

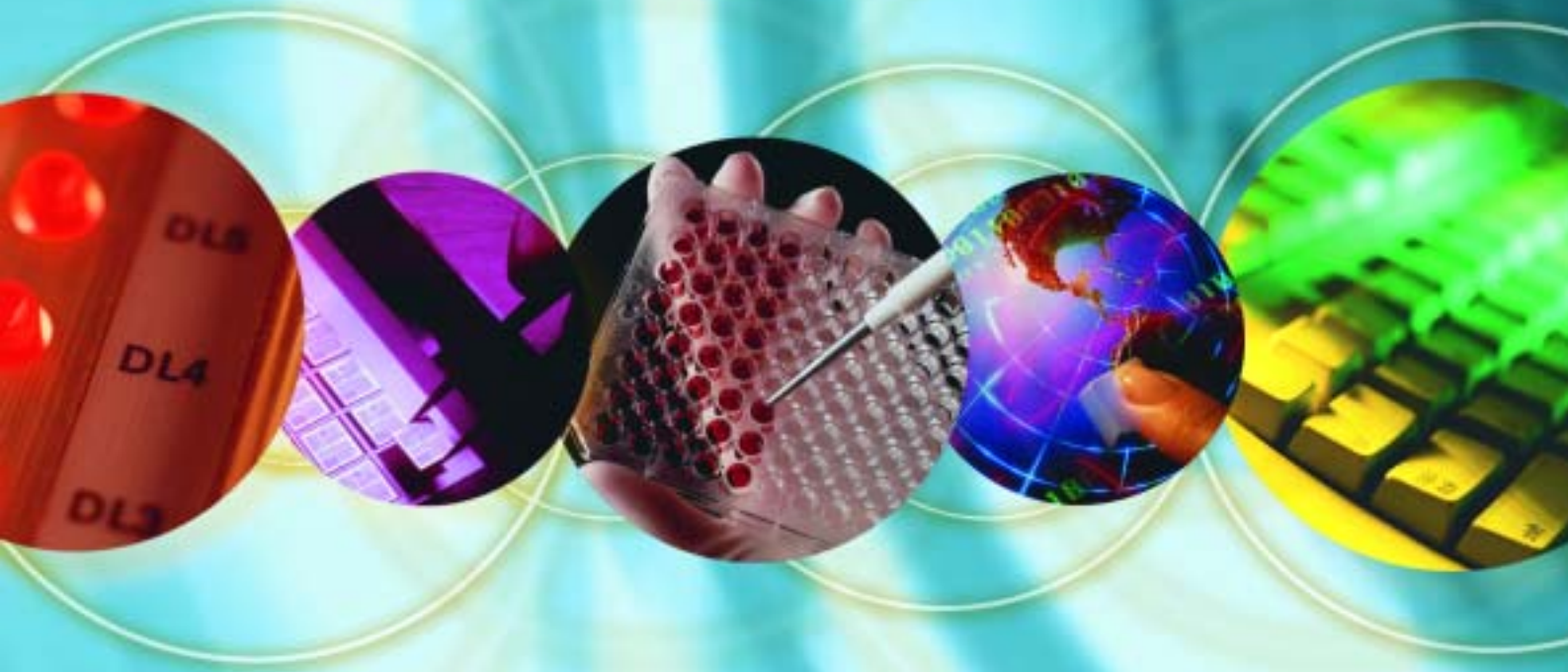


NUI MAYNOOTH

Ollscoil na hÉireann Má Nuad

# Faculty of Science

Research Report 2002





# FACULTY OF SCIENCE

## RESEARCH REPORT

### 2002

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## DEAN'S INTRODUCTION



I am very pleased to introduce the annual research report from the Faculty of Science at NUI Maynooth for the year 2002. The year 2002 was one of continued growth and progress for the Faculty. Despite the continuing decline in the numbers of students taking Leaving Certificate science subjects, our teaching programmes and student numbers remain buoyant - over 900 undergraduate students participated in BSc degree programmes in the Faculty. In September 2002 the first students for the new denominated degree in Biological Science were enrolled, and in the same month our first cohort of 29 students graduated from the Computer Science and Software Engineering denominated degree programme. In September 2003 the first students for the new denominated BSc degree programmes in Psychology and in Chemistry with Pharmaceutical Chemistry were enrolled. The vision and flexibility shown by

Faculty staff in reviewing and expanding their academic programmes, developing exciting new courses and ensuring their relevance to a modern Ireland is commendable. There was a strong demand this year for places on these two new denominated entry courses and for the other undergraduate BSc courses at NUI Maynooth. Faculty staff were very pleased to learn that the number of first preference applications to the CAO in 2003 for places on our undergraduate BSc courses had increased by 7%. In October 2002 the first postgraduate students funded under the IRCSET Embark Initiative Postgraduate Scholarship Scheme commenced their research projects. We were very pleased to welcome 15 Embark Initiative Scholars to the Faculty of Science at NUI Maynooth. In all, 165 students were registered for postgraduate degrees by research in the Faculty in 2002.

NUI Maynooth has internationally acclaimed scientists in a variety of research areas ranging from astrophysics to molecular biology, quantum computing and software engineering. The research and publication record of Faculty staff have facilitated the University in securing funding for a number of strategic, specialist research initiatives. These include two Institutes: The Institute for Bioengineering & Agroecology and The Institute for Immunology which were established under the Irish Higher Education Authority PRTL I initiative. One of the highlights of 2002 was the completion of a new building to house these two Institutes. This new facility was officially opened by Mr. Noel Dempsey, TD, Minister for Education and Science in January 2003. A third research institute, The Hamilton Institute, established in July 2001 and funded by Science Foundation Ireland (SFI) was formally opened by Dr. William C. Harris, Director General of SFI in September 2002. Research in the Hamilton Institute builds upon the natural synergies which exist between Computer Science, Mathematics, Physics and Engineering with a particular focus on computer controlled systems.

This report highlights the achievements by members of the Faculty in different fields of scientific research and scholarship. We are a relatively small Faculty, comprising at present 63 permanent academic staff and 17 full-time contract academics, yet this small group of staff produced a range of high profile research publications in Journals such as *Nature*, *Journal of Virology*, *Journal of Bacteriology*, *Journal of Clinical Microbiology*, *Journal of Biological Chemistry*, *Polyhedron*, *Astroparticle Physics*, *Applied Optics*, *Physics Review Letters*, *Journal of High Energy Physics*, *Bulletin of the London Mathematical Society* and *Inventiones Mathematicae*. A publication from the Department of Experimental Physics in *Physical Review E* was selected for the November 2002 issue of the *Virtual Journal of Ultrafast Science* which is a multi-journal compilation of links to articles covering frontier research on ultrafast phenomena in physics, optics, chemistry, and biology. A publication in *Nature* in October 2002 by Professor Vladimír Buzek and colleagues was selected by *PhysicsWeb* as one of the top ten highlights of year 2002 in Physics. In its citation *PhysicsWeb* commented that this publication marked a major breakthrough in quantum optics. *PhysicsWeb* noted that while it is not certain that optical methods will be used in a real quantum computer, it is likely that such techniques would be used in quantum cryptography, in which encoded optical signals would be transmitted over long distances. Professor Buzek, a co-author of this paper is an SFI ETS Walton Fellow in the Department of Mathematical Physics at NUI Maynooth on leave from the Slovakian Academy of Science.

In addition to producing a range of high profile publications, researchers in the Faculty have also been successful in attracting major research grants from The European Union, The European Space Agency, The Leverhulme Foundation, The Wellcome Foundation, The Engineering and Physical Research Council (UK) and other international funding bodies and also from national funding bodies such as Science Foundation Ireland, Enterprise Ireland, The Irish Research Council for Science, Technology and Engineering, The Health Research Board, The National Advisory Committee on Drugs and industrial sponsors. Further evidence of the strong research performance in the Faculty is the number of highly competitive Enterprise Ireland Basic Research grants currently held by Faculty members. In 2003 Enterprise Ireland and IRCSET funded 87 projects out of 570 applications, a success rate of 15%. Twenty three percent of NUI Maynooth's applications for Basic Research grants were funded - this was the highest success rate of any University in the state. The current committed research funds to researchers in the Faculty is in excess of €27 million.

During July 2002 the Science Faculty opened its laboratories and teaching facilities to over 140 second-level students as part of the Maynooth Science Camp. A week full of experiments and laboratory work, games, competitions and field trips drew a very positive response from students, parents and teachers alike. This initiative demonstrated how the second-level and third-level sectors can work together to encourage and support students in opting for science, both as subjects for study and a genuine career option. In August 2003 the Maynooth Science Camp was run for a second year. This year the camp was for designed for senior students only and the focus was on a more in depth introduction to aspects of Science and Engineering. Sessions included astronomy, forensics, the chemistry of fireworks, the science of flight, the building of robots, molecular machines and the biology of cells. I thank the Camp director, Dr. Paul Gibson, the Camp sponsors, and all the academic and technical staff of the Faculty who participated, on a voluntary basis, in the running of the Science Camp, for donating their time to this exciting venture.

This 15th Annual Report from the Faculty of Science at NUI Maynooth illustrates the contribution of Faculty members to research, teaching and public service in the year 2002. I thank the members of the Faculty for their productivity, commitment and significant achievements in the past year.

Ann M. Burnell  
Dean of Science  
NUI Maynooth

Tel 353 1 7083840

E-mail: [ann.burnell@may.ie](mailto:ann.burnell@may.ie)



**Faculty of Science**

**Research Report 2002**

**Biology**



# BIOLOGY

## ACADEMIC STAFF\*

**Professor K. Ohlendieck**, DipBiol, MSc (Konstanz), PhD, Head of Department (2002-)

**Professor A.M. Burnell**, BSc, MSc, PhD (1974-)

**Professor P.J. Dix**, BSc, PhD (Leicester), FIBioll, EurBiol (1980-)

**Professor M.J. Downes**, MAgrSci, PhD, FIBioll (1973-)

**Dr. N. Curran**, BSc, PhD (2001-)

**Dr. D. Doherty**, BA (Mod), MSc, PhD (London) (2000-)

**Dr. B. Dowds**, BA (Mod), PhD (Dublin) (1987-2002)

**Dr. S. Doyle**, BSc, PhD (1997-)

**Dr. C.T. Griffin**, BSc, PhD (Dublin) (1992-)

**Dr. P. Johnson**, BSc, PhD (QUB) (2000-)

**Dr. K.A. Kavanagh**, BSc, PhD (1994-)

**Dr. B.P. Mahon**, BSc (Kent), PhD (Open University) Wellcome Trust Fellow (1998-)

**Dr. G. McCormack**, BSc, PhD (2001-)

**Dr. J. McInerney**, BSc, PhD (1999-)

**Dr. J. Nugent**, BSc, MSc, PhD (Michigan) (1995-)

**Dr. D. Roche**, BSc, PhD (2002-)

## ADJUNCT PROFESSORS

**Professor J. Burke**, BAgSci, MSc, PhD (2002-)

**Professor L. Downey**, PhD (Reading), DSc, LLD (2002-)

## PROFESSOR EMERITUS

**Professor P. Whittaker**, BSc (Liverpool), PhD (Leicester), FIBiol, CBiol, FIBioll, EurBiol (1978-)

## PRINCIPAL INVESTIGATOR

**Dr. S. O'Dea**, BSc, PhD (2001-)

## RESEARCH FELLOWS

**Dr. C. Meade**, BSc, PhD (Dublin) (2000-)

**Dr. K. Brady**, BSc, PhD (2002-)

**Dr. J. Browne**, BA (Mod), PhD (2001-)

**Dr. D. Casey**, BSc, PhD (2000-)

**Dr. A. Corcoran**, BSc (DCU), PhD (2001-)

**Dr. P. Daly**, BSc, PhD (1999-)

**Dr. C. Dempsey**, BSc, PhD (2000-)

**Dr. I. Dix**, BSc, PhD (Szeged) (1984-)

**Dr. K. Dolan**, BSc, PhD (2001-)

**Dr. P. Fitters**, BSc, PhD (1999-)

**Dr. E. Kane**, BSc, MAgrSci, PhD (Florida) (1997-)

**Dr. L. Madrigal**, BSc (Madrid), PhD (Dublin) (2002-)

**Dr. M. McCabe**, BSc, PhD (Nottingham) (2000-)

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\* Unless otherwise stated the higher degrees listed are those of the National University of Ireland.

