



School of Mathematics, Statistics and Applied  
Mathematics Research Day  
1 May 2014

**Programme**

09:30-9:45	Ray Ryan	Opening remarks
09:45-10:00	Pól Ó Dochartaigh (Registrar)	Research at NUI Galway
10:00-10:30	Martin Meere	Some mathematical models for drug delivery
10:30-11:00	Tea and Coffee	
11:00-11:30	Emma Holian	Clustering longitudinal profiles using P-splines and mixed effects models applied to time-course gene expression data.
11:30-12:00	Tim Downing	DNA variation in a pathogen outbreak: past, present and predictions
12:00-12:30	Aisling McCluskey	Categorising properties of road systems
12:30-2:00	Lunch in Concourse	
14:00-14:40	Rosemary A. Bailey	Circular designs balanced for neighbours at distances one and two
14:40-15:30	Blitz Session	
15:30-17:00	Poster Session in Concourse	
17:00	Reception and Presentation of Poster Prizes in Staff Club, Quadrangle	

# 1 Introduction

Welcome to the annual Research Day of the School of Mathematics, Statistics and Applied Mathematics. The programme for the day shows the breadth of activity in the School, ranging from basic research to applications and collaborations in Biology, Biomedical Science, Engineering and other areas. And we are delighted to welcome Professor Rosemary Bailey from the University of St Andrews, who will give a lecture on statistical design of experiments.

This year, we welcomed three new members of staff:

- **Sejong Park** was awarded his PhD by the University of Aberdeen. He works on modular representation theory of finite groups, fusion systems and related homological algebra, Mackey functors and biset functors.
- **Alexander Rahm** was awarded his PhD jointly by the Universities of Grenoble and Göttingen. He works on classifying space for proper actions, discrete subgroups of Lie groups, discontinuous groups of transformations and isometries of hyperbolic space.
- **Giuseppe Zurlo** was awarded his PhD by the University of Pisa. He works on continuum mechanics, with particular emphasis on biomechanics, non-linear elasticity, rubber elasticity and electroelasticity.

The School has restructured its research activity in order to optimize the use of our resources and focus on some of the key themes that support the strategic aims of the University. Building on the example of the very successful SFI funded De Brun Centre, we have established three research clusters:

- **The De Brún Centre for Mathematics** supports mathematical research across a spectrum of areas, including Algebra, Analysis, Geometry and Mathematics Education.
- **The Biostatistics/Bioinformatics Cluster** covers the areas of biostatistics and bioinformatics and is engaged in collaborative work with researchers in genomics and other areas, and with clinicians, through the Clinical Research Facility (CRF).
- **The Stokes Applied Mathematics Cluster** applies advanced mathematical skills to the modeling of computational, physical and biological phenomena, with the aim of fostering interdisciplinary research across the NUI Galway campus and beyond.

As well as making significant resource allocations to the clusters, the School has also provided administrative support. **Ms Collette McLoughlin**, a member of the administrative staff of the School, now has responsibility for providing research support, including liaison with the Research Office, tracking funding opportunities, managing IRIS pages and producing research reports. In addition, the School's new workload model gives explicit recognition to research and postgraduate supervision. We feel that this new strategic focus will enable the School to maximize the impact of our research, to be able to respond to the University's new strategic plan and to be well placed to seek out new funding opportunities.

We have been very fortunate in being able to recruit high quality PhD students and the past year has been no exception, with particular success in IRC Scholarships. One of the challenges facing us is to identify new sources of support to ensure that we maintain our excellent body of postgraduate students. The unprecedentedly large number and quality of applicants for college fellowships this year is a good indication of our potential for growth. Our thriving graduate school includes students from as far afield as Kenya, Iran, China, Vietnam and Argentina, along with students from all parts of Ireland. The poster session on the Concourse will display the wide range of excellent work being carried out by them. As always, they do us proud.

Ray Ryan,  
Head of School

## 2 Presentations

### DNA variation in a pathogen outbreak: past, present and predictions

**Tim Downing**

School of Mathematics, Statistics and Applied  
Mathematics, NUI Galway

Mixing between genetically distinct pathogens within a population leads to novel combinations with altered host virulence and drug resistance. Such unique specimens represent either undiscovered lineages or re-assortments between established groups: comparison with known DNA patterns (haplotypes) provides a framework for determining ancestry and predicting biological traits. Current methods of allele frequency correlation, variant distribution modality and admixture modelling are effective for breeding between sub-species, but are untested for monomorphic populations where discriminatory mutations are rare. Haplotype distribution, size and length provided sufficient power to distinguish samples with just 3.4 mean pairwise SNPs/Mb in a sample of 191 Indian subcontinent clinical isolates of *Leishmania donovani* sampled in 2002-11 during two drug treatment eras. Model-based population clustering identified six genetically homogeneous populations with little evidence of recent interbreeding. These originated in the 1850s and showed a genetic bottleneck-recovery signature from anti-parasite pesticide spraying campaigns ending in the 1960s. Population-free membership assignment, phylogenetic trees and admixture statistics indicated six recent isolates were discovered whose haplotypes were mixes of these populations, despite as few as 60 genome-wide polymorphisms differentiating the main groups. These six hybrids were distinguishable from seven rare lineages whose haplotype structure did not resemble any previous sample. Predicting resistance to future second-line or combination drug therapies using genetic data is now a tangible goal.

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### Some mathematical models for drug delivery

**Martin Meere**

School of Mathematics, Statistics and Applied  
Mathematics, NUI Galway

Drug-eluting stents are now commonly used in the treatment of coronary artery disease. These devices increase the flow of blood through blocked arteries and provide mechanical support to the artery wall. They also protect the artery from re-blockage due to inflammation by releasing an anti-inflammatory drug into the surrounding tissue from a polymer that coats the stent. However, the permanent presence of a polymer in the body is now thought to increase the likelihood of a dangerous blood clot forming on the stent. Consequently, a new generation of stents are being developed that do not rely on a polymer to release the drug.

In these polymer-free stents, the drug is either sprayed directly onto a bare metal surface or infused in a metallic porous medium. Polymer free stents are a relatively new technology and no mathematical models have yet been developed to describe drug release from them. In this talk, some preliminary ideas for the modelling of polymer free stents are presented. The proposed models are based principally on dissolution theory and the theory of diffusion in porous media.

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### Clustering longitudinal profiles using P-splines and mixed effects models applied to time-course gene expression data

**Emma Holian, Norma Coffey and John Hinde**

School of Mathematics, Statistics and Applied  
Mathematics, NUI Galway

Time-course microarray analyses involve measuring the expression levels of thousands of genes repeatedly through time. Multivariate clustering methods such as principal components analysis, k-means clustering, finite mixture models etc. have difficulties handling missing values, require uniform sampling for all genes, fail to account for the correlation between measurements made on the same gene or do not facilitate the removal of noise from the measured data thus ignoring any smoothness that may be evident in the expression profiles. This talk proposes the use of curve-based clustering, which can handle the latter issues. We use the linear mixed effects model representation of penalized spline smoothing to

estimate the gene expression curves which provides a framework for simultaneously determining a smooth estimate of the mean expression profile in each cluster, determining estimates of the gene-specific expression profiles within a cluster through the use of additional random effects and clustering expression profiles using mixtures of mixed effects models.

Coffey, N., J. Hinde, and E. Holian. "Clustering longitudinal profiles using P-splines and mixed effects models applied to time-course gene expression data." *Computational Statistics & Data Analysis* 71 (2014): 14-29.

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### Categorising properties of *road systems*

**Jorge Bruno, Aisling McCluskey**  
School of Mathematics, Statistics and Applied  
Mathematics, NUI Galway

A *road system* on a nonempty set  $X$  is a family  $\mathcal{R}$  of nonempty subsets of  $X$  such that:

- (i)  $\{a\} \in \mathcal{R}$  for all  $a \in X$ .
- (ii) for all  $a, b \in X$ , there is  $R \in \mathcal{R}$  such that  $a, b \in R$ .

Each road system  $(X, \mathcal{R})$  gives rise to an  $R$ -relation  $[\cdot, \cdot]_{\mathcal{R}}$  on  $X$  as follows:  
 $[a, b, c]_{\mathcal{R}}$  holds if each road  $R$  containing  $a$  and  $c$  also contains  $b$ .

We explore some properties that are characteristic of  $R$ -relations using a categorical framework.

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## 3 Blitz Session

- Kevin Jennings, *Spaces of Matrices with lots of different ranks*
  - Anh Thai Nhan, *Uniform convergence via conditioning*
  - Isaac Burke, *Algebraic properties of log-linear independence models*
  - Michel Destrade, *Mechanics of brain matter*
  - James McTigue, *Partial matrices of constant rank*
  - Artur Gower, *Using an on board camera to track a train's motion*
  - Jim Cruickshank, *A brief history of rigidity*
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## 4 Poster Session

### Evaluating the epigenomic landscape of colonic cell lineages.

**Alan Barnicle**

**Supervisors:** Laurence Egan & Cathal Seoighe

DNA methylation is an epigenetic mark, essential for transcriptional regulation, silencing of repetitive DNA elements and genomic imprinting. It happens predominantly in Cytosine-Guanine dinucleotides (CpGs). CpGs tend to cluster around CpG islands, found predominantly around the transcription start site of human protein coding genes. The majority of the genome is methylated at 70-80

Recent evidence suggests that closely related cell types have distinct methylation patterns and that cell purification should always be considered prior to investigating epigenetic phenomena. However the epigenomic profile of individual cell types has not been fully elucidated in vivo. Here we utilize the heterogeneous cell composition of colonic pinch biopsies to find differentially methylated regions of interest (primarily around transcription start sites and enhancers) between a purified epithelial cell population and a non-purified mixture of cell lineages. The data generated from this study will determine the necessity of cell purification and reveal the epigenetic signature of specific cell types on a genome wide scale.

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### Genomic Architecture of Nucleolar Organiser regions.

**Sofia Barreira**

**Supervisors:** Brian McStay & Cathal Seoighe

Nucleolar Organiser Regions, NORs, comprised of tandem arrays of ribosomal DNA and responsible for the formation of a major functional domain of the nucleus dedicated to ribosome biogenesis, the nucleolus, are positioned on the short arms of the five human acrocentric chromosomes (13, 14, 15, 21 and 22). These regions and those adjacent to the NORs are missing from the current human genome assembly. The identification and characterisation of these sequences is of critical importance, as nucleoli

have a central role in growth-regulation and a long-established connection to tumorigenesis, and more importantly, ribosomes serve as the primary site of biological protein synthesis. My work focuses in the organisation of rDNA repeats, in extending and characterising the sequences on the distal side (DJ) of the NORs and establishing the organisation/structure of DJ chromatin.

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### On the classifying space of cubical crystallographic group

**Anh Tuan Bui**

**Supervisors:** Graham Ellis

This paper introduces a new method which attempts to find a cubical classifying space for a family  $\mathfrak{F}$  of subgroups of a crystallographic group  $G$  in two cases. The main case is when  $\mathfrak{F} = \{1\}$  the family with just the trivial subgroup, we obtain  $EG$ , a contractible  $G$ -CW-complex whose quotient  $BG$  is the classifying space for principal  $G$ -bundles, which can be used to find the cohomology ring structure for group  $G$ . We also provide a brief comment for the case,  $\mathfrak{F} = \mathfrak{Fin}(G)$  the family of all finite subgroups of  $G$ . The corresponding classifying space for proper actions is denoted  $\underline{EG}$  and its quotient space  $\underline{BG} = \underline{EG}/G$  which can be used to find Bredon homology for  $G$ .

- [1] M. Röder, HAPcryst – A HAP extension for crystallographic groups, Version 0.1.11 (2013), an official package for the GAP computational algebra system.  
(<http://www.gap-system.org/Packages/hapcryst.html>)
- [2] G. Ellis, J. Harris and E. Sköldbberg, “Polytopal resolutions for finite groups”, *J. reine angewandte Mathematik*, 598 (2006) 131–137.
- [3] C.T.C. Wall, “Resolutions of extensions of groups”, *Proc. Cambridge Philos. Soc.* 57 (1961), 251–255.

