University) <https://www.siam.org/>
"Monitoring Country-Level Changes in Family-Planning Indicators Over Time"
- **3-3:30pm: Break**
- **3.30pm: Faiza Alssaedi** (NUI Galway)
"Parameter robust methods for fourth-order real-valued singularly perturbed problems"

NUIG SIAM STUDENT CHAPTER

President: **Victoria Sánchez Muñoz**
v.sanchezmunoz@nuigalway.ie

Vice-president: **James Blackwell**
Treasurer: **Michael Flaherty**
Secretary: **Sophie Flunket**

Faculty Advisor: **Niall Madden**

→ CCM: ...

Figure 3: Slide of the program for the International Day of Maths 2022.