**Dr. A. Murphy**, BSc, PhD (2001-)  
**Dr. G. Nugent**, BSc, PhD (RMIT, Melbourne) (2000-)  
**Dr. T. O'Connor**, BSc, PhD (2001-)  
**Dr. E. Reeves**, BSc, MSc, PhD (London) (2002-)  
**Dr. M. Sekiya**, BSc, PhD (Cornell) (1998-)  
**Dr. C. Stack**, BSc, PhD (1999-)

## POSTGRADUATE RESEARCH STUDENTS

**Mr. A.M. Aeshwika**, BSc (Al Fateh University, Tripoli) (2002-)  
**Ms. H. Asrafel**, BSc (Derna University, Tripoli) (2002-)  
**Mr. D. Bergin**, BSc (2002-)  
**Ms. C. Brady**, BA (Mod) (Dublin) (2001-)  
**Mr. M. Brennan**, BSc (1999-)  
**Ms. E. Burbridge**, BSc (1997-)  
**Ms. S. Cloney**, BA (Mod) (Dublin) (2000-)  
**Ms. J. Commins**, BSc (2002-)  
**Ms. L. Corrigan**, BSc (2002-)  
**Ms. P. Dagg**, BSc (1996-2002)  
**Ms. S. Delaney**, BSc (2000-)  
**Ms. A. Dillon**, BSc, MSc (London) (1998-)  
**Ms. P. Donoghue**, BSc (2002-)  
**Mr. P. Doran**, BSc (2002-)  
**Mr. P. Dowling**, BSc (2002-)  
**Mr. D. Ennis**, BSc (2000-)  
**Mr. R. Enright**, BSc (1997-)  
**Ms. C. Finnerty**, BSc (2002-)  
**Ms. E. Fitzgibbon**, BSc (1998-)  
**Mr. D. Fitzpatrick**, BSc (2000-)  
**Ms. M. Flynn**, BSc (2000-)  
**Ms. R. Geraghty**, BSc (2002-)  
**Mr. P. Geraghty**, BSc (2000-)  
**Ms. B. Henley**, BSc (1999-)  
**Ms. J. Kelly-Rogers**, BA (Mod) (Dublin) (2000-)  
**Ms. R. Kinsella**, BSc (2001-)  
**Mr. J. Lohan**, BSc (2002-)  
**Ms. T. Lola-Luz**, BSc (TEI, Thessaloniki), MSc (Edinburgh) (2000-)  
**Ms. J. Martin**, BSc (1999-)  
**Ms. L. Maye**, BSc (IT Tallaght) (1998-)  
**Ms. E. McCarthy**, BSc (2000-)  
**Mr. I. McEvoy**, BSc (2002-)  
**Mr. H. McWeeney**, BA (Mod) (Dublin) (2000-)  
**Ms. M. Moran**, BSc (Manchester), MSc (2002-)  
**Ms. C. Neville**, BSc (2000-)  
**Ms. T. Nguyen Thi**, BSc (Ho Chi Minh Univ), MSc (Freie Univ, Berlin) (2000-)  
**Ms. C. Noone**, BA (Mod) (Dublin) (2002-)  
**Ms. K. O'Callaghan**, BSc (2000-)  
**Ms. M. O'Connell**, BSc (2000-)  
**Ms. M. O'Gorman**, BSc (2002-)  
**Mr. D. O'Halloran**, BSc (2000-)  
**Mr. J. O'Keefe**, BSc (2000-)  
**Ms. C. O'Reilly**, BSc (2002-)  
**Ms. M. Pentony**, BSc (2000-)

**Ms. G. Philip**, BSc (2002-)  
**Ms. M. Poage**, BSc (Texas Tech) (2002-)  
**Mr. W. Reardon**, BSc (1998-)  
**Ms. S.O. Regeai**, BSc, MSc, (Al Fateh University, Tripoli) (2002-)  
**Mr. A. Rolston**, BSc (Exeter) (2000-)  
**Ms. E. Ryan**, BSc (QUB) (2002-)  
**Mr. A. Shannon**, BSc (2002-)  
**Ms. K. Shiel**, BSc (1999-)  
**Mr. S. Travers**, BSc (2001-)  
**Mr. T. Tyson**, BSc (2001-)  
**Ms. I. Vickers**, BSc (2002-)  
**Ms. D. Vicuna**, BSc (Toulouse) (2001-)  
**Ms. S. Waters**, BSc (1999-)

## RESEARCH ASSISTANTS

**Ms. S. Cahill**, BSc (North London), HDipMicro, MSc (1999-)  
**Mr. C. Creevey**, BSc, MSc (2002-)  
**Ms. O. Deegan**, BSc, MSc (2002-)  
**Ms. M. Foxe**, BSc (2002-)  
**Ms. G. Gray**, BSc (DCU) (2002-)  
**Mr. T. Kavanagh**, BSc (2000-)  
**Ms. E. Lewis**, BSc (2001-)  
**Ms. J. Masterson**, BSc (2002-)  
**Ms. G. Murphy**, MSc (London) (1996-)  
**Ms. C. Noone**, BA (Mod) (Dublin) (2001-)

## TECHNICAL STAFF

**Ms. A. Butler**, (1985-)  
**Ms. P. Colton**, (1994-)  
**Ms. M. Finnegan**, GI Biol (1985-)  
**Ms. E. Hewson**, (1993-)  
**Mr. A. Hildebrand**, (1976-)  
**Ms. G. Lynch**, BSc (2000-)  
**Mr. J. O'Sullivan**, BSc, DipBiol (Open Univ) (1978-)  
**Mr. A. Power**, BSc (1992-)  
**Dr. F. Tinley**, BSc, PhD (1998-)

## ADMINISTRATIVE STAFF

**Ms. C. Batchelor**, BSc (Coventry) (2001-)  
**Ms. R. Bradshaw**, (2002-)  
**Ms. J. Burbridge**, (1995-)  
**Dr. R. Dempsey**, BSc, MSc, PhD (Dublin) (2001-)  
**Ms. T. Roche**, (1977-)  
**Ms. N. Travers**, BTheol, HDipEd (2001-)

## HEAD OF DEPARTMENT'S REVIEW OF THE YEAR

By the end of 2002 the construction of the Biosciences Building was complete and the Minister of Education and Science, Mr. Noel Dempsey TD, officially opened the new facility in January 2003. The biosciences facility houses two research institutes and a variety of core equipment for biological and biomedical research, which are closely associated with the Biology Department. The scientific directors of the Institute of Immunology and the Institute of Bioengineering and Agroecology, Dr. Bernard Mahon and Professor Martin Downes, have assembled teams of internationally recognised researchers who have attracted considerable amounts of external funding underpinning the core support under PRTL. The Biology Department continues to be highly active in basic research with strong international collaborative links to research groups in the European Union and the United States. Members of staff are again to be congratulated on their success in obtaining funding in a very competitive environment. Ongoing research in 2002 was supported by grants totalling in excess of €11.5 million! In particular, 2002 saw Dr. Sean Doyle and Dr. Kevin Kavanagh being granted €1.7M funding under HEA PRTL Cycle 3, towards the establishment of The National Institute for Cellular Biotechnology, which is co-ordinated by Professor Martin Clynes, DCU. Substantial Science Foundation Ireland grants were also awarded to Professors Ann Burnell and Philip Dix, and to Dr. Shirley O'Dea who is a Principal Investigator for the Institute of Immunology.

The research spectrum of the department was complemented by a Muscle Biology Laboratory. The new Chair of Biology brought with him an established research team focusing on the biochemistry and molecular cell biology of supramolecular membrane complexes. The Department of Biology is working towards establishing a proteomics facility including high-throughput protein analysis and mass spectrometry. Proteomics will be used for the large-scale screening of protein complements and the determination of protein-protein interactions involved in biological function.

We are pleased at the recent appointment by the University of two Adjunct Professors, Professor James Burke and Professor Liam Downey, who are associated with the Department of Biology. We also welcomed Dr. Declan Roche to the lecturing staff of the department in 2002. Declan's research interests lie in the area of Bacterial Molecular Genetics. We were, however, saddened to lose two distinguished members of the Biology Department, Dr. Barbara Dowds and Professor Kingston Mills who have left us to take up positions elsewhere. We wish them every success in the future.

New postdoctoral fellows joining the Department in 2002 were Killian Brady (Population Ecology), John Browne (Nematode Genetics) and Emer Reeves (Medical Mycology). We also welcomed new postgraduate students Ahmed Mohamed Aeshwika, Hamed Asrafel, David Bergin, Jennifer Commins, Laura Corrigan, Pamela Donoghue, Philip Doran, Paul Dowling, Caroline Finnerty, Rachel Geraghty, James Lohan, Ian McEvoy, Mary Moran, Mary O'Gorman, Sassia Omar Regeai, Clare O'Reilly, Gayle Philip, Miranda Poage, Eimear Ryan, Adam Shannon and Imelda Vickers. We would like to congratulate John Browne, Emma Burbridge, Amanda Corcoran, Pamela Dagg and Declan Roche who successfully completed their PhD studies and examinations this year, and Marc Brennan and Orla Deegan, who obtained MScs in 2002.

2002 saw the first class of students for the new denominated honours degree in Biological Science. This degree is unique in that it allows students combine study of an arts subject with an in-depth analysis of Biology. The new degree prompted much interest and the initial class contained seven students who received University Entrance Scholarships for attaining more than 500 points in their Leaving Certificate. We are now also in the second year of the new Computational Biology & Bioinformatics denominated honours degree.

## RESEARCH INTERESTS OF STAFF

### Bacterial Molecular Genetics Laboratory

#### Dr. Barbara Dowds

Research in the Bacterial Molecular Genetics Laboratory is centred on bacteria (*Photorhabdus temperata*) which are pathogenic to insect pests and which live in the gut of nematodes (*Heterorhabditis spp.*) in a mutualistic partnership. Apart from their value in biological pest control in agriculture and horticulture, these bacteria are interesting for use as model organisms in gaining understanding of a number of fundamental biological processes. Thus, they may be used to examine the overlap between different types of symbiotic relationship, and secondly, they are studied for a unique form of phenotypic variation they exhibit which supports their survival in changing environments. We work on genes and mutants affecting the regulation of phenotypic variation and on genes needed for infection of the insect host.

### Bioinformatics and Pharmacogenomics Laboratory

#### Dr. James McInerney

The principal activities of the Bioinformatics and Pharmacogenomics Laboratory centre on the computational analysis of molecular data. There are four Research divisions in the Bioinformatics and Pharmacogenomics Laboratory – Software and Algorithms, Human Genome, Bacterial Genomes and Viral Genomes. We have developed software for the analysis of adaptive evolution in protein-coding genes. Adaptive evolution is said to occur when there has been a rate of amino acid replacement substitutions that is higher than would be expected. One frequent result of adaptive evolution is a change in protein structure or function. We have also developed algorithms and software for phylogenetic supertree construction. In order to construct phylogenetic trees from many gene sequences and from complete genomes it is necessary to develop methods that can deal with missing data – since every genome does not have the same complement of genes. We have developed a number of methods that deal with this issue and we are currently working on large supertree problems. We are working on a number of bacterial genome sequences including the bacteria that cause meningitis and tuberculosis. The complete genome sequences from multiple strains of these bacteria are known and we are working on identifying what they have in common, what is different and how things have changed in the recent past. Our viral genome work involves the analysis of HIV sequences. HIV is the aetiological agent of the human Acquired Immune Deficiency Syndrome (AIDS), a disease so deadly that unfortunately it needs no introduction. We are trying to identify factors in the genome sequences that are of vital importance to the virus order for it to survive.