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### Universal Gröbner Bases of Determinantal Ideals

**Isaac Zebulun Burke**  
**Supervisor: Dr. Emil Sköldbberg**

Here we study the algebraic properties of log-linear independence models [1], considering in particular  $2 \times 2 \times \dots \times 2$  independence models. The fiber polytopes of these models are a special class of  $n$ -way transportation polytopes, the general properties of which have been well documented for  $n = 2, 3$ , see e.g. [2] and references therein.

Given a generic  $m \times n$  matrix  $A$  over a field  $\mathbb{k}$  whose entries are algebraically independent variables  $x_{ij}$ , the set of  $k$ -minors ( $0 < k \leq m$ ,  $k \leq n$ ) of  $A$  generates a determinantal ideal  $I \subset \mathbb{k}[x_{ij}]$ . We associate such a determinantal ideal  $I$  with each independence model and seek to enumerate the elements of the universal Gröbner basis of  $I$ , drawing on results of Sturmfels [3] (see chapter 7) while making use of the software systems `polymake` and `gfan`. Implications are discussed in relation to the problem of describing graphs of  $n$ -way transportation polytopes for  $n \geq 4$ .

- [1] DRTON, M., STURMFELS, B. and SULLIVANT, S. (2009). Lectures on Algebraic Statistics. *Oberwolfach Seminars*, **Vol.39**.
- [2] DE LOERA, J.A., KIM, E.D., ONN, S. and SANTOS, F. (2009). Graphs of transportation polytopes. *Journal of Combinatorial Theory*, **Vol.116**, pp. 1306-1325.
- [3] STURMFELS, B., (1996). Gröbner Bases and convex polytopes. *University Lecture Series*, *AMS*, **Vol.8**.

Supported by the Irish Research Council (IRC).

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## Dynamics on evolving networks

**Richard Burke**  
**Supervisors: Petri Piiroinen**

My research project is a study of self-evolving asymmetric complex networks. A network is a set of agents (called nodes) which may be connected to one another via relational links (edges or arcs). The focus is on edge-based evolution, where the relational links

between agents in the ensemble grow or decrease in strength thus imparting a stronger or weaker influence on each other over time. The dynamic interplay between agents in this way can give rise to fascinating collective phenomena. We generate mathematical networks using differential equations which define the communication rules between the respective agents in the ensemble and drive our networks from disconnected states of disarray toward stable configurations (synchronisation). A number of different edge-based evolution strategies are considered and both numerical and analytical methods are employed to discern the conditions conducive to synchronisation and the structural properties of the emergent networks when synchrony has been reached.

- [1] “Complex Networks: Structure and Dynamics”, S. Boccaletti, V. Latora, Y. Moreno, M. Chavez, D. U. Hwang, *Physics Reports* 424 pp. 175-308 (2006).
- [2] “Evolution of Complex Networks via Edge Snapping”, P. DeLellis, M. diBernardo, F. Garofalo and M. Porfiri, *IEEE Transactions on circuits and systems-1: regular papers*, vol. 57, pp. 2132-2143 (2010).
- [3] “The structure and function of complex networks”, M. E. J. Newman, *SIAM Rev.*45, pp. 167-256 (2003).

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## Model considerations for impacts with friction

**Shane Burns**  
**Supervisor: Petri Piiroinen**

There are many different impact laws used to model collisions between two bodies, where some disregard friction and some include friction. Similarly, some impact laws consider the impact with compliance of the contact region during impact while others consider the impact as being completely rigid. Non-compliant impact models, the focus of this work, are based on the rigid-body formulation which assumes contact occurs at an isolated number of points and that the impact occurs over an infinitesimal time period. Due to

the assumptions present in this formulation, various inconsistencies are inherent to all impact mappings. Our work resolves some of these inconsistencies and highlights some interesting phenomenon using a comparison between two different impact mappings.

- [1] S.J. Burns, P.T. Piiroinen : The complexity of a basic impact mapping for rigid bodies with impacts and friction. Regular and Chaotic dynamics 19, 1 (2014) 20-36.
- [2] A. Nordmark, H. Dankowicz, A. Champneys: Discontinuity-induced bifurcation in systems with impacts and friction: Discontinuities in the impact law. International Journal of Non Linear Mechanics 44 (2009) 1011-1023.
- [3] W.J. Stronge: Impact Mechanics. Cambridge University Press (2000) 1-3.

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### Harnessing related species and samples data to create and optimise draft genome sequences for *Leishmania* species

**Simone Coughlan**

**Supervisors:** Tim Downing, Cathal Seoighe

Effective molecular tools for monitoring the emergence of novel pathogens in domestic and peridomestic reservoir hosts are urgently required. Taxonomically classifying unknown samples of ambiguous origin and identifying optimal protocols for their genome assembly using short-read data is required for comparison with known species. DNA was sampled from two Colombian dogs with leishmaniasis and from an Ethiopian rat harbouring a new species called *L. arvicanthis*. These samples were sequenced to produce paired-end short read Illumina libraries. A genome assembly pipeline that iteratively optimised and transformed the short read data into high quality draft genomes was developed, including the current *L. braziliensis* genome data [1] as a reference control. Phylogenetic markers were extracted from the genomes and compared with markers from a panel of known *Leishmania* species, identifying two of them as members of the *L. braziliensis* complex: *L. naiiffi* and

*L. shawi*. The assembly pipeline implemented here involves stringent QC filtering, de-novo assembly, iterative gap-filling and base correction steps before identifying and removing potential mis-assemblies. Then, using reference genome data (*L. braziliensis* [1] and *L. tarentolae* [2] here), it aligns, orders and orients scaffolds into pseudo-chromosomes and transfers the reference annotation onto the new draft genome. Short read coverage and allelic diversity determined variation across four levels in the draft genomes: ploidy, whole chromosome copy number, structural changes and SNPs. While *L. naiiffi*, *L. shawi* and *L. arvicanthis* were diploid, aneuploidy was also observed in all three species, highlighting the universality of multi-levelled genome plasticity in differing environments.

- 1 Rogers, M. B., Hilley, J. D., Dickens, N. J., Wilkes, J., Bates, P. a, Depledge, D. P., & Mottram, J. C. (2011). Chromosome and gene copy number variation allow major structural change between species and strains of *Leishmania*. Genome Research, 21(12), 2129-42.
- 2 Raymond, F., Boisvert, S., Roy, G., Ritt, J.-F., L'AlgarÃe, D., Isnard, A., & Corbeil, J. (2012). Genome sequencing of the lizard parasite *Leishmania tarentolae* reveals loss of genes associated to the intracellular stage of human pathogenic species. Nucleic Acids Research, 40(3), 1131-47.

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### Mathematical modelling of seasonal migration

**John Donohue**

**Supervisors:** Dr Petri Piiroinen

The breeding success of many species depends on the synchronisation of the period of maximum demand of offspring with a period of food abundance. The trend towards higher spring temperatures in recent decades has caused such windows to advance [1]. In this work, we propose a population-based dynamical system framework in which the interplay of different seasonal factors both within and between years can be better understood. The breeding and survival

stages are modelled as separate annual regimes in a time-dependent switching system. Steady state solutions are used to measure the extent to which the population can sustain itself over long time-scales and repeated breeding events.

We then use a simple switching model to assess the impact of persistent temporal mismatches brought about by changing climatic conditions. We show the negative effect that an advance in the food season, relative to a fixed reproductive window and migration schedule, can have on population size, with a sufficiently severe shift bringing about a total collapse. Two obstacles to achieving resynchronisation of breeding and food supply are considered - a shortage of food early in the breeding season [2] and a constraint on arrival date to the breeding quarters [3].

- [1] Gian-Reto Walther, Eric Post, Peter Convey, Annette Menzel, Camille Parmesan, Trevor J. C. Beebee, Jean- Marc Fromentin, Ove Hoegh-Guldberg, and Franz Bairlein. Ecological responses to recent climate change. *Nature*, 416:389-395, 2002.
- [2] I.R. Stevenson and D.M. Bryant. Climate change and constraints on breeding. *Nature*, 406:366-367, 2000.
- [3] Christiaan Both and Marcel E. Visser. Adjustment to climate change is constrained by arrival date in a long-distance migrant bird. *Nature*, 411:296-298, 2001.

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## Shift Representations on 2-Cocycles

**Ronan Egan**

**Supervisor:** Dane Flannery

Let  $R$  be a ring. A matrix  $M \in \text{Mat}(n, R)$  is *cocyclic* over a group  $G$  with cocycle  $\psi : G \times G \mapsto \{R\}$  if  $M = [\psi(g, h)\phi(gh)]_{g, h \in G}$  for some set map  $\phi$ . The cocycles from a group  $G$  to an abelian group  $U$  form a group  $Z^2(G, U)$  under pointwise composition. The set of all cocycle classes form the 2-cohomology group  $H^2(G, U)$ . Cohomology does not preserve orthogonality in cocycles, a requirement for the development

of many *Pairwise Combinatorial Designs* [1], in particular the Hadamard matrices.

We are investigating the relatively new idea of *shift representations*, which are derived from an action of  $G$  on  $Z^2(G, U)$  (discovered by Horadam [2]) that preserves both cohomology and orthogonality. We prove new results in relation to fixed points under this action, building on the work of Horadam in [3]. We also answer a number of questions concerning the reducibility of  $\Gamma$ , the linear representation of the shift action of  $G$  on  $Z^2(G, U)$ , and give some computational results regarding orthogonality.

- [1] Warwick de Launey and Dane Flannery, *Algebraic design theory*, Mathematical Surveys and Monographs, vol. 175, American Mathematical Society, Providence, RI, 2011.
- [2] K. J. Horadam, *The shift action on 2-cocycles*, Journal of Pure and Applied Algebra, vol. 188, pp. 127-143, Elsevier, 2003.
- [3] K. J. Horadam, *Hadamard matrices and their applications*, Princeton University Press, Princeton, NJ, 2007.

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## Modelling Heterogenous Populations under Joint Progressive Type-II Censoring

**Author:** Lida Fallah

**Supervisors:** Prof. John Hinde, Dr. Haixuan Yang

Comparative life testing is commonly used in an industrial setting to study differences between items produced by different manufacturing lines and similar approaches may be used to compare the survival of subgroups of patients in the medical setting, for example males and females. Here, we limit ourselves to two groups and suppose that we have two independent samples of sizes  $m$  and  $n$  that are put on test or followed up over time. The study is terminated as soon as some fixed number,  $r$ , of failures are observed, i.e. a Type-II censoring scheme. However, to save costs this is combined with

joint progressive censoring in which at each observed failure time a number of units is randomly withdrawn from study, joint progressive Type-II censoring. Here we consider the use of mixture models to account for heterogeneity in populations undergoing life-testing under joint progressive Type-II censoring scheme. We discuss model formulation and maximum likelihood parameter estimation using the EM algorithm. We study the behavior of the estimators through a simulation study and present an illustrative example.

**Achcar, J.A. and Pereira, G.D.A.** (1999). Mixture models for Type-II censored survival data in the presence of covariates *Journal of Computational Statistics*, **14**, pp. 233–250.

**Kuo, L. and Peng, F.** (2000). *Generalized linear models: A Bayesian Perspective*. New York: Marcel Dekker, pp. 255–270.

**Rasouli, A. and Balakrishnan, N.** (2010). Exact likelihood inference for two exponential populations under joint Progressive Type-II censoring *Journal of Communication in statistics-Theory and Method*, **39**, pp. 2172–2191.

In Statistics, a nomogram is a graphical representation of a statistical model allowing a point estimate of the response variable to be made for a particular set of values for the explanatory variables (Allcock, H. J. and Jones, J. R. 1950). Nomograms are popular in cancer research to inform clinical decision making because of their ability to allow a point estimate of the probability of the event in question, such as death or recurrence (Kattan, M.W *et al.*, 2003).

In this poster dynamic nomograms are introduced that can be created automatically from any glm model object in R. In theory any model appearing in a scientific publication can be accompanied by a URL directing the 'user' to the accompanying dynamic nomogram from which the results of the models and the relative importance of each explanatory variable are directly translational.

**Allcock, H. J. and Jones, J. R.** (1950). *The Nomogram (4th Edition)*. Publisher: Pitman; 2nd edition.

**Kattan, M.W *et al.*** (2003). Counseling Men With Prostate Cancer: A Nomogram for Predicting the Presence of Small, Moderately Differentiated, Confined Tumors.

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## Incremental Elasticity and Residual Stress

**Artur Gower**

**Supervisors:** Prof Michel Destrade

I work mainly in non-linear elasticity, one of the main pillars of solid mechanics. At the moment I am investigating how to design potential energy functions for residual stressed solids, how wrinkles form in fibre reinforced materials and linearised surface waves. Supported by NUIG - Hardiman Scholarship and the Irish Research Council.

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## Using Shiny to Generate Dynamic Nomograms

**Amirhossein Jalali**

**Supervisor:** John Newell, John Hinde, Alberto Alvarez-Iglesias

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## Promiscuous mRNA splicing under the control of AIRE in medullary thymic epithelial cells

**Peter Keane**

**Supervisors:** Cathal Seoighe and Rhodri Ceredig

The expression of tissue-restricted antigens (TRAs) in the thymus is required to ensure the efficient negative selection of T lymphocytes and avoid autoimmunity. This promiscuous expression is under control of *AIRE*, a transcription factor expressed in medullary thymic epithelial cells (mTECs). The mechanisms through which *AIRE* induces TRA expression is not yet fully understood. Tissue-specific alternative splicing may also produce TRAs, but the extent to which mTECs express tissue-specific isoforms had yet to be investigated. We reanalyzed microarray and RNA-Seq datasets from mouse mTECs and other epithelial and non-epithelial cells types and found that the diversity of splice isoforms expressed in mTECs was

greater than in any of the other cell types studied. Furthermore, we found evidence that *AIRE* influences splicing diversity in mTECs. Finally, we identified a set of normally tissue-specific isoforms which are ectopically expressed in mTECs and suggest that this promiscuous splicing is under the influence of *AIRE*, representing a novel aspect of its role in maintaining immune self-tolerance.

Supported by the program for research in third level institutions and co-funded under the European regional development fund.

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## Quantum Walk

**Dan Li**

**Supervisors:** Michael Mc Gettrick

Quantum walks are the quantum counterparts of classical random walks. Due to the constructive quantum interference along the paths in the discrete or the continuous version, quantum walks provide a method to explore all possible paths in a parallel way. Quantum walks have recently emerged as a useful tool in developing quantum algorithms. Up to now, quantum walks have a large number of applications in different fields, ranging from element distinctness [1] to database searching [2,3], from constructing quantum Hash schemes [4,5] to graph isomorphism testing [6]. Also quantum walk can be regarded as a universal computational primitive.

- [1] A. Ambainis, quant-ph/0311001 (2003).
- [2] S.D. Berry and J.B. Wang, Phys. Rev. A 82, 042333 (2010).
- [3] L. Tarrataca and A. Wichert, Quant. Inf. Proc. 12, 2, pp 1365-1378 (2013).
- [4] D. Li, J. Zhang, F.Z. Guo, W. Huang, Q.Y. Wen, and H. Chen, Quant. Inf. Proc. 12, 3, pp 1501-1513 (2013).
- [5] D. Li, J. Zhang, X.W. Ma, W.W. Zhang, and Q.Y. Wen, Quant. Inf. Proc. 12, 6, pp

2167-2176 (2013).

- [6] S.D. Berry and J.B. Wang, Phys. Rev. A 83, 042317 (2011).

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## Flags of Root Systems and Their Applications

**Mohammad Adib Makrooni**

**Supervisors:** John Burns

This work studies subroots systems and flags of sub-root systems of a compact, connected Lie group  $G$  [1]. It also gives a selection of applications. We obtain a new description of the Exponents of a simple complex Lie Algebra [2] in terms of the Coxeter number and other root theoretic data associated to geometric objects. When the subroot system corresponds to a parabolic subgroup  $P$  we obtain uniform expressions for the nef values  $\tau(X, L)$  of ample line bundles  $L$  on the corresponding homogeneous complex projective variety  $X = G/P$ . Recall that  $L$  is ample if the sections of some power of  $L$  give an embedding of  $X$  in some projective space. Finally we calculate a topological invariant  $\phi$ , related to the Poincare polynomial for all complex homogeneous space  $G/H$  with non vanishing Euler characteristic.

We briefly recall two definitions of the exponents. We may pass from the first to the second using a Morse function on the associated flag manifold of  $G$  [1].

- Let  $W$  be the Weyl group of a compact, connected Lie group  $G$ . The manifold  $G$  has the same cohomology as a product of odd-dimensional spheres

$$H^*(G, \mathbb{R}) \cong H^*\left(\prod_{i=1}^l S^{2m_i+1}, \mathbb{R}\right).$$

The numbers  $m_i$  appearing above are by definition the exponents of  $G$  (or  $W$ ).

- Let  $\ell : W \rightarrow \mathbb{Z}_{\geq 0}$  be the length function. Then

$$\sum_{w \in W} t^{\ell(w)} = \prod_{i=1}^l \frac{1-t^{m_i+1}}{1-t}.$$

Again the numbers  $m_i$  are the exponents of  $W$  (or  $G$ ).

- [1] R. Carles. *Méthode récurrente pour la classification des systèmes de racines réduits et irréductibles*. C. R. Acad. Sci. Paris **276** (1973) pp 355–358.
- [2] B. Kostant, The Principal Three-Dimensional Subgroup and the Betti Numbers of a Complex Simple Lie Group, American Journal of Mathematics, Vol. 81, No. 4 (Oct., 1959), pp. 973–1032
- [3] D. M. Snow, The Nef Value and Defect of Homogeneous Line Bundles, Transactions of The American Mathematical Society, Vol. 340, No. 1 (November 1993)

Supported by School of Mathematics, Statistics and Applied Mathematics

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## Bifree subgroups of a Direct Product

**Brendan Masterson**  
Supervisors: Götz Pfeiffer

It is well known, by Goursat’s lemma, that all subgroups of a direct product  $G_1 \times G_2$  can be described by a triple which contains a section from each of the factor groups and an isomorphism between their quotient groups. We are interested in those subgroups of  $G_1 \times G_2$  whose corresponding triple contain a trivial subgroup in each of the sections. Subgroups of this form are called *bifree subgroups*. These bifree subgroups form a basis for the *bifree double Burnside ring*, a subring of the double Burnside ring. The bifree Burnside ring is currently at the centre of a great deal of research because of the insights it can offer into the double Burnside ring while having a significantly simpler structure. Here we present some of our recent research on bifree subgroups

- [1] K. Bauer, D. Sen, P.Zvengrowski, A Generalized Goursat Lemma, Preprint, 2011. arXiv:1109.0024. 47

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## Completions of partial matrices

**James McTigue**  
Supervisor: Dr Rachel Quinlan

A partial matrix over a field  $\mathbb{F}$  is a matrix whose entries are either elements of the field  $\mathbb{F}$  or independent indeterminates. We present a number of results pertaining to:

- partial matrices whose completions all have ranks that are bounded below,
- partial matrices of constant rank, and
- maximal non-singular partial matrices.

- [1] J. McTigue, R. Quinlan, *Partial matrices whose completions have ranks bounded below*, Linear Algebra Appl. (volume 435, pages 1956-1967, 2011).
- [2] J. McTigue, R. Quinlan, *Partial matrices whose completions all have the same rank*, Linear Algebra Appl. (volume 438, pages 348-360, 2013).
- [3] J. McTigue, R. Quinlan, *Partial matrices of constant rank*, Linear Algebra Appl. (volume 446, pages 177-191, 2014).

Supported by The College of Arts, Social Sciences, and Celtic Studies, NUIG

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## MCMC Simulation for Flexible Models in Survival Analysis

**Shirin Moghaddam**  
Supervisors: Prof. John Hinde, Dr Milonan Krnjajić

We apply nonparametric Bayesian (NPB) methods, which substantially enhance the flexibility of standard parametric models while providing a fully probabilistic framework for inference. Under the NPB paradigm, the unknown functions or distributions of the model are treated as random parameters with stochastic nonparametric priors, such as Dirichlet or Gaussian processes. The computational component of NPB model development involves design and implementation of MCMC simulation algorithms. As a preparatory and training step for developing MCMC samplers for a posteriori inference and prediction, a

**Shiny** (CRAN-R) application has been implemented to obtain samples from Dirichlet process (DP) and a simple DP location mixture model, which illustrates how the sample paths from the DP process are affected by changes in the main model parameters.

**Escobar, M.D. and West, M. (1995)** .

Bayesian Density Estimation and Inference Using Mixtures. *Journal of the American Statistical Association*, 90, pp. 577–588.

**Kottas, A. and Krnjajić, M. (2009)** Bayesian Semiparametric Modeling in Quantile Regression, *Scandinavian Journal of Statistics*, 36, 297-319.

**Müller, P. and Quintana, F.A. (2004)**

Nonparametric Bayesian Data Analysis, *Statistical Science*, 19, 95-110.

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### Identification of translational *cis*-regulatory SNPs in human HeLa cancer cells line using allele-specific gene expression analysis

**Trung Thong Nguyen, Thanh Ngoc Nguyen**  
Supervisors: Cathal Seoighe

Regulation of the mRNA translation level plays an important role in determining protein abundance in cells and point mutations causing single nucleotide polymorphisms (SNPs) that lead to differences in protein synthesis rate between alleles of same genes (*cis*-acting variants) may result in genetic diseases in human. However, recent allele-specific expression studies have been extensively explored at the level of transcription but not translation. Here we developed a computational pipeline to infer the variations in the level of proteins translated from alternative alleles, which are referred to as allele-specific translation (AST). Publicly available RNA-seq and Ribo-seq data of human cervical cancer HeLa cell lines generated from RNA-seq and Ribosome profiling experiments [1] were mapped to 1) our constructed from high-throughput sequencing data and 2) high-quality reference haplotype-resolved genomes of HeLa [2] to identify genes with evidence of AST. We found a total of 171 genes (for part 1) and 198 genes (for part

2) associated with AST. The SNP rs9660 in the 5' UTR of ATP5H gene (from part 1) and rs114238154 in the start codon of NQO1 gene (from part 2) with strong evidence of AST (around 10-fold change in protein abundance between alternative alleles) have been chosen for next experimental validation.

[1] Guo, H. et al. Mammalian microRNAs Predominantly Act to Decrease Target mRNA Levels. *Nature* 466, 835–840 (2010).

[2] Adey, A. et al. The Haplotype-Resolved Genome and Epigenome of the Aneuploid HeLa Cancer Cell Line. *Nature* 500, 207-211 (2013).

Supported by Irish Research Council

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### The Rational Canonical Form of a Matrix

**Olga O'Mahony**

Supervisor: Dr Rachel Quinlan

The Rational Canonical Form (RCF) of  $A \in M_n(\mathbb{F})$  (or  $T \in \text{End}_{\mathbb{F}}(V)$ ) is explored beginning with some definitions and the main theorem. The main sections include:

- The RCF of a Matrix; definitions and theorem,
- Some facts about the RCF, and
- A detailed example including how to find a basis of  $\mathbb{F}^n$  with respect to which  $T$  is in Rational Canonical Form.

[1] D. Dummit, R. Foote *Abstract Algebra*, United States of America: Wiley; 3 edition (July 14, 2003). Print. (pages 456-491).

Supported by The College of Science, NUIG

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### A multiscale sparse grid finite element method for a two-dimensional singularly perturbed reaction-diffusion problem

**Stephen Russell**

Supervisor: Dr. Niall Madden

Standard finite element methods (FEMs), such as the Galerkin method with the usual polynomial basis functions are impractical for very large problems, especially in higher dimensions. Sparse grid methods try to break this “curse of dimensionality” by delivering the same order of accuracy as a classical FEM but, through careful choice of basis functions, with far fewer degrees of freedom (ideally, independent of the problem dimension).