### Biotechnology Laboratory

#### Dr. Sean Doyle

The main thrust of the research work in the Biotechnology group is the further understanding, diagnosis and treatment of human and animal disease. To this end, my laboratory has established, and will continue to develop (i) a highly trained research group with key skills in the areas of protein expression/characterisation, immunotechnology and molecular biology and (ii) research contacts with the key players in the area of human disease. More specifically, my group has an ongoing interest in the mechanism of immunity against parvovirus B19 and we have been amongst the first to explore and characterise the nature of the cellular immune response against this virus. We are currently investigating, in an EU-funded project, host factors which may affect viral infectivity during infection of the pregnant woman. We are currently expressing a number of parasite antigens in the baculovirus expression system with a view to assessment of both vaccine and diagnostic potential. In addition, a number of molecular diagnostic assays to detect parvovirus B19, *E. coli* and equine herpesvirus-1 have been developed which we aim to commercialise in due course. An emerging area of interest in my laboratory, in collaboration with Dr. Kevin Kavanagh (NUI Maynooth), is the functional genomic analysis of *Aspergillus spp.* and we are currently investigating and attempting to characterise non-ribosomal peptide synthesis in this species using both molecular biological and bioinformatic approaches. Current collaborators include Dr. Bernard Mahon, Institute of Immunology, NUI Maynooth, Professor John Dalton, DCU (parasitic disease), and Dr. Kevin Kavanagh, NUI Maynooth (medical mycology in the immunocompromised person). In addition I have active collaborations with a number of Biotechnology companies including Biotrin (Dublin, Ireland), Tridelta Development Limited (NUI Maynooth and Co. Wicklow).

## Ecology Laboratory

### Professor Martin J. Downes

The work of the laboratory has to do mainly with fundamental and applied aspects of biological control of pest and pathogen populations. This includes studies of predatory mites, fungi and entomopathogenic nematodes. The objectives are to understand fundamental aspects of how genetic and geographic biotype boundaries are created and maintained, to recognise components of ecological competence, which are important in the success of biological control agents, and to find or build new organisms for better commercial biological control.

## Environmental Physiology and Behaviour Laboratory

### Dr. Christine T. Griffin

Research of this laboratory has two related foci: the behaviour and physiology of nematode parasites, and use of insect parasitic nematodes as biological pesticides.

A specialised infective juvenile transmits many nematode parasites from host to host. We are interested in the survival and infection strategies of these infective juveniles, and generally use species of insect parasitic nematode as models in this research. We are currently investigating the complex manner in which several factors interact to influence infectivity, including factors operating during development (such as resource availability) and those operating during ageing of the infective juveniles. One of our lines of investigation is into the importance of starvation as a factor modifying the foraging behaviour of infective juveniles, and also as a mortality factor for them.

The second main strand of our research is the development and utilisation of insect parasitic nematodes as biological control agents. Pest species currently targeted include pine weevil (*Hylobius abietis*) in reforestation, black vine weevil (*Otiorhynchus sulcatus*) in soft fruits, and sciarid and phorid flies in mushroom cultivation.

## Epithelial Immunobiology Laboratory

### Dr. Shirley O'Dea

As the principle organs of gas exchange in the body, the lungs are constantly exposed to the vast array of substances present in inhaled air, yet they are lined by just a single layer of epithelial cells. The main functions of the cells lining the conducting airways involve protection against harmful inhaled substances as well as warming and humidifying the air before it reaches the delicate alveolar regions where gas exchange takes place. My team is studying the lung epithelium and the signalling networks that influence its functions in health and disease.

The airway epithelium is not merely a passive barrier preventing the entry of harmful substances into the host. The cells within the epithelium carry out a range of specialised functions including detoxification of harmful substances and active defence against microorganisms as well as communicating directly with the immune and inflammatory systems. To carry out these essential functions, the epithelium must be intact and contain the appropriate subpopulations of specialised cells. Chronic exposure to harmful substances and underlying genetic factors can compromise defence and repair mechanisms in the lungs, leading to long term damage and disease.

My group is interested in interactions between the lung epithelium and its microenvironment and the ways in which lung epithelial cells, mesenchymal cells and immune and inflammatory cells modulate each other's functions in health and disease. In particular, we are interested in mechanisms of regeneration within damaged airways and we are investigating both normal repair processes and the alterations in these pathways that lead to the development of disease. We are examining the effects of signals emanating from 1. inflammatory and immune cells, 2. underlying mesenchymal cells and extracellular matrices and 3. neighbouring epithelial cells on epithelial cell proliferation and function. Understanding these signalling networks should result in the identification of potential areas for intervention strategies to prevent, treat and cure lung disease. In addition, we are examining stem and progenitor cell pathways operating within the epithelium in order to identify potential target cells for regeneration therapies, gene therapy and cancer treatments.

## Gene Flow Laboratory

### Dr. Conor V. Meade

Our main interest is developing models for the spread of genes through wild and cultivated plant populations, and the impact GM crops may have on these patterns. Currently we are investigating gene-flow in Irish populations of *Brassica rapa* L. (wild turnip), *Lolium perenne* L. (perennial ryegrass) and *Avena sativa/fatua* (cultivated and wild oats).

We use a variety of PCR-based fragment analysis techniques including microsatellites (SSRs), AFLPs and RAPDs to investigate genetic diversity, gene-flow, hybridisation and inheritance patterns in these species. Data is being generated from wild and cultivated populations and from controlled experimental crosses. Much of our work is done in collaboration with the Teagasc Crop Research Centre at Oakpark, Co. Carlow.

Other research interests include the taxonomy and systematics of the Annonaceae (Custard Apples) in South and Southeast Asia, the phytogeography of Asia and phylogenetics.

## Lymphocyte Biology Laboratory

### Dr. Derek G. Doherty

Immune recognition and successful elimination of tumours, viruses, bacteria and multicellular parasites all require distinct cell types that mediate the appropriate effector functions and regulatory mechanisms. The Lymphocyte Biology Laboratory is focused on the mechanisms by which the immune system distinguishes between harmless antigens and different types of danger, and selectively activates the appropriate effector functions. These functions appear to be controlled by multifunctional lymphocyte subpopulations, including  $\gamma\delta$  T cells, natural killer (NK) cells and natural killer T (NKT) cells that recognise common structures on target cells that signify danger and initiate immune responses. We are attempting to identify the receptors and soluble factors that control their functions and their interactions with other cells of the immune system. We have evidence that the above-mentioned cells play a crucial role in immunity against hepatitis C virus (HCV). HCV infects over 400 million people worldwide, and while about 20% of infected individuals successfully clear the virus, the majority develop chronic liver disease which appears to be mediated by the immune system. We are therefore investigating the roles of NK cells,  $\gamma\delta$  T cells and NKT cells in resolution and persistence of HCV infection as well as in healthy individuals. These studies may lead to the elucidation of mechanisms whereby the immune system distinguishes between different types of danger and may ultimately lead to the development of therapeutic strategies for the treatment of immune-mediated diseases including HCV.

## Medical Mycology Unit

### Dr. Kevin Kavanagh

Fungal pathogens are recognised as a significant cause of illness and death among patients immunocompromised as a result of disease (AIDS, cancer) or therapy (immunosuppressive therapy prior to organ transplantation). Most fungal pathogens are normal components of the body flora but in the event of an underlying disease they can become invasive and colonise many organs with deleterious consequences. In the Medical Mycology Unit we are concerned with understanding the mechanisms employed by fungi to colonise human tissue, with designing novel means of detecting fungal infection and with developing therapies to complement existing anti-fungal strategies.

The pathogenic yeast *Candida albicans* is the dominant cause of oral candidosis ('thrush') in humans. The mitochondrion is the energy producing organelle in the cell and disruption of its function may represent a novel means of reducing the ability of *C. albicans* to colonise human tissue. Our primary objective is to develop a therapy, which targets the mitochondrion, and to use this in combination with the conventional anti-fungal agents so that resistance to this latter group of agents may be overcome.

*Aspergillus fumigatus* is a filamentous fungus which is associated with a range of pulmonary diseases, a number of which can disseminate to distant sites in the body and have a mortality rate of 95%. Together with Dr. Sean Doyle (Department of Biology) we are developing novel diagnostics which will detect the presence of fungal toxins and enzymes in human blood as an early indicator of fungal infection. Our objective is to make earlier detection of fungal infection feasible so that anti-fungal therapy can be initiated with a consequent reduction in patient mortality. In addition, we have embarked on a project to selectively knock-out genes associated with the production of secondary metabolites that may have a role in tissue invasion.

Conventional anti-fungal therapy relies upon the use of a range of azole and polyene drugs. While these are effective in the majority of cases, many have reduced efficacy due a range of adverse side effects and to the advent of drug resistance among pathogenic fungi. Together with Dr. Malachy McCann (Department of Chemistry) we are assessing the efficacy of novel metal-based anti-fungal drugs with a view to their possible use in treating a range of superficial fungal infections. To date we have identified the mode of action of these drugs and established their potential for controlling the growth of fungi by acting synergistically with conventional anti-fungal drugs.

## **Molecular Phylogenetics and Systematics Laboratory**

### **Dr. Grace McCormack**

The focus of research in this laboratory is currently on the molecular evolution of HIV-1, in collaboration with the London School for Hygiene and Tropical Medicine and the Central Public Health Laboratory in London, UK. The introduction and spread of HIV-1 in the rural Karonga District (located in Malawi, a small country in central East Africa), has been monitored since 1982 as part of a large research programme are on leprosy and TB. HIV-1 prevalence has increased here from 0.1% of the population in the early 1980s to over 10% in the late 1990s. The dynamics of the HIV-1 epidemic over the twenty-year period is being studied using the latest molecular phylogenetic and population genetic techniques to give insight into changes in the HIV-1 population over time both between and within hosts and the diversity of the virus in this population. HIV-1 Subtype C accounts for over 50% of worldwide HIV-1 infection being responsible for HIV-1 epidemics in southern Africa, India and China. The prevalence of this subtype increased from 55% of cases in Karonga in the early 1980s to over 90% by the late 1980s. Why this HIV-1 subtype is spreading so successfully in the heterosexual community, in these areas, is also the focus of research.

Research into the molecular systematics of sponges, of mites of agricultural and veterinary importance, and of echinoderms is also being pursued in collaboration with other researchers.

## **Mucosal Immunology Laboratory**

### **Dr. Bernard Mahon**

Our airways are constantly exposed to foreign material and yet for the most part are maintained as a healthy, functioning system. The goal of our laboratory is to understand how microbes colonise this mucosal surface, compromise our health and how the immune system operates to return us to homeostasis. The work focuses on a fundamental question: how is the local immune response in the airways induced? Recently we have made significant advances in answering this question by identifying the biochemical signals that are involved in recruiting sentinel dendritic cells to the trachea. We have identified three mechanisms whereby respiratory pathogens corrupt this process to hinder immunity and prolong infection. The results are also giving us unexpected insights into asthma, and new mucosal vaccines. When we understand how immunity is induced, or evaded by microbes, we will be close to understanding a fundamental aspect of human biology. We will also be able to rationally devise new vaccines and medications for both respiratory infections, and indeed other conditions with an immune component such as allergies and asthma.

## Muscle Biology Laboratory

### Professor Kay Ohlendieck

The functional performance of skeletal muscle is based on refined physiological mechanisms that couple the electrical depolarisation of the surface membrane to motor protein activation, generally referred to as excitation-contraction coupling. Our laboratory focuses on the biochemical and physiological characterisation of supramolecular membrane complexes involved in the regulation and stabilisation of this relatively unique signal transduction mechanism. In mature fast fibres, direct physical coupling between the voltage-sensing receptor of the transverse tubules and the calcium release channel complex of the sarcoplasmic reticulum initiates contraction, while the energy-dependent re-uptake of calcium ions causes muscle relaxation. Using blot overlay assays with conjugated proteins, two-dimensional gel electrophoresis and chemical crosslinking and various immunochemical techniques we are characterising the role of protein-protein interactions in ion homeostasis. Muscle fibres exhibit enormous plasticity and can adapt efficiently to changes in activity by atrophy, hypertrophy and/or fibre type shifting. Employing chronic low-frequency electro-stimulation to fast fibres, we are studying the effect of the fast-to-slow transition process on isoform expression patterns of key muscle proteins. Diseases affecting muscle proteins usually have devastating consequences for the organism, i.e. muscular dystrophy or sarcopenia of old age. To elucidate the molecular pathogenesis of these diseases, we are examining naturally occurring animal models, such as the dystrophic mdx mouse. The long-term aim of our laboratory is to make major advances in the understanding of excitation-contraction coupling by focussing on the elucidation of the molecular architecture of the triad junction, the molecular cell biology and functional interactions between ion-regulatory elements and on the pathophysiology of neuromuscular diseases arising from abnormalities in calcium handling. In conjunction with two research networks funded by the European Commission, our laboratory is currently involved in a proteomics-based approach to identify all integral membrane proteins responsible for the assembly and maintenance of the junctional sarcoplasmic reticulum during myogenesis, transformation and ageing.