Sparse grid methods can be described as either two-scale or multiscale. In [1], a two-scale sparse grid method is applied to a reaction-diffusion problem on a Shishkin mesh. This method requires only  $\mathcal{O}(N^{3/2})$  degrees of freedom compared to  $\mathcal{O}(N^2)$  for the Galerkin FEM, but with no loss of accuracy.

In this poster, we discuss recent work on extending the analysis of [1] to a multiscale method that requires only  $\mathcal{O}(N \log N)$  degrees of freedom, [2]. The main ingredient in the design and analysis of the method is the construction of a special interpolation operator. We conclude with the results of numerical experiments that support the theoretical findings.

[1] Fang Liu, Niall Madden, Martin Stynes, and Aihou Zhou (2009). A two-scale sparse grid method for a singularly perturbed reaction-diffusion problem in two dimensions. *IMA J. Numer. Anal.*, 29(4):986–1007.

[2] Stephen Russell and Niall Madden (2014). A multiscale sparse grid finite element method for a two-dimensional singularly perturbed reaction-diffusion problem. (*submitted*).

Supported by College of Science fellowship, National University of Ireland, Galway.

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## Building a Model of the Industry Space & Skill Space of Ireland

**Eoghan Staunton**

**Supervisors:** Petri Piironen, Srinivas Raghavendra, Jim Duggan

Spatial agglomeration of economic activities and unequal growth of urban centres are a major topic of economic interest. Our aim is to model and analyse these uneven spatial economic dynamics by setting up

an agent-based simulation environment. Our model is to be composed of multiple overlapping networks across space and time. The characteristics of each node are then determined by these network layers and the links between them. We introduce our approach to modelling the *industry space* layer, the *skill space* layer and the interactions between them. We also look briefly at some motivating official statistics from the Central Statistics Office and Higher Education Authority.

[1] M. Kaiser and C.C. Hilgetag, Spatial growth of real-world networks, *Phys. Rev. E* 69 (2004), 036103.

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## An Efficient Preconditioner for a Singularly Perturbed Problem

**Thái Anh Nhan**

**Supervisor:** Niall Madden

Our goal is to develop an optimal iterative solution strategy for linear systems of equations arising from the finite element discretization of singularly perturbed reaction-diffusion problems on layer adapted meshes. This develops on an earlier paper [1], which dealt with finite difference methods. The finite element methods considered here are used much more widely in practice. However, the analysis of the resulting linear system is much more complicated.

Our model problem is the singularly perturbed reaction-diffusion problem:

$$-\varepsilon^2 u'' + b(x)u = f(x), \quad \text{with } u(0) = u(1) = 0. \quad (1)$$

Here,  $b$  is a positive function on  $[0, 1]$ , but  $\varepsilon$  may be arbitrarily small. The finite element discretization of (1) on a mesh with  $N$  intervals leads to a linear system to be solved:

$$AU = F \quad (2)$$

where  $A$  is a tridiagonal, symmetric positive definite  $(N - 1) \times (N - 1)$  matrix.

These systems can be solved by direct methods. However, the direct solvers are of limited use in higher dimensions because the computational cost grows exponentially with the number of dimensions. Therefore, iterative solvers, which scale well, are needed.

Our starting point is the one-dimensional problem (1). However, the condition number of the discrete system (2) depends badly on  $\varepsilon$ : it is unbounded as  $\varepsilon \rightarrow 0$ . This shortcoming can be addressed by designing a suitable preconditioner, by which we mean, choosing a matrix  $M$  such that  $M \approx A$  (in the sense of spectral equivalence), but for which the linear system  $M\mathbf{x} = \mathbf{b}$  is easy to solve. Then, instead of solving (2), we solve  $M^{-1}AU = M^{-1}F$ , if  $M$  is a good preconditioner, then this solution process is efficient, and robust with respect to  $\varepsilon$ .

We propose a *boundary layer preconditioner* which is motivated by the physical distribution of layer fitted meshes. We prove its optimality, in the sense of spectral equivalence. A suitable stopping criterion, in the context of the numerical analysis of (1), is also derived [2].

- [1] Scott Maclachlan and Niall Madden, Robust Solution of Singularly Perturbed Problems Using Multigrid Methods, SIAM J. Sci. Comput., 35 (2013), pp. A2225-A2254.
- [2] Scott Maclachlan, Niall Madden and Tháí Anh Nhan, Boundary layer preconditioners for finite element discretizations of reaction-diffusion problems in one and two dimensions, in preparation.

Supported by IRC under Grant No. RS/2011/179.

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## Analysis of T cell receptor diversity using high throughput sequence data

**Yaxuan Yu**

**Supervisor:** Cathal Seoighe

The immune response driven by the adaptive immune system is based on the large diversity of lymphocytes. And the antigen specificity of lymphocytes is determined by its receptors, namely the T cell receptor for T lymphocytes and Immunoglobulin for B-lymphocytes. Here in this study we mainly focused on T cell receptor, which is a molecule formed by somatic genomic recombination in order to recognize different types of antigens. Therefore, analyzing the diversity of TCR can give us a clearer understanding of the process of immune system under infection, cancer and aging. In this study, we present two

bioinformatics pipelines for analyzing high throughput TCR sequencing data by using Decombinator[1] and Mitcr[2].

## 5 Abstracts of PhD Theses

### Mathematical Models of Centromere Associating Proteins

**Kevin Doherty**

Supervisors: Martin Meere & Petri Piironen

#### Abstract

This thesis describes the development and analysis of new mathematical models of Centromere Protein A (CENP-A) incorporation in mammalian centromeres, intermolecular autophosphorylation and Aurora B kinase activity in prophase and metaphase. The models are all developed using a dynamical systems approach.

CENP-A is incorporated as part of nucleosomes at centromeres and is required for correct chromosome segregation in mitosis. A first mathematical model of CENP-A incorporation is developed in Chapter 3. The results of simulations of this model are presented in Chapter 4. The model correctly produces the behaviour of the system and helps explain apparently conflicting experimental results.

In Chapter 5, a generic model of intermolecular autophosphorylation is developed. The model includes dephosphorylation by a phosphatase of constant concentration, and predicts a threshold concentration for the phosphorylation of enzyme and the possible existence of a bistable switch.

Aurora B is a mitotic kinase that localises to centromeres in prophase and metaphase and is vital in ensuring correct attachment of kinetochores to microtubules. A first model of Aurora B binding and activation is developed in Chapter 6 based on the autophosphorylation model of Chapter 5. The model supports the hypothesis that it is possible for soluble Aurora B in the cytoplasm to activate due to binding at centromeres.

Both CENP-A and Aurora B play important roles in cellular regulation and have been identified as targets of cancer therapies due to their roles in cell division. The mathematical models developed in this thesis help to shed light on key mechanisms in the functioning of the cell.

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**Observational Studies, Matching and**

### Propensity Scores: Applied to Colorectal Cancer Data

**Cara Dooley**

Supervisors: John Hinde & John Newell

#### Abstract

The analysis of observational studies is somewhat complex, given the lack of design and randomisation in an observational study and there is often large imbalances in the distributions of covariates, in the treatment groups. This imbalance in the observed covariates would usually be accounted for in the design of a study and randomisation would balance over the unobserved covariates. This imbalance affects subsequent analysis and usual statistical methods are often not enough to correct for this imbalance, leading to biased estimates of treatment effects.

The differences between observational studies and randomised control trials are discussed. Following this, methods to allow observational studies to be analysed in a meaningful and correct manner are presented, particularly the propensity score. The use of the propensity score is a powerful tool which can be used to correct for the lack of balance in a study. This can be implemented in many ways, including through matching and inverse probability weighting. However, when the size of the dataset is large, estimation of the propensity score is not always straightforward. Issues in estimation are shown and methods to improve the estimation of the propensity score are given. Throughout, the ideas are illustrated in a survival analysis setting with reference to a study on the effect of inflammatory bowel disease on survival in colorectal cancer patients from the Irish Cancer Registry.

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### Genus Two Zhu Theory for Vertex Operator Algebras

**Tom Gilroy**

Supervisor: Michael Tuite

#### Abstract

In this thesis we consider the recursive properties of correlation functions for a vertex operator algebra on a genus two Riemann surface formed by sewing two

tori together. We derive a system of formal recursive identities, which allow us to express an arbitrary genus two  $n$ -point correlation function in terms of  $(n - 1)$ -point functions. This generalises Zhu reduction for genus one correlation functions. We apply these recursive identities to compute the genus two Heisenberg  $n$ -point correlation functions, the genus two Virasoro  $n$ -point functions and the genus two Ward Identity. We define a formal differential operator with respect to the sewing parameters and derive differential equations for holomorphic 1-forms, the normalised 2-form, the Heisenberg partition function and the partition function for the Virasoro  $(2, 5)$ -minimal model. We prove that this formal differential operator is defined on an open subset of the sewing domain.

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## Novel Insights into Chromatin Structure and Gene Regulation through Integrative Analysis of High Throughput Genomics Data

**Thong Nguyen**

Supervisor: Cathal Seoighe

### Abstract

Genetics and epigenetics research has evolved dramatically over the last decade, owing to rapid developments in high-throughput genomics techniques. Analysis of the resulting quantities of data requires advanced computational strategies. In this thesis, we use computational and statistical methods to tackle biological questions relating to two major research topics. First, we carried out integrative analysis of next generation sequencing data to answer questions regarding chromatin biology and epigenetics. Second, we performed genome-wide analysis of the effects of genetic variants on gene expression, focussing on two key processes: mRNA decay and mRNA translation. The first question investigated genome-wide distribution of the histone variant H2AX, a key factor in the DNA damage response pathway. We assessed the genomic landscape of H2AX in human U2OS cells using H2AX ChIP-seq data. Strikingly, we found that H2AX was enriched in heterochromatic regions. Heterochromatin has previously been shown to be refractive to damage signalling through H2AX phosphorylation and, consequently, we hypothesized that the

greater abundance of H2AX in heterochromatin helps to ensure sufficient H2AX phosphorylation to signal DNA damage events.

We next turned to characterizing the chromatin organization of the genomic regions that are distal (distal junction – DJ) and proximal (proximal junction – PJ) to human nucleolar organizer regions (NORs). Because they are absent from the reference genome assembly, these regions represent a major gap in our understanding of the epigenetic configuration of the human genome. An integrative analysis of ChIP-seq, RNA-seq, FAIRE-seq and DNase-seq data, generated by the ENCODE consortium, revealed that the DJ resembles euchromatic regions and, surprisingly, harbours transcripts that are transcribed by RNA polymerase II. Laboratory experiments showed that the DJ is localized to the periphery of the nucleolus, where it anchors the ribosomal DNA arrays. This study sheds new light on the role of NORs in nucleolar formation and function, and enables further investigation of the link between nucleoli and human pathologies.

The focus then shifts to studying genetic variation in gene expression. First, we set out to identify transacting genetic variants that influence RNA stability. We demonstrate that perturbation of RNA stabilization is detectable from mRNA expression data. Using the mRNA expression data generated from 726 HapMap3 samples, we calculated the relative expression of long-lived RNAs versus short-lived RNAs for each sample (referred to as RNA stability score or RS-score). Treating RS-score as a quantitative trait, we applied genome-wide association and identified a SNP, rs6137010, with which it is strongly associated in two Asian populations: Han Chinese from Beijing (CHB) and Japanese from Tokyo (JPT). This SNP is a cis-eQTL for SNRPB (a core component of the spliceosome) in CHB and JPT. Thus, we propose that the association between this SNP and inter-individual variation in RS-score is likely mediated by changes in SNRPB expression levels.

The final question investigated the effects of genetic variants on mRNA translation. We developed a computational pipeline to identify genetic variants that influence allele-specific mRNA translation rate (AST). Analysis of allele-specific events is severely biased by the fact that short read sequences favour mapping to the reference allele. Thus, our pipeline

first constructs a haplotype-resolved genome for a given cell-type by making use of high-throughput sequencing data that are publicly available for that cell-type. Both RNA-seq and Ribo-seq data are then mapped to the resulting haplotype-resolved genome in order to identify genes that show evidence of AST. Applying this pipeline for the datasets from HeLa cells, we found 171 protein-coding genes that are associated with AST. Inspection of heterozygous SNPs located in the AST genes revealed two interesting mutations, within the 5'UTR of two genes: ATP5H and SLCO4A1, that appear to inhibit translation initiation of these genes.

To sum up, this thesis presents novel computational strategies for integrative analysis of large volumes of high-throughput genomics data. By addressing biological questions in the areas of chromatin biology and gene regulation, this thesis yields key insights into the DNA damage response, the role of NORs in nucleolar formation and function, and the effects of genetic variants on mRNA stability and mRNA translation.

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## Integration of Genetic Biomarkers in Prognostic Models for Breast Cancer Survival

**Deirdre Wall**

Supervisors: John Newell

Abstract

The main aim of my PhD is to create a prognostic model for invasive breast cancer patients for disease recurrence and death. The data were collected retrospectively and are comprised of 647 invasive breast cancer patients with patient characteristics and genetic markers measured. An additional complexity exists due to the presence of missing data. A complete case analysis with both clinical and pathological biomarkers reduces the number of cases to 103 patients. A major challenge is how best to build a prognostic model for breast cancer in the presence of missing data.

The Kaplan Meier estimate of the survival function is the most commonly used method for the representation of the distribution of survival times. Extensions to graphical comparisons of these survival estimates

were developed. Classical approaches to modelling survival data using complete case analysis are examined and then an empirical simulation study is used to examine the effect of missing data on variable selection and to compare the performance of variable selection techniques in imputed data.

The final model identified Bilateral, Lymph Node status, Mitotic Count, Metastasis and UICC staging as good predictors of Disease Free Survival and a subset of these for Overall Survival (Mitotic Count, Metastasis and UICC staging). These models have good concordance and were calibrated both internally and externally.

Classification and Regression Trees (CART) are a non-parametric approach to regression modelling. The main feature of CART is the data are recursively partitioned into groups and a simple prediction model fitted to each partition. A novel approach using surrogate splits to create alternative competing trees with comparable prediction power are introduced. This helps identify underlying structure in the data.

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## On the collection of topologies, generalized metrics and continuity spaces.

**Jorge Bruno**

Supervisors: Aisling McCluskey

Abstract

This thesis is concerned with the order-theoretic aspects of several collections of topological structures, the study of generalized metrics and the categorical duality between topologies and distance-assignment structures. In particular, the latter focuses on a complete reformulation of topology based solely on the intuitive notion of distance between points.

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## 6 Abstracts of Masters Theses

### Sparse Grid Methods for the Two-Dimensional Poisson Problem

**Stephen Russell**

Supervisors: Niall Madden

This thesis is concerned with finite element methods for computing numerical solutions to boundary value problems. Standard finite element methods, such as the Galerkin finite element method, become impractical for large problems and those in higher dimensions. Sparse grid methods can be employed to overcome these difficulties. As we shall see, the main ingredient in designing and analysing such methods is the construction of a special interpolation operator. We describe and analyse the so called two-scale sparse grid interpolation method. We then prove that the resulting finite element method has the same order of accuracy as the standard Galerkin method, but with significantly lower computational cost. Next, we propose a multi-scale interpolation that is a natural extension of the two-scale one. We give a novel analysis for the error of this interpolant that is clear and understandable. We then outline the analysis required to show that the accuracy of the resulting Finite Element Method is comparable to the standard Galerkin method, and provide numerous supporting results from numerical experiments along with illustrative examples. We conclude by demonstrating the huge savings in computational time and memory.

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## 7 Research Activity from 1 Jan 2013 to 31 Dec 2013

### Permanent and Contract Staff

**Burns, John**

#### Current Research Interests

My current research interests are in the areas of Algebra (Lie algebras, Lie groups, Weyl groups) and Differential Geometry (Homogeneous manifolds, Symmetric spaces, manifolds with multiple conjugate points). Research in all of the above areas is ongoing with various authors:

Adib Makrooni and I are studying ample line bundles on homogeneous complex projective varieties and topological invariants (related to the Poincaré polynomial) of complex homogeneous spaces with non vanishing Euler characteristic.

Patrick Browne and I are finishing work on the geometry of certain homogeneous submanifolds of non-compact symmetric spaces. They are particularly interesting as they turn out to be a very large class of Einstein manifolds.

#### Publications

#### Research Activities

Publications appearing in calendar year 2013: "On the Jacobi equation and manifolds with multiple conjugate points", *Mathematical Proceedings of the R.I.A.* 113A (2013), 19-30 (with D. Wraith and E. Staunton). // Invited talks: Dublin City University, Nov. 2013. // Refereeing: 1 paper. // Conferences and workshops: A Panorama of Geometry, ETH - Zurich, June 2013. Irish Geometry Conference 2014 (co-organizer) May 2014. // Postgraduate supervision: 1 Ph.D. student. // Examiner: One (internal) Ph.D thesis. // Visitors: Tristan Audam, École Centrale de Marseille, France (March-August 2014). conferences, visits, invited talks, research visits, papers refereed, math reviews, editorships, memberships, external posts, etc

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**Cruickshank, James**

### Current Research Interests

- [1] Geometric graph theory - in particular rigidity of bar-joint frameworks and other related structures.
- [2] Rank properties of spaces of matrices
- [3] Random geometric graphs

### Publications

- [1] *Unitary groups over local rings*. James Cruickshank, Allen Herman, Rachel Quinlan, Fernando Szechtman. *J. Algebra App.* **13**, Issue 2, March 2014

### Research Activities

Graduate Students: Christine Marshall (cosupervised with Colm O Riordan, Discipline of Information Technology)

Conference presentation: Geometric and Topological Graph, University of Bristol, March 2013 (contributed talk)

Invited talk: Lancaster University, October 2013 (department colloquium)

Editorships: Editorial board of the Bulletin of the IMS

Journal Submissions: 2 articles submitted (both since accepted for publication)

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**Destrade, Michel**

### Current Research Interests

I am mostly interested in applying the principles of Continuum Mechanics to the modelling of soft matter, including biological tissues and gels. The equations of motion can be written down to take into account all physical characteristics of these materials, including coupling with other fields such as electromagnetism or fluid dynamics. However great care must be taken when large deformations are envisaged, especially in the elaboration of adequate boundary conditions, with crucial repercussions in the correct formulation of numerical simulations. I am mainly working in problems and application of elastic wave

propagation, elastic stability, and proper computational solid mechanics.

Keywords: Stability of soft solids; Acousto-elasticity with application to soft tissues; Mechanical modelling of Human Skin and of Brain Tissue, Numerical implementation of Solid Mechanics.

### Publications

Numbers of publications appearing in calendar year 2013: 10

Four significant publications

- [1] B. Rashid, M. Destrade, M.D. Gilchrist. Mechanical characterization of brain tissue in simple shear at dynamic strain rates, *Journal of the Mechanical Behavior of Biomedical Materials*, 28 (2013) 71-85.
- [2] L. Vergori, M. Destrade, P. McGarry, R.W. Ogden. On anisotropic elasticity and questions concerning its Finite Element implementation, *Computational Mechanics*, 52 (2013) 1185-1197.
- [3] A.L. Gower, M. Destrade, R.W. Ogden. Counter-intuitive results in acousto-elasticity, Wave Motion, Special Issue in Honour of V.I. Alshits [invited contribution], 50 (2013) 1218-1228.
- [4] P. Ciarletta, M. Destrade, A.L. Gower. Shear instability in skin tissue, *Quarterly Journal of Mechanics and Applied Mathematics*, 66 (2013) 273-288.

### Research Activities

Research grants: Postgraduate IRC Fellowship (co-I), NUI Galway start-up grant, NUI Galway Hardiman Scholarship, Italian Institute of Higher Mathematics (INdAM) Visiting Professor Programme, INdAM Marie Curie COFUND Fellowship for L. Vergori, Royal Society International Joint Project (co-I), New Foundations Grant from the Irish Research Council;

Numbers of graduate students: 1;

Conferences/Seminars: 4;

Outreach talks: 8;

Guest Visits: 3; Host Visits: 3;

Papers/Grants refereed: 20;

Editorships: Quarterly Journal of Mechanics and Applied Mathematics, International Journal of Applied Mechanics, International Journal of Non-Linear Mechanics, Proceedings of the Royal Society A, Journal of the Acoustical Society of America;

Memberships: Acoustical Society of America, Society for Industrial and Applied Mathematics, International Society for the Interaction of Mechanics and Mathematics;

External positions: Visiting Professor of Mechanical Engineering (University College Dublin); Directeur de Recherche, Institut d'Alembert, CNRS, Paris, France (on leave); International Brain Mechanics and Trauma Lab (Oxford); Biomechanics Research Centre (NUI Galway).

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### Detinko, Alla

#### Current Research Interests

Computational group theory, linear groups, arithmetic groups, algebraic groups.

#### Publications

Most significant recent publications

- [1] A. Detinko, D. Flannery, E. O'Brien Algorithms for linear groups of finite rank, *Journal of Algebra*, 393 (2013), 187-196.
- [2] A. Detinko, D. Flannery, E. O'Brien, 'Recognition of finite matrix groups over infinite fields', *Journal of Symbolic Computation*, 50 (2013), 100-109.
- [3] A. Detinko, D. Flannery, W. de Graaf Integrality and arithmeticity of solvable linear groups, *Journal of Symbolic Computation*, to appear, 2014.
- [4] A. Detinko, D. Flannery, A. Hulpke Algorithms for arithmetic groups with the congruence subgroup property, submitted, 2014.

#### Research Activities

- Selected talks (2013).

1. 'Recent advances in computing with infinite linear groups' Groups St Andrews 2013 (University of St Andrews, UK), August 2014.

2. 'Computing with linear groups of finite rank', Questions, Algorithms, and Computations in Abstract Group Theory, (Braunschweig, Germany), June 2013 .

- Reviewing: 5 reviews for Mathematical Reviews.
- Membership: member of the American Mathematical Society.

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### Downing, Tim

My research focuses on using genomics, population genetics and models of evolution to infer the origin, history and spread of single-cell parasites and bacteria. Insights into the genetic pathways and mechanisms of drug resistance in pathogens can be determined from DNA and RNA sequences in large collections of samples. Identifying mutations in populations provides information on their evolutionary and epidemiological history as well as a means to distinguish novel samples that may be hybrid combinations of other ones. This can be applied to explore the origins of monomorphic clonal outbreaks as well as new pathogen species.

#### Current Research Interests

Genome assembly, population genetics, experimental evolution of drug resistance.

#### Publications

Most significant recent publications

- [1] Downing T, Rogers MB, et al. Genomic confirmation of hybridisation and recent inbreeding in a vector-isolated *Leishmania* population. *Plos Genetics* (2014) e1004092.
- [2] Connell S, Meade KG, Allan B, Lloyd AT, Downing T, et al. Genome-wide association analysis of avian resistance to *Campylobacter jejuni* colonization identifies risk locus spanning the CDH13 gene. *G3* (2013) 3(5):881-90.

- [3] Coughlan S, Barreira S, Seoighe C, Downing T. Genome-wide variant discovery using sequence assembly, mapping and population-wide analysis. Book chapter in *Bioinformatics and data analysis in microbiology* (2013).