## Nematode Genetics Laboratory

### Professor Ann M. Burnell

Research in this laboratory is concentrated mainly on the biology and genetics of nematodes. We work on several nematode species, among them *Caenorhabditis elegans*, which is widely used as a research model in molecular genetics and whose genome has been fully sequenced; *Heterorhabditis bacteriophora* and *Steinernema carpocapsae*, parasites of insects which are commercially produced and marketed for the biological control of soil dwelling insect pests; and *Aphelenchus avenae* and *Panagrolaimus*, nematodes which are able to survive desiccation to 0% relative humidity.

One project concerns the identification of immediate/early gene transcription products in infective stage juveniles of the nematode *Heterorhabditis bacteriophora*. We have cloned over 1,000 genes which are expressed by the nematode during the early stages of insect infection by *H. bacteriophora*. This project is likely to provide information of value in the design of antihelminthic drugs and it is facilitating the construction of a molecular linkage map of *H. bacteriophora* expressed genes. In a separate project we are investigating chemoreceptor genes in *H. bacteriophora* – chemoreception is extremely important in host finding by parasites.

We are also working on an EU funded project aimed at using insect parasitic nematodes (especially *Steinernema carpocapsae*) and other biological control agents to gain a sustainable biological control of diamondback moth in China and Indonesia. The diamondback moth is a major pest of vegetable crops, especially brassicas, in tropical and subtropical areas world wide and it is now resistant to all available chemical insecticides. The work at Maynooth is aimed at developing desiccation resistant strains of *S. carpocapsae* for use in foliar applications against the diamondback moth.

Although water is essential for life, a number of organisms can enter a state of suspended animation which allows them to survive in a dry state for indefinite periods. This remarkable ability is called anhydrobiosis ('life without water'). Our project on anhydrobiosis in *Aphelenchus avenae* is being carried out with in association with the University of Cambridge and is funded by a Royal Irish Academy/Royal Society Joint Research Project and by the Leverhulme Trust, UK. In January 2003 we began a second anhydrobiosis project with the nematode *Panagrolaimus* which is funded by Science Foundation Ireland. We expect that this project will lead to the discovery of several novel genes and may ultimately lead to the development of new methods of preserving biological materials that do not normally survive drying.

In association with DevGen, a biotechnology company based in Belgium, we are involved in an EU funded research project aimed at identifying the genes responsible for the enhanced longevity phenotype of certain long lived mutant strains of the nematode *Caenorhabditis elegans*. The ultimate aim of this project is to identify homologues of these 'enhanced life maintenance genes' in humans.

## Plant Biology Laboratory

### Dr. Jacqueline M. Nugent

The research of this laboratory focuses on a number of different aspects of plant molecular biology and evolution. One of our research projects is aimed at understanding the role the plant hormone ethylene plays in regulating plant physiology and development. We are concentrating on cloning ACC synthase genes from *Antirrhinum majus* (snapdragon). Ultimately we will use a PCR-based 'reverse genetic' approach to selectively inactivate individual ethylene signalling during plant development. A long-term goal is to focus on the role of ethylene during flower development. We are also interested in understanding how plant developmental processes evolve. *Plantago lanceolata* (plantain) has regular, wind-pollinated, flowers that have evolved from irregular, animal pollinated ancestors similar to those of *Antirrhinum majus*. Three genes *cycloidea*, *dichotoma*, and *divericata* play a major role in controlling flower shape in *Antirrhinum*. We are currently investigating what role, if any, the homologues of these genes play in controlling flower shape in *Plantago*. This study should aid in the elucidation of a general model for how changes in floral shape are achieved as well as providing insight on the associated changes in pollination syndrome. A third project is aimed at characterising the mitochondrial genome of *Antirrhinum majus*. This study will address how plant organelle genomes are evolving as well as how organelle/cooperativity in the cell is evolving. The other main research area in the lab is the development of plants as model systems for the production of human and veterinary oral vaccines. We are developing the plastid as a 'factory' for the production of large amounts of recombinant antigenic proteins.

## Plant Cell Biology Laboratory

### Professor Philip J. Dix

The research in this group is directed to the *in vitro* genetic manipulation of plants through genetic transformation. The objectives are both fundamental and applied. The generation and molecular characterisation of antibiotic resistant mutants of Solanaceous plants has led to several chloroplast genetic markers which are being used for studies on segregation and recombination in chloroplast genomes, as well as functional analysis of the genes. They also provide the basis for a novel chloroplast transformation procedure developed at Maynooth. This fundamental research is carried out with tobacco (a model species), but through EU-funded projects we are extending the plastid transformation work to include other crop species, including Brassica crops (cauliflower, broccoli, oilseed rape), and to explore agriculturally useful traits, including insect and herbicide resistance, phytoremediation, and (in collaboration with J. Nugent) oral vaccine production.

Another major area of investigation is the regulation of peroxidase genes, the targeting of the gene product and its role in plant development and stress tolerance. Tobacco plants over-expressing peroxides in the cell wall (apoplast) or cytoplasm, sometimes in combination with other oxidative enzymes (oxalate oxidase), are being evaluated for changes in such developmental features as xylem production, and in resistance to abiotic (UV, temperature, high light, ozone) and biotic (insects, pathogens) stresses.

An applied research area is the improvement in shelf life and quality of vegetable crops. Cauliflower plants expressing genes for cytokinin metabolism, under control of a senescence-associated promoter showed delayed leaf ageing, and changes in nitrogen metabolism are being studied in plants expressing a bacterial asparagine synthetase gene. The role of cytokinins in development is also being explored in transgenic apple trees.

The group is experienced in a range of methods for the genetic transformation of plants, including biolistics, the shooting of DNA-coated tungsten particles directly into the plant cells.

## **Viral Immunology Laboratory**

### **Dr. Patricia Johnston**

The research interest of this group is aimed at understanding the mechanisms involved in viral pathogenesis with emphasis on modulation of the immune response by viral infection or viral antigens. A number of specific immune mechanisms together with non-specific defence mechanisms are called into play to eliminate an infecting virus. At the same time, the virus acts to subvert one or more of these mechanisms to prolong its own survival. The outcome of the infection depends on how effectively the host defence mechanisms resist the offensive tactics of the virus. A major goal of research has been to develop a better understanding of this interplay between an infectious organism or its antigenic components and the host immune response to design safer, more effective therapeutic agents and vaccines against viral disease.

As part of a collaborative EU project we are currently developing and clinically evaluating a novel bivalent vaccine against childhood respiratory viral diseases, human parainfluenzaviruses (PIV) type 3 and respiratory syncytial virus (RSV). Respiratory viruses such as RSV and PIV cause severe lower respiratory tract diseases in infants and children throughout the world. Together these two agents account for up to 30% of all hospitalisations of infants and young children for respiratory tract disease. Despite the clinical and economic importance of these infections efforts to develop an efficacious RSV or PIV vaccine have been unsuccessful to date.

In addition to applied research and vaccine development the Viral Immunology Group has a strong interest in fundamental aspects of immunity to viruses. Research has focused on possible subversion of the immune response by influenza virus. It appears that the host is severely immunosuppressed during infection with influenza virus allowing secondary bacterial infections, a consequence of which can be serious/fatal illness such as pneumonia. We have identified key viral molecules that may contribute to immunosuppression *in vitro* and in experimental animal models. Armed with this knowledge we plan to deepen our understanding of the mechanisms involved in immunosuppression by viral infection or components of viruses to further elucidate the factors involved in the induction, regulation and function of immune responses to other pathogens. Identification of molecules that modulate or regulate the immune responses has far reaching therapeutic consequences. Several debilitating syndromes such as autoimmunity, hypersensitivity and allergy result from a dysfunction of immune processes and require intervention in the form of immune regulation or suppression. Molecules from infectious agents that modulate or regulate immune processes may therefore provide more appropriate alternative or novel treatments for such conditions.

In a broader context the Viral Immunology Group aims to promote a better understanding of the basic concepts underlying viral immunology and to exploit these findings to generate innovative therapies for a range of clinical syndromes.

## RESEARCH GRANTS

'Life without water: the genetics of anhydrobiosis in nematode worms'. Royal Irish Academy/Royal Society Exchange Scheme Joint Research Project in collaboration with the University of Cambridge, UK, 2000-2002, £5,628 (Professor A.M. Burnell).

'Chemoreception and chemoreceptor genes in entomopathogenic nematodes'. HEA PRTL Cycle 1, 2000-2002, €131,826 (Professor A.M. Burnell).

'Identification and characterisation of genes controlling longevity and ageing in an animal model (the nematode *Caenorhabditis elegans*)'. The European Union, CT-1999-02071, 2000-2003, €210,600 (Professor A.M. Burnell).

'Life without water: the molecular biology of anhydrobiosis in nematodes'. The Leverhulme Trust, 2001-2004, UK£70,765 (Professor A.M. Burnell).

'An integrative strategy for the sustainable control of diamondback moth by conservation of natural enemies and application of biocontrol agents'. The European Union ICA4-CT-2001-10003, 2001-2004, €241,000 (Professor A.M. Burnell).

'The exploitation of anhydrobiotic genes for the preservation of intact proteins, cells and tissues in a dry state'. SFI Investigator Award, 2003-2006, €882,000 (Professor A.M. Burnell, Dept. of Biology and Dr. John McCaffrey, Dept. of Chemistry).

'Peroxidases in agriculture, the environment and Industry'. EU Training and Mobility of Researchers (TMR), 1998-2002, €128,000 (Professor P.J. Dix).

'The plastid factory.' EU Fifth Framework Programme – Quality of Life and Management of Living Resources, 2000-2003, €258,000 (Professor P.J. Dix).

'The effect of plastidial expression of reactive oxygen species-detoxifying enzymes on stress responses in plants'. Enterprise Ireland Basic Research Grant, 2001-2005, €126,079 (Professor P.J. Dix).

'Macrochloroplasts as a model for the study of calcium fluxes in plant cells in response to abiotic stress'. Enterprise Ireland Basic Research Grant, 2002-2005, €165,000 (Professor P.J. Dix).

'Metabolic engineering of the chloroplast for health and industry'. Science Foundation Ireland, Investigator Award, 2002-2006, €638,870 (Professor P.J. Dix).

'Characterisation of CD1-restricted T cells in the human liver'. Health Research Board Project Grant, 1999-2002, £49,164 (Dr. D.G. Doherty).

'Activation and regulation of human NKT cells'. Enterprise Ireland Basic Research Grant, 2000-2003, £57,190 (Dr. D.G. Doherty).

'The role of intrahepatic  $\gamma\delta$  T cells in immunity against hepatitis C virus'. Health Research Board Project Grant, 2001-2004, £129,260 (Dr. D.G. Doherty).

'The functional significance of diversity in human natural killer cell receptors'. Enterprise Ireland Basic Research Grant, 2002-2004, €154,044 (Dr. D.G. Doherty).

'Non-target effects of genetically-modified field crops'. Teagasc, 2000-2003, £40,000 (Professor M.J. Downes).

'Control of disease in two integrated strawberry production systems'. (FRAGRA), The Department of Agriculture, Food and Rural Development Research Stimulus Fund, 2001-2004, €220,000 (Professor M.J. Downes).