### Research Activities

I am supervising one PhD student (Simone Coughlan) funded by an NUIG fellowship, who has one paper in preparation. I have several papers in preparation through collaborations with the Wellcome Trust Sanger Institute, the Institute of Tropical Medicine Antwerp, Strathclyde University, and Charite University Berlin. Within NUIG, I have two papers in preparation through collaborations with Prof. Charlie Spillane and Dr. Thomas Barry. I have planned a project with Prof. Jim O’Gara on genetic analysis of induced drug-resistance in *S. aureus* bacteria. I won travel funding from FP7 Enterprise Ireland, organised the Virtual Institute of Bioinformatics and Evolution conference here in NUIG, compiled a few rejected research proposals, and refereed for a variety of journals.

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### Dane Flannery

#### Research

Algebraic design theory; computational group theory; linear group theory; arithmetic groups.

#### Publications

- [1] A. S. Detinko, D. L. Flannery, and W. de Graaf, *Integrality and arithmeticity of solvable linear groups*, Journal of Symbolic Computation, to appear 2014.
- [2] A. S. Detinko, D. L. Flannery, and E. A. O’Brien, *Algorithms for linear groups of finite rank*, Journal of Algebra, 393 (2013), 187-196.
- [3] A. S. Detinko, D. L. Flannery, and E. A. O’Brien, *Recognition of finite matrix groups over infinite fields*, Journal of Symbolic Computation, 50 (2013), 100-109.

- [4] A. S. Detinko, D. L. Flannery, and A. Hulpke, *Algorithms for arithmetic groups with the congruence subgroup property*, submitted, 2014.

### Research Activities

- Principal Investigator, Research Frontiers Programme 11/RFP.1/MTH3212.
- Team leader, ‘Groups, Computing, Designs’.
- PhD supervision: Ronan Egan; Hardiman fellowship and Irish Research Council scholarship.
- Editorship, Journal of the Australian Mathematical Society.
- Organizer, ‘Algebraic design theory with Hadamard matrices: applications, current trends and future directions’, Banff International Research Station, Canada.
- Reviewer for the European Science Foundation.
- Distinguished visitor: Professor Willem de Graaf, University of Trento, Italy (September 2013).
- Referee for CRC Press/Chapman & Hall (1), LMS Journal of Computation and Mathematics (2), Journal of Algebra (1), Journal of Combinatorial Designs (1).
- 3 Mathematical Reviews.
- ‘Computing with arithmetic groups’, Groups St Andrews 2013 (University of St Andrews, UK), August 2014.

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### Hinde, John

#### Current Research Interests

Statistical modelling, particularly generalized linear models and random effects and mixture models; statistical computing and statistical software; likelihood theory and inference; applications of statistics in biological, medical and social sciences.

## Publications

Most significant recent publications

- [1] Coffey, Norma, Hinde, John and Holian, Emma (2014) Clustering longitudinal profiles using P-splines and mixed effects models applied to time-course gene expression data. *Computational Statistics and Data Analysis*, **71**, 14-29.
- [2] Urbano, Mariana Ragassi, Hinde, John and Demétrio, Clarice Garcia Borges (2013) Bioassays with natural mortality: handling overdispersion using random effects. *Journal of Agricultural, Biological and Environmental Statistics*, **18**, 594-610,
- [3] Coffey, Norma, Hinde, John and Garcia, Augusto Franco. (2013) Finite mixture model clustering of SNP data. In *Statistical Modelling: Papers in Biostatistics and Bioinformatics*, eds MacKenzie, G. and Peng, D., Springer.
- [4] Martinez, Marie-José and Hinde, John (2013) Random effects ordinal time models for grouped toxicological data from a biological control assay. In *Statistical Modelling: Papers in Biostatistics and Bioinformatics*, eds MacKenzie, G. and Peng, D., Springer.

## Research Activities

Graduate students: 2

Journal submissions: 1 accepted, 1 under review

Conferences: Invited Speaker 2; Contributed presentations 3

Invited talks:

*glms 40+ years on: a Personal Perspective* - 58th Reuniao Anual da RBras, Brazil & ESALQ/USP, Piracicaba, Brazil

*Observational studies, matching and propensity scores; an application to colorectal cancer data* - ROeS 2013, Dornbirn, Austria

Research Visits: ESALQ/USP, Brazil – July & December 2013

Editorships: Statistics and Computing (Associate); Computational Statistics and Data Analysis (Associate); Statistical Modelling (Advisory Board).

President of the International Biometric Society (2013-2017)

Review Panel Member for Group Biomedical Sciences/ L-BioStat Cluster, K. U. Leuven, Belgium (2013)

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## Holian, Emma

### Current Research Interests

Mixture modelling to cluster longitudinal data profiles and to model the group features via generalized linear mixed models and penalized smoothing models, leading to the formulation of the Regression Cluster Model (RCM). Analysis into capability of the RCM to handle missing data within profiles or profiles measured at variable time-points. Extension of the RCM to longitudinal profiles measured on discrete or categorical scales. P-Splines and mixed effects model clustering. Applications in microarray analysis.

### Publications

Recent publications pending review

- [1] Coffey, N., J. Hinde, and E. Holian. “Clustering longitudinal profiles using P-splines and mixed effects models applied to time-course gene expression data.” *Computational Statistics & Data Analysis* 71 (2014): 14-29.
- [2] Martinez, Marie-José, and Emma Holian. “An alternative estimation approach for the heterogeneity linear mixed model.” *Communications in Statistics-Simulation and Computation* just-accepted (2013).
- [3] Martinez, Marie-José, and Emma Holian. “An alternative estimation approach to fit a heterogeneity linear mixed model.” *ERCIM 2013-6th International Conference of the ERCIM Working Group on Computational and Methodological Statistics*. 2013.

### Research Activities

Memberships: Irish Statistical Association.

Affiliations: Staff member Biostatistics Unit. HRB Clinical Research Facility, Galway, (CRFG).

Collaborative work: Statistical Consultation, Dr.

Roisin Dwyer, REMEDI, NUIG, microarray analysis in Mesenchymal Stem Cells and Breast Cancer.

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### Krnjajić, Milovan

#### Current Research Interests

My research interest focuses on the development of statistical methods and models for analysis of structured data arising in applied problems of science, engineering, finance and medicine. In particular, I work on the development of new Bayesian non-parametric models in regression and classification, and algorithms for MCMC simulation. I am also interested in inverse problems, Bayesian model specification and model choice.

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### Madden, Niall

#### Current Research Interests

I am interested in the theory and application of numerical methods (finite element; finite difference) for solving ordinary and partial differential equations whose solutions feature boundary and interior layers. I am especially interested in highly efficient algorithms, such as *hp*-finite elements, sparse-grid methods, and fast linear solvers. I am also interested in the use of modern numerical techniques that accelerate computer models of physical phenomena.

#### Publications in 2013

- [1] S. MacLachlan and N. Madden. Robust solution of singularly perturbed problems using multigrid methods. *SIAM Journal on Scientific Computing*, 35(5), pp. A2225-A2254, 2013.
- [2] C. Xenophontos, M. Melenk, and N. Madden. *hp*-Finite Element Methods for Fourth Order Singularly Perturbed Boundary Value Problems. Dimov, FaragÅş, Vulkov (Eds.): *Proc. NAA 2012, Springer Lecture Notes in Computer Science*, Vol 8236, pp. 532-539, 2013.
- [3] C. G. Enright, M. G. Madden, and N. Madden. Bayesian networks for mathematical models: Techniques for automatic construction and

efficient inference. *International Journal of Approximate Reasoning*, 54(2):323 – 342, 2013.

#### Research Activities

During 2013, I submitted two papers, both on the topic of *hp*-finite element methods for coupled systems and high-order differential equations.

In May, I gave a talk at the 10<sup>th</sup> *Annual Workshop on Numerical Methods for Problems with Layer Phenomena*, hosted by the University of Cyprus. In June, I spent a week visiting the Tufts University, MA, and later that month gave a talk at the 25<sup>th</sup> *Biennial Numerical Analysis Conference*, at the University of Strathclyde.

I am currently supervising two Ph.D. students: Thái Anh Nhan, and Stephen Russell. Thái is developing optimised iterative linear solvers, and Stephen is working on sparse grid methods.

I refereed papers for several international journals during 2013: the IMA Journal of Numerical Analysis, International Journal of Numerical Analysis and Modelling, Numerical Methods for Partial Differential Equations, and Numerical Algorithms.

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### McCluskey, Aisling

#### Current Research Interests

My research interests reside primarily within analytic topology, with a particular fascination in how order theoretic structures mesh with topology. Considerable insight into the structure of  $Top(X)$  as a particular type of order-theoretic object has been accomplished by my graduate student Jorge Bruno, whilst new avenues of research, with a categorical flavour, have unfurled in collaboration with Ittay Weiss (University of South Pacific). Other ongoing research concerns continua theory in the context of both a natural associated order (a notion of "betweenness"), and of discrete dynamical systems.

Additionally, my research interests also encompass research in undergraduate mathematics education. Specifically, and in collaboration with Hardiman scholar Michelle Duane, I am interested in the development of and facility with proof and proving in ab-

stract analysis-based mathematical subjects typically taken in mathematics-major degree programmes.

## Publications

Numbers of publications appearing in calendar year 2013: 4

Most significant publications

- [1] J. L. Bruno and A. E. McCluskey, "Topologies as points within a Stone space: lattice theory meets topology", *Topology Appl.* 160 (2) (2013), 273 - 279.
- [2] J. L. Bruno and A. E. McCluskey, "Topologies on  $X$  as points within  $2\hat{P}(X)$ ", *Topology Appl.* 159 (13) (2012), 3027 - 3032.
- [3] Aisling E. McCluskey, "What are our Senior Undergraduates in Mathematics Learning? A Mathematician's Hope", *Proceedings of Volcanic Delta 2011*, 278 - 291.
- [4] A. E. McCluskey and R. W. Knight, "A consistent counterexample in  $P(R)$ ", *Topology Appl.* 156 (11) (2009), 1943 - 1945.

## Research Activities

Publications:

Topology - 2 peer reviewed Journal Articles Published; Mathematics Education - 2 peer reviewed Articles in Conference Proceedings published.

Publishing contract with Oxford University Press awarded to produce undergraduate topology textbook with co-author Brian McMaster, QUB.

Conferences: Hosted 16th Galway Topology Colloquium (GalTop16) at NUI Galway, July 8 - 10, 2013. Participant of the Fifth Conference on Research in Mathematics Education, Dublin, September 2013.

Appointed as host of the annual international Summer Conference in Topology and Its Applications (SUMTOPO30) at NUI Galway in 2015.

Appointed to the International Steering Committee of DELTA 2013

Research funding: 7500 euros secured for SUMTOPO30.

Research visitors: Professor Jiling Cao, Auckland University of Technology (3 weeks) - funded by Millennium Fund.

Professor Ivan Reilly, University of Auckland - 2 weeks.

Professor Alev Kanibir, Hacettepe University, Turkey - 2 months.

Professor Sadik Bayhan, Mehmet Akif Ersoy University, Turkey - 2 months.

Professor Judy Paterson, University of Auckland - 4 days

Professor Salvador Garcia Ferreira, UNAM, Mexico - 1 week.

Graduate students: 2, one of whom successfully defended his PhD thesis in November 2013; 2 further applications in process.

Reviewer of papers submitted to *Topology and its Applications* and *Central European Journal of Mathematics*.

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## Mc Gettrick, Michael

### Current Research Interests

Quantum Computing and Quantum Information Theory: In particular, quantum random walks and quantum game theory.

### Publications

Most significant recent publications

- [1] "Quantum walks with memory on cycles", M. Mc Gettrick and J. A. Miszczak, *Physica A*, Vol. 399, pp. 163-170 (2014)
- [2] "Measurement-induced generation of spatial entanglement in a two-dimensional quantum walk with single-qubit coin", C. Di Franco, M. Mc Gettrick, T. Machida, T. Busch, *Journal of Computational and Theoretical Nanoscience* 10, 1613 (2013)

## Research Activities

- Currently a member of the Irish Mathematical Society and the American Mathematical Society.
- Participated in the “Workshop on Physics and Information” at the Institut Henri Poincaré (Paris), April 2013.
- In June 2013 I obtained a millennium travel grant to give an invited lecture at the Joint Mathematics Meeting of the American Mathematical Society (held in Baltimore, MD, January 2014).
- A scholarship was obtained from the Chinese Scholarship Council to enable a student from Beijing (Dan Li) to come to Galway as a visiting PhD student for a year. Dan arrived in September 2013.