'Effects of select fungi on *Hylobius abietis*, the large pine weevil, in Sitka spruce'. Enterprise Ireland Strategic Research Grant. 2000-2002, £57,000 (Professor M.J. Downes, Dr. C.T. Griffin).

'Integrated crop management system (ICMS) for soft fruit'. Teagasc, 2000-2003, £30,000 (Professor M.J. Downes, Dr. C.T. Griffin).

'Gene-flow from cultivated Irish cereals and grasses to wild relatives' Dept of Agriculture Research Stimulus Fund, 2002-2005, €180,000 (Professor M.J. Downes, Dr. C.M. Meade).

'The role of schistosome asparaginyl endopeptidase (legumain) in haemoglobin digestion', Enterprise Ireland Basic Research Grant, 2000-2002, £63,000 (Dr. S. Doyle in collaboration with Professor J.P. Dalton, DCU).

'C-Reactive Protein: Development of a novel detection product and manufacturing process'. Enterprise Ireland Innovation Partnership Grant co-funded by Enterprise Ireland and Tridelta Development Limited, 2001-2003, €44,450 (Dr. S. Doyle).

'Human parvovirus infection: towards improved understanding, diagnosis and therapy'. European Union 5th Framework Grant Code: QLK2-CT-2001-00877, 2001-2004, €224,000 (Dr. S. Doyle).

'Determination of glutathione s-transferase expression in *Aspergillus fumigatus*'. Health Research Board Summer Studentship awarded to Ms. Sharon Boyle, 2002, €1280 (Dr. S. Doyle)

'Identification, cloning and expression of *A. fumigatus* encoded cysteine proteases'. Irish Research Council for Science Engineering and Technology (IRCSET) PhD Studentship-Embark Initiative awarded to Ms. Imelda Vickers, 2002-2005, €57,150 (Dr. S. Doyle).

'The role of peptidases in the regulation of neurotransmission signalling in the parasitic helminths *Fasciola hepatica* and *Schistosoma mansoni*'. Health Research Board North-South Grant, 2003, £213,900 (Dr. S. Doyle in collaboration with Professor J.P. Dalton, DCU and Professor D.W. Halton/Dr. A. Maule, QUB).

'Novel tests for the *in vitro* detection of *Aspergillus* infection in humans and animals'. Enterprise Ireland Strategic Research Grant, 2000-2002, £83,000 (Dr. S. Doyle and Dr. K. Kavanagh, in collaboration with Dr. P. Kavanagh, TCD).

'NUI Maynooth Daniel O'Connell PhD Fellowship awarded to Ms. Claire Neville'. 2000-2003, £21,000 (Dr. S. Doyle, Dr. K. Kavanagh).

'National Institute of Cellular Biotechnology'. PRTL Cycle 3 funding with DCU and ITT, 2002-2007, €1,600,000 (Dr. S. Doyle, Dr. K. Kavanagh).

'Novel immunodiagnosics for the detection of *Aspergillus* infection'. Enterprise Ireland Advanced Technologies Research Programme (ATRP) Grant, 2001-2004, €256,540 (Dr. S. Doyle, Dr. K. Kavanagh, in association with Professor M. Clynes and Dr. E. Moran, DCU).

'Infectivity in insect-killing nematodes'. HEA PRTL Cycle 1, 2000-2002, £103,821 (Dr. C.T. Griffin).

'Pesticide reduction in mushroom cultivation in Europe', EU Craft, 2002-2004, €144,303 (Dr. C.T. Griffin).

'Nematodes for control of phorid flies in mushroom cultivation'. Teagasc Walsh Fellowship, 2002-2005, €55,000 (Dr. C.T. Griffin).

'Virus variants and host immune responses in the resolution and progression of chronic liver disease following hepatitis C infection'. Health Research Board Hepatitis C Unit Grant, 1997-2002, £741,972 (Dr. J. Hegarty, Dr. D. Kelleher, Dr. W. Hall, Dr. C. O'Farrelly, Dr. D.G. Doherty).

'Role and mechanism of immunomodulation by Haemagglutinin (HA) from Influenza Virus in the predisposition to bacterial disease during influenza infection'. HRB fellowship to fund undergraduate summer studentship. Health Research Board, 2002, €1,500 (Dr. P. Johnson).

'Novel intranasal vaccines'. European Union, 2002-2005, €240,000 (Dr. P. Johnson).

'An investigation of the role of bacterial and *Demodex* associated antigens in the induction of Rosacea'. National Rosacea Society, (USA), 2000-2004, \$46,700 (Dr. K. Kavanagh).

'Design, synthesis, purification and evaluation of pharmaceuticals as chemotherapeutics and anti-microbials'. Higher Education Technology Accreditation Council (HETAC) - Strand 3. ITT, DIT & NUI Maynooth, 2002-2006, €317,000 (Dr. K. Kavanagh).

'Mucosal immunology of the respiratory tract'. Health Research Board/Wellcome Trust New Blood Lectureship Grant, 1998-2003, UK£298,000 (Dr. B. P. Mahon).



'Role of the chemokine CCL28 in respiratory disease'. Health Research Board Research Project Grant, 2001-2004, €120,000 (Dr. B. P. Mahon).

'Use of siRNA as novel immunomodulators'. Enterprise Ireland Basic Research Grant, 2002-2004, €148,000 (Dr. B.P. Mahon).

'The role of human CCL28 in asthma'. Host laboratory to IRCSET Scholar Mary O'Gorman. Irish Research Council for Science Engineering and Technology, 2002-2005, €40,000 (Dr. B.P. Mahon).

'Adaptive Evolution in Protein-coding genes of Pathogenic Microorganisms'. Health Research Board (RP124/2000), 2000-2003, £48,500 (Dr. J.O. McNerney).

'The Institute for Biopharmaceutical Sciences'. Higher Education Authority (HEA PRTLII II), 2000-2003, £200,000 (Dr. J.O. McNerney).

'Sequence variation, lateral gene transfer and adaptive evolution in the meningococcal and *Gonococcal neisseriae*'. Enterprise Ireland Project Grant, 2001-2004, £77,000 (Dr. J.O. McNerney).

'Large piece of equipment grant'. (This grant has been awarded to support research and teaching in Bioinformatics at NUI Maynooth). Higher Education Authority, 2002, €189,000 (Dr. J.O. McNerney).

'Probiotic genomes initiative'. Higher Education Authority (HEA PRTLII III) (in collaboration with NUI Cork), 2002-2005, €150,000 (Dr. J.O. McNerney).

'EMBO workshop at NUI Maynooth'. European Molecular Biology Organisation (EMBO), April 2003, €25,000, (Dr. J.O. McNerney).

'An analysis of adaptive evolution in the malaria parasite *Plasmodium falciparum*'. Host Laboratory to IRCSET Scholar Gayle Philip. Irish Research Council for Science, Engineering and Technology, 2002-2005, €60,000 (Dr. J.O. McNerney).

'NUI Maynooth Daniel O'Connell PhD Fellowship awarded to Ms. Rhoda Kinsella'. 2001-2004. £30,000. (Dr. J.O. McNerney).

'Collection and genetic characterisation of semi-wild populations of *Lolium perenne*'. Dept. of Agriculture, 2002-2004, €16,000 (Dr. C.M. Meade).

'Evolution of mitochondrial protein genes in *Antirrhinum majus*: Cellular location and developmental expression patterns'. Enterprise Ireland Basic Research Grant, 1999-2002, £52,194 (Dr. J. Nugent).

'Plant based vaccines'. Irish Higher Education Authority Programme for Research in Third Level Institute Funding, 2000-2002, £111,119 (Dr. J. Nugent).

'The Plastid Factory'. EU 5th Framework Programme – Quality of Life and Management of Living Resources, 2000-2003, £151,000 (Dr. J. Nugent).

'Determination of stem cell and differentiation pathways within the lung epithelium'. Science Foundation Ireland Investigator Programme Grant, 2002-2006, €653,089 (Dr. S. O'Dea).

'Analysis of halothane-induced oligomerisation of the ryanodine receptor and associated calcium-regulatory proteins in normal and malignant hyperthermia-susceptible muscle, heart and brain tissues', Health Research Board, 1999-2002, €68,000 (Professor K. Ohlendieck).

'Isoform expression and oligomerisation of calcium-regulatory muscle proteins during low-frequency stimulation', Enterprise Ireland Basic Research Grant, 1999-2002, €60,000 (Professor K. Ohlendieck).

'Investigation on the mechanisms for maintenance and regeneration in the ageing muscle: development of guidelines, diagnostic tools and a view to therapies'. European Commission, 5th Framework Programme', 1999-2003, €165,000 (Professor K. Ohlendieck)

'Influence of motor innervation on the oligomeric status of the nicotinic acetylcholine receptor and associated components at the neuromuscular junction', Health Research Board, 2000-2003, €84,000 (Professor K. Ohlendieck).

'Development of a two-dimensional electrophoretic system for the rapid differential diagnosis for inherited muscular dystrophies', Enterprise Ireland Basic Research Grant, 2000-2003, €79,000 (Professor K. Ohlendieck).

'Molecular pathogenesis of calcium-regulatory membrane complexes in dystrophic fibres from mdx heart and diaphragm', Health Research Board, 2001-2004, €160,000 (Professor K. Ohlendieck).

'Identification of novel therapeutic targets in dystrophic muscle fibres'. Muscular Dystrophy Ireland, 2002-2005, €22,000 (Professor K. Ohlendieck).

'Proteomics analysis of adult skeletal muscle fibre transformation, a neurobiological model system of electro-stimulation therapy', Health Research Board, 2002-2005, €150,000 (Professor K. Ohlendieck).

'Excitation-contraction coupling and calcium signalling in health and disease', European Commission, 5th Framework Research and Training Programme 'Improving the human research potential and the socio-economic knowledge base', 2002-2006, €167,000 (Professor K. Ohlendieck).

'Sex and mortality factors in entomopathogenic nematodes (SEXMORT)'. IRCSET Basic Research Grant, 2002-2005, €164,000 (Mr. A. Rolston, Professor M.J. Downes).

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C.J. Armit, **S. O'Dea**, A.R. Clarke and D.J. Harrison. Absence of p53 in lung epithelial cells favours multinucleation and loss of cell cycle arrest. *BioMed Central Cell Biology* **3**, 27 (2002).

M. Brennan, D.Y. Thomas, M. Whiteway and **K. Kavanagh**. Analysis of *Candida albicans* virulence in *Galleria mellonella* larvae. *FEMS Immunology and Medical Microbiology* **34**, 153-157 (2002).

J. Browne, A. Tunnacliffe and **A. Burnell**. Plant desiccation gene found in nematode. *Nature* **416**, 38 (2002).

B. Byrne, L. Madrigal-Estebas, A. McEvoy, J. Carton, **D.G. Doherty**, D. O'Donoghue and C. O'Farrelly. Human duodenal epithelial cells constitutively express molecular components of antigen presentation but not costimulatory molecules. *Human Immunology* **63**, 977-986 (2002).

B. Coyle, **K. Kavanagh**, M. McCann, M. Devereux and M. Geraghty. Mode of anti-fungal activity of 1,10-phenanthroline and its Cu(II), Mn(II) and Ag(I) complexes. *Biometals* **16**, 321-329 (2003).

C.J. Creevey and **J.O. McInerney**. An algorithm for detecting directional and non-directional positive selection, neutrality and negative selection in protein coding DNA sequences. *Gene* **300**, 43-51 (2002).

C.J. Creevey and **J.O. McInerney**. CRANN: A program for detecting adaptive evolution in protein-coding DNA sequences. *Bioinformatics* (in press).

K. Culligan, N. Banville, P. Dowling and K. **Ohlendieck**. Drastic reduction of calsequestrin-like proteins and impaired calcium binding in dystrophic mdx muscle. *Journal of Applied Physiology* **92**, 435-445 (2002).

M.P. Cummings, **J.M. Nugent**, R. Olmstead and J.D. Palmer. Molecular and phylogenetic analysis reveals five, and implies many more, independent transfers of the chloroplast gene *rbcl* to the mitochondrial genome in angiosperms. *Current Genetics* (in press).