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**Meere, Martin**

## Current Research Interests

*Drug release modelling.* Analysis of reaction diffusion models describing drug release from affinity hydrogels. Modelling drug release from novel drug eluting stents. Modelling drug transport in nanoporous solids.

*Molecular biology.* Modelling aspects of centromere specification, and the role of the Aurora B kinase.

## Recent Publications

[1] Tuoi Vo T.N., Rongbing Yang, Fawaz Aldabbagh, William Carroll, Martin Meere & Yury Rochev, A thermally activated drug delivery system based on a thermoresponsive polymer and a cooling device: a theoretical assessment, *Journal of Thermal Science and Engineering Applications*, doi:10.1115/1.4025935 (2014)

[2] Kevin Doherty, Martin Meere & Petri Piiroinen, A mathematical model for CENP-A incorporation in mammalian centromeres, *Mathematical Biosciences*, doi: 10.1016/j.mbs.2014.01.005 (2014)

[3] William Finnegan, Martin Meere & Jamie Goggins, The wave excitation forces on a truncated vertical cylinder in water of infinite depth, *Journal of Fluids and Structures*, doi: 10.1016/j.jfluidstructs.2013.04.007 (2013)

[4] Tuoi Vo T. N. & M.G. Meere, Minimizing the passive release of heparin-binding growth factors from an affinity-based delivery system, *Mathematical Medicine & Biology*, doi:10.1093/imammb/dqs027 (2012)

## Research Activities

Completed project: In the past year, one student (Kevin Doherty, co-supervisor Dr. P. Piiroinen) has successfully completed a PhD, and one student successfully completed a Summer internship.

Invited talk at the conference *Cardiovascular Disease and Treatment: Mathematical Modelling and Clinical Insights*, University of Strathclyde, June 2013

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**Naughton, Liam**

## Current Research Interests

Computational Group Theory, Tables of Marks of finite groups and their associated Burnside Rings.

## Publications

[1] Integer Sequences realized by the Subgroup pattern of the Symmetric Group, with G. Pfeiffer, *J. Integer Seq.* 16 (2013), no. 5, Article 13.5.8, 23 pages

[2] Computing the Table of Marks of a Cyclic Extensions, with G. Pfeiffer, *Math. Comp.* 81 (2012), no. 280, 2419 - 2438.

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**Newell, John**

## Publications

Most significant recent publications

[1] Glynn, L. G., Hayes, P. S., Casey, M., Glynn, F., Alvarez-Iglesias, A., Newell, J., Ó

Laighin, G., et al. (2013). SMART MOVE - a smartphone-based intervention to promote physical activity in primary care: study protocol for a randomized controlled trial. *Trials*, 14(1), 157. doi:10.1186/1745-6215-14-157

- [2] Simpkin, A., & Newell, J. (2013). An additive penalty -Spline approach to derivative estimation. *Computational Statistics & Data Analysis*, 68, 30–43. doi:10.1016/j.csda.2013.06.007
- [3] Casey D, Murphy K, Devane D, Cooney A, McCarthy B, Mee L, Newell J, et al (2013). The effectiveness of a structured education pulmonary rehabilitation programme for improving the health status of people with moderate and severe chronic obstructive pulmonary disease in primary care: the PRINCE cluster randomised trial. *Thorax*, 1-7. doi:10.1136/thoraxjnl-2012-203103
- [4] Ingoldsby H, Webber W, Wall D, Scarrott C, Newell J, Callagy C (2013). Prediction of Oncotype DX and TAILORx risk categories using histopathological and immunohistochemical markers by classification and regression tree (CART) analysis. *The Breast*, <http://dx.doi.org/1-16/j.breast.2013.04.008>

### Research Activities

- Current research grants: 1 (Co-PI), 8 (Co-Applicant)
- Numbers of graduate students: 1, 4 joint supervision in School of Medicine
- Journal submissions: 5 in 2013
- Conferences: Presented at 34th Annual Conference of the International Society for Clinical Biostatistics, Munich 2013.
- Memberships: President of Irish Statistical Association
- External post: Adjunct Senior Research Fellow, Department of Mathematics and Statistics, University of Canterbury, Christchurch New Zealand

### Pfeiffer, Götz

#### Current Research Interests

Computational algebra, representations of finite groups and associative algebras, combinatorics and geometry of finite Coxeter groups.

#### Publications

Numbers of publications appearing in calendar year 2012: 5

Four significant publications

- [1] (with J. Matthew Douglass and Gerhard Röhrle)  
On Reflection Subgroups of Finite Coxeter Groups.  
*Comm. Algebra* **41** (2013), no. 7, 2574–2592.
- [2] (with Liam Naughton)  
Integer Sequences Realized by the Subgroup Pattern of the Symmetric Group.  
*J. Integer Seq.* **16** (2013), no. 5, Article 13.5.8, 23 pages.
- [3] (with Marcus Bishop)  
On the Quiver Presentation of the Descent Algebra of the Symmetric Group.  
*J. Algebra* **383** (2013), 212–231.
- [4] (with Marcus Bishop, J. Matthew Douglass and Gerhard Röhrle)  
Computations for Coxeter arrangements and Solomon’s descent algebra II: Groups of rank five and six.  
*J. Algebra* **377** (2013), 320–332.
- [5] (with Marcus Bishop, J. Matthew Douglass and Gerhard Röhrle)  
Computations for Coxeter arrangements and Solomon’s descent algebra: Groups of rank three and four.  
*J. Symbolic Comput.* **50** (2013), 139–158.

#### Research Activities

Numbers of graduate students: 1; Journal submissions: 3; Conferences: 3; Visits: 2; Invited talks:

2; Research visits: 3; Papers refereed: 9; Math reviews: 2; Editorships: Mathematical Proceedings of the Royal Irish Academy; Memberships: Irish Mathematical Society, American Mathematical Society;

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### Piiroinen, Petri T

#### Current Research Interests

My main research interests are in the area of discontinuous dynamical systems with application to rigid-body mechanics, economics, psychology and biological systems. I am also involved in a few projects that deal with the analysis of evolving networks. An overarching aim of my research is to bridge the gap between mathematics and numerical analysis on one hand and biology, engineering and social sciences on the other to make mathematical theories more applicable to non-theoreticians.

#### Publications

Most significant publications

- Doherty, K., Meere, M. and Piiroinen, P.T., *A Mathematical Model of CENP-A Incorporation in Mammalian Centromeres*, *Mathematical Biosciences* 249, pp. 27–43, 2014. (DOI:10.1016/j.mbs.2014.01.005)
- Burns, N. and Piiroinen, P.T., *The complexity of a basic impact mapping for rigid bodies with impacts and friction*, *Regular and Chaotic Dynamics* 19(1), pp. 20-36, 2014.
- Mason, J., Humphries N. and Piiroinen, P.T., *Numerical analysis of codimension-one, -two and -three bifurcations in a periodically-forced impact oscillator with two discontinuity surfaces*, *Mathematics and Computers in Simulation* 95, pp. 98–110, January 2014. (DOI: 10.1016/j.matcom.2012.08.010)
- O’Hora, D., Dale, R., Piiroinen, P.T. and Connolly F., *Local dynamics in decision making: The evolution of preference within and across decisions*, *Scientific Reports* 3, Article no. 2210, Nature Publishing Group, 2013. (DOI: 10.1038/srep02210)

#### Research Activities

During 2013 I supervised or co-supervised 4 PhD students and 1 MSc student. I attended 2 conferences and gave 1 academic (University of Naples Federico II (Italy)). I guest edited a Special Issue *Discontinuous Dynamical Systems: Theory and Numerical Methods* of the journal *Mathematics and Computers in Simulation* (MATCOM).

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### Quinlan, Rachel

#### Current Research Interests

My research interests are primarily in the area of linear algebra and its interactions with other areas of algebra such as field theory and representation theory. Recently I have been interested in linear and affine spaces of matrices that have special rank properties. I also have research interests in mathematical education at university level, specifically in the teaching and learning of proof and proving.

#### Publications

Most significant recent publications

- [1] James McTigue and Rachel Quinlan. Partial matrices of constant rank. *Linear Algebra and its Applications*, Vol. 446, 177–191 (2014).
- [2] James Cruickshank, Allen Herman, Rachel Quinlan and Fernando Szechtman. Unitary groups over local rings. *Journal of Algebra and its Applications*, Vol 13, no. 2 (2014)
- [3] James McTigue and Rachel Quinlan. Partial matrices whose completions all have the same rank. *Linear Algebra and its Applications*, Vol. 438, no. 1, 348–360 (2013).
- [4] Kirsten Pfeiffer and Rachel Quinlan. A proof evaluation exercise in an elementary linear algebra course. *Proceedings of the 5th National Conference in Research in Mathematics Education*, St Patrick’s College Drumcondra (2013).

#### Research Activities

I am currently supervising the research of two PhD students, James McTigue and Olga O’Mahony.

During the past year I have refereed articles for *Linear Algebra and its Applications* and for *Transactions of the American Mathematical Society*.

I am a member of the Irish Mathematical Society, the American Mathematical Society and the International Linear Algebra Society. I am currently serving as secretary of the Irish Mathematical Society.

During the past year I have presented at the following conferences

- Representations and Finite Fields, UCD, May 2013.
- International Linear Algebra Society Conference, Providence, June 2013.
- Irish Mathematical Society Annual Meeting, NUI Maynooth, August 2013.
- 5th National Conference in Research in Mathematics Education, St Patrick's College Drumcondra, September 2013.
- Irish Students Mathematical Society Conference, March 2014.

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### Seoighe, Cathal

Research interests in several areas of bioinformatics/computational biology: Genomics and epigenetics, including gene expression deconvolution, mRNA splicing and analysis of chromatin structure using high throughput sequencing data. Development and application of probabilistic models of evolution, especially the use of evolutionary models to identify immune epitopes in HIV-1. Bioinformatics is interdisciplinary and I collaborate with several other research groups on campus. A major focus of recent collaborations involves the analysis of data from high throughput sequencing technologies. These technologies can be used to sequence genomes or for studying gene expression or the binding of proteins to DNA.

### Current Research Interests

The focus of my research is on modeling molecular biological data, including epigenetic data, gene expression, alternative mRNA splicing and molecular evolution, including the evolution of viruses such as HIV-1.

### Publications

Seven journal articles appeared in 2013.

Most significant publications

- [1] Integrative analysis of mRNA expression and half-life data reveals trans-acting genetic variants associated with increased expression of stable transcripts. Nguyen TT, Seoighe C. PLoS One. 2013 Nov 18;8(11):e79627.
- [2] The shared genomic architecture of human nucleolar organizer regions. Floutsakou I, Agrawal S, Nguyen TT, Seoighe C, Ganley AR, McStay B. Genome Res. 2013 Dec;23(12):2003-12.
- [3] CellMix: a comprehensive toolbox for gene expression deconvolution. Gaujoux R, Seoighe C. Bioinformatics. 2013 Sep 1;29(17):2211-2.
- [4] Gene-set analysis is severely biased when applied to genome-wide methylation data. Geeleher P, Hartnett L, Egan LJ, Golden A, Raja Ali RA, Seoighe C. Bioinformatics. 2013 Aug 1;29(15):1851-7.

### Research Activities

My research group consisted of six PhD students in 2013. Research is supported by the IRC, through a graduate education programme in collaboration with UCD, as well as an individual PhD bursary; PRTL, through a graduate programme in simulation science and the EU, through an international training network coordinated by Leeds University. Academic community service included memberships of editorial boards of Bioinformatics and Briefings in Bioinformatics, review of grants for the Natural Sciences and Engineering Research Council of Canada and the South African National Research Foundation and refereeing for a wide range of journals, as well as membership of the Programme Board for RECOMB Comparative Genomics workshop.