A. Czaja, **D.G. Doherty** and P.T. Donaldson. The genetic bases of autoimmune hepatitis. *Digestive Diseases and Sciences* **47**, 2139-2150 (2002).

P. Daly, T. Collier and **S. Doyle**. PCR-ELISA detection of *Escherichia coli* in milk. *Letters in Applied Microbiology* **34**, 222-226 (2002).

P. Daly, A. Corcoran, **B.P. Mahon** and **S. Doyle**. High sensitivity PCR detection of parvovirus B19 in plasma. *Journal of Clinical Microbiology* **40**, 1958-62 (2002).

- P. Daly and **S. Doyle**. Development of a Competitive PCR-ELISA for the detection of equine herpesvirus-1 (EHV-1). *Journal of Virological Methods*. (in press).
- P. Daly and **K. Kavanagh**. Immobilisation of *Aspergillus fumigatus* colonies in a soft agar matrix allows visualisation of A549 cell detachment and death. *Medical Mycology* **40**, 27-33 (2002).
- O. Deegan, K. Walshe, **K. Kavanagh** and **S. Doyle**. Quantitative detection of c-reactive protein using phosphocholine-labelled enzyme or microspheres. *Analytical Biochemistry*. (in press).
- T. Deignan, M.P. Curry, **D.G. Doherty**, L. Golden-Mason, S. Norris, N. Nolan, O. Traynor, G. McEntee, J.E. Hegarty and C. O'Farrelly. Decrease in hepatic CD56+ T cells and Va24+ natural killer T cells in chronic hepatitis C viral infection. *Journal of Hepatology* **37**, 101-108 (2002).
- C.M. Dempsey and **C.T. Griffin**. Infectivity and behaviour of exsheathed and ensheathed *Heterorhabditis megidis* infective juveniles. *Nematology* **5**, (in press).
- C.M. Dempsey and **C.T. Griffin**. Phased activity in *Heterorhabditis megidis* infective juveniles. *Parasitology* **124**, 605-613 (2002).
- K.M. Dolan, J.T. Jones and **A.M. Burnell**. Detection of changes occurring during recovery from the dauer stage in *Heterorhabditis bacteriophora*. *Parasitology* **125**, 71-81 (2002).
- P. Dowling, K. Culligan and **K. Ohlendieck**. Distal mdx muscle groups exhibiting up-regulation of utrophin and rescue of dystrophin-associated glycoproteins exemplify a protected phenotype in muscular dystrophy. *Naturwissenschaften* **89**, 75-78 (2002).
- P. Dowling, J. Lohan and **K. Ohlendieck**. Comparative analysis of Dp427-deficient mdx tissues shows that the milder dystrophic phenotype of extraocular and toe muscle fibres is associated with a persistent expression of  $\beta$ -dystroglycan. *European Journal of Cell Biology* (in press).
- M. Ellabib, M. Agaj, Z. Khalifa and **K. Kavanagh**. *Trichophyton violaceum* as an important cause of tinea capitis in children in Tripoli (Libya): Results of a two year survey. *Mycopathologia* **153**, 145-147 (2002).
- M. Ellabib, M. Agaj, Z. Khalifa and **K. Kavanagh**. Yeasts of the genus *Candida* are the dominant cause of onychomycosis in Libyan women but not men: Results of a two year surveillance study. *British Journal of Dermatology* **146**, 1038-1041 (2002).
- M.S. Ellabib, Z. Khalifa and **K. Kavanagh**. Dermatophytes and other fungi associated with skin mycoses in Tripoli, Libya. *Mycoses* **45**, 101-104 (2002).
- M.S. Ellabib, A. Refaai, Z. Khalifa and **K. Kavanagh**. Isolation and identification of *Madurella mycetomatis* from two cases of Black grain Mycetoma in Libya. *Mycoses* (in press).
- M.R. Enright, **J.O. McInerney** and **C.T. Griffin**. Characterization of endospore-forming bacteria associated with entomopathogenic nematodes, *Heterorhabditis* spp., and description of *Paenibacillus nematophilus* sp. nov. *International Journal of Systematic and Evolutionary Microbiology* **53**, 435-441 (2003).
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- L. Glover, S. Quinn, M. Ryan and **K. Ohlendieck**. Supramolecular calsequestrin complex. *European Journal of Biochemistry* **269**, 4607-4616 (2002).
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- B. Hass, **M.J. Downes** and **C.T. Griffin**. Persistence of four *Heterorhabditis* spp. isolates in soil: role of lipid reserves. *Journal of Nematology*, **34**, 151-158, (2002).

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- O. Zachariadis, J.P. Cassidy and **B.P. Mahon.** 'Unconventional T populations in the respiratory tract play a non-redundant role in the early immune response to *B. pertussis*'. *Joint Congress of the British Society for Immunology and the British Society for Allergy and Clinical Immunology*, Harrogate, UK (3-6 December, 2002). *Immunology* **107** (Suppl 1) 117 (2002).

## EXTERNAL ASSIGNMENTS AND PUBLIC SERVICE

### Professor A.M. Burnell

- Member of the Senate of the National University of Ireland 2002-2007.
- Member of the Irish Research Council for Science, Engineering and Technology 2001-2005.
- Proposer and Chairman of the EU Concerted Action in Science and Technology COST 850 'Biocontrol Symbioses' 2001-2006.
- Reviewer for the following journals: *Genome*, *Nematology*, *Parasitology* and *FEMS Microbiology Reviews*.
- Reviewer of research projects for the BBSRC [Biotechnology and Biological Sciences Research Council, UK] and The Wellcome Foundation.

### Professor P.J. Dix

- External examiner of PhD thesis, University of Wales at Aberystwith.
- Evaluator of Interim and Final Reports for EU 4th and 5th Framework projects.
- Evaluator of Marie Curie Fellowships for EU 5th Framework.
- Member of evaluation panel for 'Expressions of Interest' to compile the Work Programme for the EU 6th Framework.
- Member, Food Safety Authority of Ireland Sub-committee on GMOs and Novel Foods.

### Dr. D.G. Doherty

- Reviewer for the following journals: *Journal of Hepatology*, *Immunology*, *Clinical and Experimental Immunology*, *Biomed Central Immunology*, *Gastroenterology* and *European Journal of Gastroenterology and Hepatology*.
- Committee Member, Immunology, Pathology and Mechanisms of Disease Committee of the Health Research Board.
- Secretary, Irish Society for Immunology.
- Member, British Society for Immunology, American Association of Immunologists.

### Dr. B. Dowds

- Reviewer for the following journals: *Microbiology*, *Cellular Microbiology* and *Journal of Invertebrate Pathology*.
- Member, American Society for Microbiology, Society for General Microbiology.

### Professor M.J. Downes

- Convenor of COST 850 Biocontrol Symbioses Working Group 4.
- National Representative on the European Working Group on Integrated Pest Management.
- Joint Promoter, Ceide Fields Project – Biology.
- Joint Promoter, Belderrig Institute Project – Biology.
- Member of the Advisory Board of CAB International Training.
- NUI Representative, Second Level Biology Examinations.
- Member of the *ad hoc* Committee which established the Agri-Food Biotechnology Society.
- Member of the Scientific Advisory Board, Forest Protection Centre of Excellence, Forest Research Institute, Warsaw.

**Dr. S. Doyle**

- Reviewer of research projects for the following: Enterprise Ireland ATRP Programme, Innovation Fund Programme, Innovation Partnership Programme and Health Research Board Research Project Grants - Microbiology Panel.
- Committee member of Irish Area Section of the Society of General Microbiology.
- Member of the Irish Medicines Board (IMB) expert panel concerning *in vitro* Diagnostic Medical Devices.
- Reviewer for the following journals: *Journal of Food Microbiology* and *Clinical Infectious Diseases*.

**Dr. C.T. Griffin**

- External examiner of PhD thesis, University of Reading.
- Visiting Professor on International Course on Insect Pathology, Ciudad Victoria, Mexico.
- Vice Chairwoman, COST 850, Biocontrol Symbioses (A framework for R&D collaboration Europe).
- Member of Management Committee, COST E12, Bark and Wood Boring Beetles (A framework for R&D collaboration in Europe).
- Reviewer of research projects for the following granting agencies: DEFRA (UK) and BARD (US-Israel).
- Reviewer for the following journals: *BioControl*, *Nematology* and *Biocontrol Science and Technology*.

**Dr. P. Johnson**

- Co-ordinator of research project short-listed for the Health Research Board Watts Medal Award.
- Committee member of the Irish Society for Immunology.

**Dr. K. Kavanagh**

- Member, National Commission for Microbiology, Royal Irish Academy, (1996-2002).
- Institute of Biology of Ireland, (Vice-Chairperson 2001-).
- Referee for the following journals: *Enzyme and Microbial Technology*, *Cytotechnology*, *FEMS Microbiology Letters*, *Microbiology*, *Pharmacy and Pharmacology Communications*, *British Journal of Biomedical Science*, *Journal of Pharmacy and Pharmacology* and *Microbes and Infection*.
- Examiner of PhD thesis, School of Pharmacy, Queen's University of Belfast.
- Examiner of PhD thesis, Dublin Dental Hospital, Trinity College Dublin.

**Dr. B.P. Mahon**

- Reviewer of research projects for the following: Irish Health Research Board: Microbiology panel, basic research grant scheme, panel member; Immunology and pathology panel, basic research grant scheme, panel member; Enterprise Ireland, Advanced Technology Research Fund (ATRF) and British Biotechnology and Biology Science Research Council (BBSRC).
- Committee Member, The Royal Irish Academy National Committee for Biochemistry.
- Editorial Board *Modern Aspects of Immunobiology*.
- Reviewer for the following journals: *Journal of General Virology*, *Vaccine*, *Clinical and Experimental Immunology*, *Immunology* and *Nature Publishing group*.
- Academic Representative, Health Research Board meeting with the Expert group from the Welsh Universities on *Research Impacts on the Irish Economy*.

**Dr. J.O. McInerney**

- Reviewer for the following journals: *Genome Biology*, *Nucleic Acids Research*, *Gene*, *Zoologica Scripta*, *Memoirs of the Queensland Museum*, *Molecular Biology and Evolution*, *Heredity*, *SGM Quarterly*, *Microbiology Today*, *Proceedings of the Royal Society of London (Biology Series)*, *Journal of the Science of Food and Agriculture*, *International Journal for Parasitology* and *Journal of Molecular Evolution*.
- Reviewer of Research Projects for the Health Research Board Genomics, Proteomics and Human Diseases panel.
- Lecturer at Instituto Saude Publica, São Paulo, Brazil. *Molecular Systematics and Evolution*, 28 Jan–1 Feb 2002.
- Principal lecturer at Centre for Scientific Computing (CSC), Helsinki, Finland. *Computational Phylogenetics Course*, 25–29 April 2002.
- Principal lecturer at the Instituto Gulbenkian de Ciencia, Oieras, Portugal. *Bioinformatic Analysis of DNA and Protein Sequences*, 7-11 October 2002.
- Examiner of MSc thesis, University College Cork.

**Dr. J. Nugent**

- Reviewer of Enterprise Ireland Basic Science Research Grant Scheme 2002.
- External Examiner of MSc Thesis, Genetics Dept., Trinity College Dublin.
- Member of the Scientific Advisory Board of the European Plant Genomic Meeting, Berlin, 2002.
- Committee member of the Irish Research Scientists Association.

**Professor K. Ohlendieck**

- Member of the Neuroscience Committee of the Health Research Board.
- Member, Editorial advisory board of the scientific journal '*Basic and Applied Myology*' (Unipress, Pavia, Italy).
- Reviewer for the following journals: *American Journal of Pathology*, *Brain Research*, *Cellular and Molecular Life Sciences* and *Journal of Applied Physiology*.
- Reviewer of Research Projects for the following funding agencies: Italian Telethon for muscular dystrophy and French Muscular Dystrophy Association.
- Symposium Co-Chair at the '5th International Symposium on Molecular Medicine' in Hersonissos, Crete (10-12 October, 2002).
- HEA-funded exchange visit for third level educators, Max-Planck Institute for Molecular Genetics, Berlin, Germany (19-21 August, 2002).
- Committee member of the Irish Area Section of the Biochemical Society.
- Member, American Society for Biochemistry and Molecular Biology, American Society for Cell Biology, Biochemical Society, UK, British Society for Cell Biology.