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### Sheahan, Jerome

### Current Research Interests.

Sequences of various kinds, including iid and dependent sequences.

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### Tuite, Michael

#### Current Research Interests

Vertex operator algebras (VOAs), Riemann surfaces, elliptic and modular functions in number theory and combinatorics. I am particularly interested in computing partition and correlation functions on higher genus Riemann surfaces for various VOAs. I am also interested in exceptional VOAs and their relationship to Virasoro constraints.

#### Publications

2 publications in calendar year 2013 and three other papers in press.

- [1] 39. M.P. Tuite, Some generalizations of the MacMahon Master Theorem, *J. Comb. Th. Series A* **120** (2013) 92-101.
- [2] D. Hurley and M.P. Tuite, On the torus degeneration of the genus two partition function, *Int. J. Math.* **24**, 1350056 (2013).

#### Research Activities

- I currently hold one SFI RFP grants.
- I supervised 1 PhD student in 2013.
- I refereed 3 papers.
- I was an external PhD examiner.
- Invited speaker at Irish Quantum Foundations Meeting, Maynooth, May 2013.
- Invited speaker at Workshops on “Majorana Theory, the Monster and Beyond” in Imperial College London, Sept 2013.

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### Ward, James

#### Current Research Interests

Permutability and subnormality criteria in certain classes of infinite soluble groups.  
The study of  $\mathcal{N}_1$  groups (groups with all subgroups

subnormal).

History of Mathematics: Transmission of Greek and Arabic Mathematics in the early medieval era.

Reception of Galois Theory in 19th century University Mathematics teaching.

Professors of Mathematics in Queen’s College, Galway.

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### 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.

#### Publications

Most significant recent publications

- [1] Radivojac, Predrag *et al.* A large-scale evaluation of computational protein function prediction. *Nature Methods* 10 (3), 2013.
- [2] Pierre C. Havugimana *et al.* A census of human soluble protein complexes. *Cell* 150 (5), 1068-1081, 2012.
- [3] Haixuan Yang, Tamas Nepusz, Alberto Paccanaro. Improving GO semantic similarity measures by exploring the ontology beneath the terms and modelling uncertainty. *Bioinformatics* 28 (10), 1383-1389, 2012.
- [4] Prajwal Bhat, Haixuan Yang, Laszlo Buggre, Alessandra Devoto, Alberto Paccanaro. Computational Selection of Transcriptomics Experiments Improves Guilt-by-Association Analyses. *PloS one* 7 (8), e39681, 2012.

#### Research Activities

I worked as Program Committee of the following three conferences: PRIB2013 & CIBB2013

(Eighth IAPR International Conference on Pattern Recognition in Bioinformatics & Tenth International Meeting on Computational Intelligence Methods for Bioinformatics and Biostatistics); The 2013 IEEE/WIC/ACM International Conference on Web Intelligence, and the 5th Asian Conference on Machine Learning. I reviewed papers for Bioinformatics, and Web Intelligence and Agent Systems: An International Journal. Moreover, I reviewed an application for General Research Fund, RESEARCH GRANTS COUNCIL, Hong Kong.

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## Visitors

### de Graaf, Willem

Dates of visit: September 2013

#### Research Interests

Carried out research with A. Detinko and D. Flannery on SFI RFP project. Planned future collaboration, joint funding applications, and conference participation. Delivered School seminar.

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### Cao, Jiling

Dates of visit: July 10 - 19th

#### Research Interests

Joint research on quasicontinuous functions.

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### Reilly, Ivan

Dates of visit: July 10 - 21st

#### Research Interests

Group project on types of continuity.

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### Kanibir, Alev

Dates of visit: June 20 - August 18th

#### Research Interests

Group project on types of continuity.

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### Bayhan, Sadik

Dates of visit:

#### Research Interests

Group project on types of continuity.

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### Paterson, Judy

Dates of visit: March 20 - 23rd

**Research Interests**

Research in Mathematics Education.

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**Garcia Ferreira, Salvador**

Dates of visit: July 5 - 12th

**Research Interests**

Development of research proposal.

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**Moral, Rafael**, ESALQ/USP, Piracicaba, Brazil

Dates of visit: April 17th to June 14th

**Research Interests**

Rafael de Andrade Moral visited NUI Galway for a 2-month period in 2013 as part of his Master's studies to work under the supervision of Prof. John Hinde. His research involves statistical modelling of the ecological interactions among species of agricultural significance, including pests and natural enemies. His supervisor at ESALQ/USP is Prof. Clarice G. B. Demétrio.

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**Reeh, Sune**

21–25 October:

**Research Interests**

We had discussions on bisets for fusion systems. This is closely related to the Burnside ring, one of the main topics studied in de Brún Center.

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**Díaz, Antonio**

5–10 November:

**Research Interests**

This is an ongoing collaboration on homological algebra over fusion systems, specifically vanishing of higher derived limits of almost-Mackey functors over categories related to fusion systems. This is closely related to the group cohomology, one of the main topics studied in de Brún Center.

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## Postgraduate Researchers

### Current Postgraduate Research Students

<b>Student</b>	<b>Degree</b>	<b>Supervisor</b>	<b>Supervisor</b>
Nhan Anh Thai	PhD	Niall Madden	
Bui Anh Tuan	PhD	Graham Ellis	
Alan Barnicle	PhD	Cathal Seoighe	Laurence Egan
Sofia Barreira	PhD	Cathal Seoighe	Brian McStay
Isaac Burke	PhD	Emil Sköldberg	
Richard Burke	PhD	Petri Piironen	
Shane Burns	PhD	Petri Piironen	
Simone Coughlan	PhD	Tim Downing	Cathal Seoighe
John Donohue	PhD	Petri Piironen	
Liam Doonan	PhD	Uri Frank	Cathal Seoighe
Michelle Duane	PhD	Aisling McCluskey	
Ronan Egan	PhD	Dane Flannery	
Lida Fallah	PhD	Haixuan Yang	John Hinde
Artur Gower	PhD	Michel Destrade	
Amirhossein Jalali	PhD	John Newell	John Hinde
Peter Keane	PhD	Cathal Seoighe	Rod Ceredig
Dan Li	PhD (visiting)	Michael McGettrick	
Adib Makrooni	PhD	John Burns	
Brendan Masterson	PhD	Götz Pfeiffer	
James McTigue	PhD	Rachel Quinlan	
Shirin Moghaddam	PhD	John Hinde	Milovan Krnjajic
Olga O'Mahony	PhD	Rachel Quinlan	
Thanh Ngoc Nguyen	PhD	Cathal Seoighe	
Stephen Russell	PhD	Niall Madden	
Yaxuan Yu	PhD	Cathal Seoighe	

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## Seminars

- [1] Shane O'Rourke, Cork Institute of Technology **Ordering tree-free groups** 8/1/2013
- [2] Ann O'Shea, NUI, Maynooth **Student Engagement with Mathematics and Mathematics Support** 17/1/2013
- [3] Haixuan Yang, NUI, Galway **A non-linear regression/classification model and its potential applications** 24/1/2013
- [4] Eberhard Mayerhofer, Dublin City University **A free boundary problem arising from Finance** 19/1/2013
- [5] Laura O Dwyer, Boston College **Randomized Experiments in Education** 28/2/2013
- [6] Peter McNamara, Bucknell University **Symmetric polynomials and the skew Pieri rule** 7/3/2013
- [7] Maria Meehan, University College Dublin **Theory to Practice: Mathematics education research impacting practice in an advanced mathematics module** 14/3/2013
- [8] Judy Paterson, University of Auckland **Talking about Mathematics And Teaching: Team-Based Learning in Mathematics and Statistics** 26/3/2013
- [9] Steve Buckley, NUI, Maynooth **Finite rings with many idempotents** 8/4/2013
- [10] Jim Cruickshank, NUI, Galway **On Graver's conjecture on the generic rigidity of bar and joint frameworks in 3-space** 11/4/2013
- [11] Javier Aramayona, NUI, Galway **Finite rigid subsets in curve complexes** 18/4/2013
- [12] Alice Niemeyer, University of Western Australia **The complexity of multiplication in finite polycyclic groups** 19/4/2013
- [13] Claus Köstler, University College Cork **What can noncommutative probability tell about representation theory?** 25/4/2013
- [14] Rod Gow, University College Dublin **Rank Problems for Subspaces of Hermitian Matrices over Finite Fields** 9/5/2013
- [15] Greg Campbell, U.S. Food and Drug Administration (FDA) **Bayesian Statistics in Clinical Trials: Some Progress and Some Challenges** 13/6/2013
- [16] Padraig O Cathain, University of Queensland **Nesting symmetric designs** 23/7/2013
- [17] Willem de Graaf, University of Trento **Computation with linear algebraic groups** 12/9/2013
- [18] Sejong Park, NUI, Galway **Fusion, bisets and cyclic subgroups** 19/9/2013
- [19] Jeong-Sook Im, NUI, Galway **Applications of a boundary integral method for unsteady water waves** 26/9/2013
- [20] Antonio Augusto Franco Garcia, ESALQ/USP, Brazil **Statistical**

- models for genetic mapping in autopolyploids, with applications in sugarcane** 2/10/2013
- [21] John Burns, NUI, Galway **The Geometry of Maximal Tori, Continuous and Discrete** 10/10/2013
- [22] Ray W. Ogden FRS, University of Glasgow **Elasticity of biopolymer filaments and cross-linked F-actin networks with compliant binding proteins** 16/10/2013
- [23] Shaun Mahony, Penn State University **Characterizing context-dependent transcription factor activity during direct motor neuron programming** 17/10/2013
- [24] Sune Reeh, University of Copenhagen **Burnside rings and fusion systems** 24/10/2013
- [25] Sebastian Schoennenbeck, RWTH Aachen **Resolutions for unit groups of maximal orders** 31/10/2013
- [26] Antonio Díaz, Universidad de Málaga **A generalization of the Lyndon-Hochschild-Serre spectral sequence** 7/11/2013
- [27] Ted Hurley, NUI, Galway **Algebraic structures for communications** 14/11/2013
- [28] Bent Nielsen, Oxford University **Inference and forecasting in the age-period-cohort model with unknown exposure with an application to mesothelioma mortality** 21/11/2013
- [29] Grant Lythe, University of Leeds **Stochastic modelling and immunology: how many populations? how many cells? how many encounters?** 28/11/2013
- [30] Rupert Levene, University College Dublin **Distance formulae** 5/12/2013
- [31] Martin Stynes, University College Cork **A finite difference method for a two-point boundary value problem with a Caputo fractional derivative** 12/12/2013
- [32] Anthony Cronin, University College Dublin **Three Problems in Matrix Theory** 19/12/2013
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- Specialist seminar series**
- Homotopy type theory (Organiser: **Emil Sköldbberg**)
  - Fusion systems (Organiser: **Sejong Park**)
  - Canonical forms of matrices (Organiser: **Rachel Quinlan**)
  - Bioinformatics seminar series & journal club (Organisers: **Cathal Seoighe & Tim Downing**)
  - Statistics reading group (Organiser: **John Hinde**)
  - MathSoc seminar series (Organisers: **MathSoc**)
- 
- Conferences and Workshops**
- Virtual Institute of Bioinformatics and Evolution (VIBE, Irish Bioinformatics meeting)

Organisers: Tim Downing, Cathal  
Seoighe

Date: November 15, 2013

- Innovative Clinical Study Design for  
Medical Devices

Organisers: John Newell

Date: June 12, 2013

- 16th Galway Topology Colloquium

Organisers: Aisling McCluskey & Jorge  
Bruno

Date: July 8-10, 2013

- Groups in Galway 2013

Organisers: Javier Aramayona and  
Claas Röver.

Date: 10 - 11 May, 2013

- Algebraic design theory with Hadamard  
matrices: applications, current trends  
and future directions (Banff Interna-  
tional Research Station, Canada)

Date: 10-13 July

Organisers: Dane Flannery (with R.  
Craigén, H. Kharaghani).

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