**CONFERENCES HOSTED**

**Dr. J.O. McInerney**, 4th NUI Maynooth International Bioinformatics Summer School (24-28 June, 2002).

**Dr. J. Nugent**, **Dr. P. Dix**, Dr. E. Kane and Dr. G. Nugent. *Irish Botanists Meeting*, NUI Maynooth (3-5 April 2002).



**Faculty of Science**

**Research Report 2002**

**Chemistry**



# CHEMISTRY

## ACADEMIC STAFF\*

**Professor C.M. Quinn**, BSc (QUB), MA (Oxford), PhD (QUB), DSc (Birmingham), MRIA (1977-)  
**Dr. J.M. Briody**, BSc (London), PhD (London) (1978-)  
**Dr. M. McCann**, BSc (UUC), PhD (QUB) (1983-)  
**Dr. C.B. Breslin**, BSc, PhD (1990-)  
**Dr. M.F. Heaney**, BSc (QUB), PhD (QUB) (1999-)  
**Dr. J.P. Lowry**, BSc, PhD (1998-)  
**Dr. J.G. McCaffrey**, BSc, PhD (Toronto) (1991-)  
**Dr. A.D. Rooney**, BSc (QUB), PhD (QUB) (1994-)

## POST-DOCTORAL FELLOWS

**Dr. D. Bannerman**, BSc (Bristol), PhD (Edinburgh) (1995-)  
**Dr. A.M. Fenelon**, BSc, PhD (1999-)

## TECHNICAL STAFF

**Ms. A. Cleary**, BSc (1990-)  
**Ms. B. Coleman**, BSc (1995-)  
**Ms. R.G. Collery-Walsh**, MIOSH (1978-)  
**Dr. K. Maddock**, BSc, PhD (1994-)  
**Mr. N. Williams**, BSc (DCU), MEng (DCU) (1997-)  
**Ms. B. Woods**, BSc (QUB) (2001-)

## EXECUTIVE ASSISTANT

**Ms. O. Redmond** (2002-)

## POSTGRADUATE RESEARCH STUDENTS

**Ms. S. Abuskhuna**, BPharm (Al Fateh University, Tripoli, Libya) (2002-)  
**Ms. B. Alcock**, BSc (2002-)  
**Mr. A. Al-Gawari**, BSc (Sebha University, Libya) (2002-)  
**Mr. F. Bass**, BSc (RTC, Waterford) (1997-)  
**Mr. F. Bolger**, BSc (2002-)  
**Mr. F. Brown**, BSc (1999-)  
**Mr. M. Collier**, BSc (2000-)  
**Mr. K. Conroy**, BSc (1999-)  
**Mr. B. Coyle**, BSc (2000-)  
**Ms. M. Dalton**, BSc (1999-)  
**Mr. K. Doyle**, BSc (1998-)  
**Mr. S. Dunne**, BSc (1999-)  
**Mr. S. Earley**, BSc (2001-)  
**Ms. S. Farrell**, BSc (2000-)  
**Ms. J. Fenlon**, BSc (1998-)  
**Ms. M. Gallagher**, BSc (2000-)  
**Ms. J. Jago**, BSc (2002-)  
**Ms. E. Lawless**, BSc (2000-)

\* Unless otherwise stated the higher degrees listed are those of the National University of Ireland.

**Mr. T. McCarthy**, BSc (1999-)

**Mr. I. McColgan**, BSc, HDipEd (2000-)

**Ms. C. O'Brien**, BSc (2000-)

**Ms. M. Quigley**, BSc (2001-)

**Ms. S. Reilly**, BSc (2000-)

**Ms. E. Sheridan**, BSc (2001-)

**Ms. K. Uhlemann**, BSc (2002-)

## HEAD OF DEPARTMENT'S REVIEW OF THE YEAR

The strong commitment of the Department of Chemistry at NUI Maynooth to research and the training of postgraduate students in research methodology is evident again in this review of the academic year 2002-03. A number of peer-reviewed research papers have been published in the important international journals. Staff members have been invited to present the results of their research at major international conferences frequently.

Once again, the department has attracted considerable research funding from outside agencies, to support the research of the different research groups. One award, in particular, merits especial mention. Dr. J.G. McCaffrey together with his colleague, the Dean of Science, Professor Burnell, made a successful application for more than €882,000. In total, some €3,000,000 in research funding has been awarded for the period 2002–2005.

Four postgraduate students, Ms. Anna Fenelon, Ms. Margaret Quigley, Ms. Julie Fenlon and Mr. Ross Fitzgerald completed their postgraduate education. Ms. Fenelon and Ms. Fenlon were awarded PhD degrees, while Ms. Quigley and Mr. Fitzgerald completed MSc degrees at the beginning of this academic year.

Two staff members, apart from their hard work in undergraduate and postgraduate education and the management of their research groups, found time to add to the departmental family. Congratulations to Frances Heaney and Denise Rooney on the birth of their daughters Sinéad and Claire.

## RESEARCH INTERESTS OF STAFF

### Dr. C.B. Breslin

Research in the Electrochemistry and Corrosion Science laboratory ranges from fundamental studies on electrochemical processes to fundamental and applied studies on processes that occur during the corrosion of metals, alloys and coated surfaces. Ongoing projects in the group include studies on electropolymerization, which is used in the synthesis of conducting polymer films and coatings, electrochemical, photoelectrochemical and spectroelectrochemical characterisation of conducting polymers, and the doping of these conducting polymers for applications in electrocatalysis, electrochromic devices, biomedical materials and corrosion protection. In addition, we are investigating the electrosynthesis of chiral electrodes that are capable of recognising and discriminating between the enantiomers of potential drugs.

### Dr. J.M. Briody

Dr. Briody's research interests are focused on the following topics: the development of synthetic pathways for the production of combinatorial libraries of substituted imidazoles for evaluation as drug precursors; the use of derivatives of imidazole as chiral auxiliaries in asymmetric synthesis and analytical chemistry and the synthesis and application of novel ionic liquids.

### Dr. M.F. Heaney

Dr. Heaney's research interests lie in the field of synthetic and mechanistic organic chemistry, she is especially interested in heterocyclic chemistry. She has been studying the generation of new 1,3-dipoles and their cycloaddition reactions for the synthesis of novel and unusual ring systems containing nitrogen and oxygen atoms. The mechanistic aspects of this chemistry form an important aspect of ongoing research.

### Dr. J.P. Lowry

Research in the Bioelectroanalysis Laboratory (Sensors Development Unit & Neurochemistry Research Unit) focuses on the development, characterisation and direct application of sensor and biosensor systems for biomedical research. The Sensors Development Unit now has four graduate students working on the design, development and characterisation of microelectrochemical sensors for various biologically important species including glucose, lactate, glutamate and nitric oxide. The Neurochemistry Research Unit, in which these devices are used directly in fundamental physiological research on the mammalian brain, was granted its site licence for *in vivo* experimentation in October 1999. The Department of Chemistry at NUIM is thus the only such department in the country to hold a site licence.

#### **Dr. M. McCann**

Research is conducted on the design, synthesis and biological testing of new transition metal complexes. Emphasis is placed on complexes that may exhibit bioactivity and, thus, are potential candidates for new pharmaceutical drugs. The activities of complexes are assessed for their ability to inhibit the growth of pathogenic microbes, such as the yeast *Candida albicans* and the bacterium *Escherichia coli*. New compounds are required in this area in order to combat problems where the microbes are acquiring increased resistance to the current prescription drugs. *In vitro* testing has revealed that a number of our new complexes have marked antimicrobial activity. In addition, several of the new metal complexes have also demonstrated marked activity, *in vitro*, against a number of cancer cell lines.

#### **Dr. J.G. McCaffrey**

Time-resolved, optical luminescence spectroscopy of matrix-isolated metal atoms is used to examine the behaviour of these elementary solid state systems, i.e., guest atoms isolated in the face-centered-cubic, solid rare gas hosts. This experiment has its origins in measurements conducted since 1993 by the Maynooth research group at the Synchrotron Radiation (SR) laboratory HASYLAB at DESY in Hamburg. Theoretical work done on the luminescence spectroscopy of atomic zinc isolated in the solid rare gases (Zn/RG) based on the use of sums of diatomic Zn·RG pair potentials for a Zn·RG<sub>18</sub> cluster species, has allowed identification of the vibrational modes dominating emission in the solid state. In the spectral simulations the potential energy surfaces of the Jahn-Teller active vibrational modes of the <sup>1</sup>P<sub>1</sub> state of atomic Zn isolated in the solid rare gases Ar, Kr and Xe have been calculated using spectroscopically determined Zn·RG interaction potentials. A recent collaboration with Dr. Claudine Crepin at the CNRS, Orsay France has utilised molecular dynamics calculations to simulate isolation of species in low temperature solids. FTIR and fluorescence techniques are being utilised in spectroscopic studies of proteins in sugar glasses to establish their stability with respect to anhydrobiosis. This work is being done in collaboration with Professor Ann Burnell, Department of Biology NUI Maynooth. Collaborative research is also being carried out with the following researchers: Professor W.H. Breckenridge, Chemistry Department, University of Utah, Salt Lake City, Utah, USA; Dr. C. Crepin, Laboratoire de Photophysique Moléculaire du CNRS, Orsay, France and Dr. B. Soep, Laboratoire Francis Perrin, CEA, Saclay, France.

#### **Professor C.M. Quinn**

Research continues into aspects of cluster and electronic structure problems. In collaboration with his long standing collaborators Patrick Fowler at Exeter and David Redmond at NUI Maynooth, Professor Quinn has devoted much of his research effort in this past year to the completion of Volume II in his series on Computation Quantum Chemistry. This second volume will provide those in research who need to apply Group Theory to Chemistry problems with an interactive 'calculator', which returns an extensive range of results based only on the input of structural details. This second volume will be published by Elsevier – Academic Press in 2004.

#### **Dr. A.D. Rooney**

Research continues into time-resolved spectroscopic and low-temperature matrix isolation studies on transient intermediates involved in the reaction mechanisms of organometallic complexes. In order to utilise the synthetic capabilities of organometallics to an even greater extent it is essential to gain a better understanding of how they act as catalysts or synthetic reagents. To achieve this it is necessary to determine what intermediates occur along the reaction pathway. Ongoing research projects can be divided into three sections; (1) the study of charge-transfer interactions between Lewis acids and organometallic complexes, (2) the study of the photochemical reactions of metal carbenes with respect to their ability to act as reagents for the formation of cyclic organic compounds and (3) the development of chromium complexes as catalysts for alkene polymerization.

## RESEARCH GRANTS

'Corrosion protection using conducting polymer films'. Enterprise Ireland Research Innovation Grant, 2002-04, €127,010 (Dr. C.B. Breslin).

'Chiral conducting polymers: electrosynthesis, characterization and enantioselective catalytic activity'. Enterprise Ireland Basic Science Research Grant, 2001-04, €89,280 (Dr. C.B. Breslin).

'A study on the inclusion of HAP particles into conducting polymer films on orthopaedic implant materials'. Health Research Board, 2001-04, €93,700 (Dr. C.B. Breslin and Dr. J.P. Lowry).

'Studies on dynamic localised corrosion phenomena using a scanning vibrating electrode technique'. Enterprise Ireland Basic Science Research Grant, 1999-2002, €110,566 (Dr. C.B. Breslin).

Analytical Grand Prix Final: Runner-up Prize. Royal Society of Chemistry, 2002-2004, €1,275 (Dr. J.P. Lowry).

'The role of astrocytes in brain energy metabolism'. Health Research Board Research Project Grant - Neuroscience, 2002-2005, €124,728 (Dr. J.P. Lowry).

'Functional dissociations within the hippocampus'. The Wellcome Trust Research Project Grant, 2001-2004, €397,021 (Dr. J.P. Lowry and J.N.P. Rawlins, University of Oxford).

'*In vivo* voltammetry: The development of biosensors for real-time *in vivo* monitoring'. NUI Maynooth New Investigator Award, 2000-2002, €5,079 (Dr. J.P. Lowry).

'Time resolved luminescence study of the motion of atoms in low temperature solids', Enterprise Ireland Basic Research Grant, 1998-2001, €123,165 (Dr. J.G. McCaffrey).

'A pair-potentials study of the solvation of atomic mercury in solid rare gases', NUI Maynooth, Research Enhancement Fund, 2001-2004, €26,000 (Dr. J.G. McCaffrey).

'Life without water – gene discovery and functional analysis of anhydrobiosis in nematodes', SFI Investigator programme, 2002-2006, €882,050 (Dr. J.G. McCaffrey and Professor A.M. Burnell, Dept of Biology NUI Maynooth).

Member of the Pharma Research & Development Team centered in the Institute of Technology Tallaght and founded in 2002. 2003-2006, funding €317,000 to TIT (Dr. M.McCann).

'Organometallic complexes containing alkyne chains: novel non-linear optical materials', Enterprise Ireland Basic Research Grant, 2000-2003, €91,440 (Dr. A.D. Rooney).

'Ruthenium and rhodium carbenes; defined catalysts for alkene metathesis', Enterprise Ireland Basic Research Grant, 2000-2003, €51,308 (Dr. A.D. Rooney).

## PUBLICATIONS IN REFEREED JOURNALS

V. Amir-Ebrahimi, J.G. Hamilton, J. Nelson, J.J. Rooney, **A.D. Rooney** and C.J. Harding. 'Free radical forming activity of the Grubbs catalyst and related organometallics' *Nato Science Series II: Mathematics, Physics and Chemistry Kluwer Press*, **56**, 217-226 (2002).

K.G.Conroy and **C.B. Breslin**. The electrochemical deposition of polyaniline at pure aluminium: Electrochemical activity and corrosion protection properties. *Electrochimica Acta* (in press).

B. Coyle, K. Kavanagh, **M. McCann**, M. Devereux and M. Geraghty. Mode of anti-fungal activity of 1, 10-Phenanthroline and its Cu(II), Mn(II) and Ag(I) Complexes. *BioMetals*, (in press).

B. Coyle, **M. McCann**, V. McKee and M. Devereux. Synthesis and X-ray crystal structure of a tetracyclic gem-cis-bis(aminal) formed from N,N'-bis(2-aminophenyl)ethylenediamine and 1,10-phenanthroline-5,6-dione. *ARKIVOC*, (in press).

M. Devereux, M. McCann, V. Leon, V. McKee and R. J. Ball. Synthesis and catalytic activity of manganese(II) complexes of heterocyclic carboxylic acids: X-ray crystal structures of  $[\text{Mn}(\text{pyr})_2]_n$ ,  $[\text{Mn}(\text{dipic})(\text{bipy})_2] \cdot 4.5\text{H}_2\text{O}$  and  $[\text{Mn}(\text{chedam})(\text{bipy})] \cdot \text{H}_2\text{O}$  (pyr = 2-Pyrazinecarboxylic acid; dipic = Pyridine-2,6-dicarboxylic acid; chedam = Chelidamic acid (4-Hydroxypyridine-2,6-dicarboxylic acid); bipy = 2,2-Bipyridine). *Polyhedron*, **21**, 1063-1071 (2002).

B.M. Dixon, **J.P. Lowry** and R.D. O'Neill. Oxygen dependence of an enzyme/polymer biosensor for monitoring brain glucose *in vivo*. *Journal of Neuroscience Methods*, **119**, 135-142 (2002).

A.M. Fenelon and **C.B. Breslin**. The electrochemical synthesis of polypyrrole at a copper electrode: corrosion protection properties. *Electrochimica Acta* **47**, 4467-4476 (2002).

A.M. Fenelon and **C.B. Breslin**. The electropolymerization of pyrrole at a CuNi electrode: corrosion protection properties. *Corrosion Science* (in press).

M. Fillenz, **J.P. Lowry**, M.G. Boutelle, M. Miele, R.S.J. Frackowiak, P.J. Magistretti, R.G. Shulman, J.S. Altman and M. Adams. *In vivo* determination of activation-dependent metabolic coupling. In *Neuroenergetics: Relevance for functional brain imaging*, (Eds.) Human Frontier Science Program, Workshop XI, Strasbourg; **11**, 151-159 (2002).

**J.P. Lowry**, S.O. Dunne and M. Fillenz. *In vivo* evidence supporting compartmentalisation in brain energy metabolism. *Irish Journal of Medical Science*, **170**, 103-104 (2002).

**M. McCann**, B. Coyle, J. Briody, F. Bass, N. O'Gorman, M. Devereux, K. Kavanagh and V. McKee. Synthesis and antimicrobial activity of (Z)-3-(1H-imidazol-1-yl)-2-phenylpropenenitrile and its metal complexes: X-ray crystal structures of the Zn(II) and Ag(I) complexes. *Polyhedron*, (in press).

W.T. O'Connor, J.J. O'Connor, **J.P. Lowry**, and R.D. O'Neill. *In vivo* methods: monitoring molecules in neuroscience. *Journal of Neuroscience Methods*, **119**, 105-107 (2002).

## CONFERENCE PROCEEDINGS

**C.B. Breslin** and K.G. Conroy. 'Indium-induced localized corrosion of aluminium'. *202nd International Meeting of the Electrochemical Society*, Salt Lake City, Utah, USA (20-26 October, 2002).

**C.B. Breslin**, A.M. Fenelon and K.G. Conroy. 'Surface engineering: corrosion protection using conducting polymers'. *1st International Conference on Materials and Tribology*, Dublin, Ireland (4-8 September, 2002).

F.O. Brown, T. Finn and **J.P. Lowry**. 'A new amperometric sensor for real-time monitoring of regional cerebral blood flow'. *54th Irish Universities Chemistry Research Colloquium*, Queen's University, Belfast (10-12 April 2002).

M. Collier and **J.G. McCaffrey**. 'Luminescence spectroscopy of atomic manganese isolated in rare gas solids'. *CNRS seminar series on Molecular Photophysics*, CEA Saclay, France (4 July, 2002).

K.G. Conroy and **C.B. Breslin**. 'Corrosion inhibition by conducting polymers and metal-oxide glass (sol-gel) coatings on aluminium and aluminium alloys'. *202nd International Meeting of the Electrochemical Society*, Salt Lake City, Utah, USA (20-26 October, 2002).

K.G. Conroy and **C.B. Breslin**. 'Remediation of toxic environmental pollutants using conducting polymer surfaces'. *2nd Annual Conference on Analytical Science in Ireland*, Tallaght, Ireland (4-6 April, 2002).

B. Coyle, M. Devereux, **M. McCann**, K. Kavanagh and V. McKee. 'Metal complexes in the battle against fungal infections'. *9th Irish Inorganic Conference*, National University of Ireland, Maynooth (5-6 September, 2002).

B. Coyle, **M. McCann** and M. Devereux. 'Synthesis, structure and activity of new metal-based anti-fungal drugs'. *Irish Universities Chemistry Conference*, Queen's University Belfast (10-12 April, 2002).

S.O. Dunne and **J.P. Lowry**. 'Monitoring brain extracellular glutamate using glutamate oxidase-based amperometric biosensors'. *54th Irish Universities Chemistry Research Colloquium*, Queen's University, Belfast (10-12 April 2002).

S.T. Farrell and **C.B. Breslin**. 'Copper-modified polyaniline composites as a potential photoelectrocatalyst for chromium(VI) reduction'. *202nd International Meeting of the Electrochemical Society*, Salt Lake City, Utah, USA (20-26 October, 2002).

S.T. Farrell and **C.B. Breslin**. 'Electrocatalytic and photoelectrocatalytic properties of copper-modified polyaniline films'. *2nd Annual Conference on Analytical Science in Ireland*, Tallaght, Ireland (4-6 April, 2002).

S.T. Farrell and **C.B. Breslin**. 'The photoelectrocatalytic properties of a polyaniline composite electrode in the oxidation of polyhydroxy compounds'. *54th Irish Universities Chemistry Research Colloquium*, Belfast (10-12 April, 2002).

A.M. Fenelon and **C.B. Breslin**. 'An investigation into the electropolymerization and corrosion protection properties of polypyrrole on copper and copper-based alloys'. *202nd International Meeting of the Electrochemical Society*, Salt Lake City, Utah, USA (20-26 October, 2002).

A.M. Fenelon and **C.B. Breslin**. 'The use of conducting polymers to prevent the release of metal ions into the environment'. *2nd Annual Conference on Analytical Science in Ireland*, Tallaght, Ireland (4-6 April, 2002).

M.M. Gallagher, J.G. Hamilton, M.B. Mula, **A.D. Rooney** and J.J. Rooney. 'The importance of catalyst basicity for the metathesis of functionalised olefins. ROMP of matched pairs of monomers using Grubbs' initiators'. *The 20th International Conference on Organometallic Chemistry*, Corfu (7-12 July 2002).

**J.P. Lowry**. 'In vivo voltammetry: real-time neurochemical monitoring using microelectrochemical sensors'. *School of Chemical Sciences Seminar Series*, Dublin City University, Ireland (3 April, 2002).

**J.P. Lowry**. 'Brain neurochemistry: real-time studies using *in vivo* voltammetry'. *Royal Society of Chemistry, Analytical Research Forum* (presentation - Analytical Grand Prix Final), Kingston University, UK (15-17 July, 2002).

**J.P. Lowry**. 'Brain neurochemistry: real-time studies using *in vivo* voltammetry'. Department of Pharmaceutical Chemistry, School of Pharmacy, Trinity College Dublin (18 September, 2002).

**M. McCann**. 'Metal complexes for fighting fungal infections'. Trinity College Dublin, *Chemistry Seminar Series* (20 February 2003).

**M. McCann**. 'Pathogens in the Seminary - A Holy War'. *Seminar in honour of Professor George Ferguson*, Dublin City University (24 April 2003).

**M. McCann** and M. Devereux. 'New metal-based antimicrobial agents'. *6th Annual Conference Drug Discovery Technology Europe*, Stuttgart, Germany (16 April 2002).

C.T. O'Brien, K.O. Doyle and **A.D. Rooney**. 'A study of the photochemical and redox properties of novel heterobimetallic complexes'. *The 20th International Conference on Organometallic Chemistry*, Corfu (7-12 July 2002).

D. O'Shea, B. Coyle, R. Kelly, M. Devereux, **M. McCann** and K. Kavanagh. 'Novel copper complexes: possible alternatives to azole and polyene anti-fungal drugs'. *7th European Copper Research Group Meeting*, London (14 April 2002).

D. O'Shea, B. Coyle, R. Kelly, N. Grace, M. Devereux, **M. McCann**, K. Kavanagh and V. McKee. 'Metal-based anti-fungal drugs'. *The Royal Society of Chemistry Coordination Chemistry Discussion Group Meeting*, Loughborough, England (18 July 2002).

M. Quigley and **J.G. McCaffrey**. 'Spectroscopy of matrix-isolated atomic sodium – a luminescence spectroscopy/pair-potentials study'. *CNRS Seminar Series on Molecular Photophysics*, Université de Paris-Sud, Orsay, France (9 July, 2002).

M. Quigley and **J.G. McCaffrey**. 'Luminescence spectroscopy of sodium atoms and dimers in low temperature solids'. *CNRS Seminar Series on Molecular Energy Transfer*, Université Paul Sabatier, Toulouse, France (23 July, 2002).

## EXTERNAL ASSIGNMENTS AND PUBLIC SERVICE

### Dr. C.B. Breslin

- Member of the Executive Committee of the European Section of the Electrochemical Society (2002-2004).
- NCEA External Examiner for the National Diploma in Science and Analytical Chemistry at Athlone Institute of Technology.
- Reviewer of research proposals for the Enterprise Ireland Research Innovation Partnership Programme, the European Commission and the UK Engineering and Physical Sciences Research Council.
- Reviewer for the following journals: *Journal of the Electrochemical Society*, *Electrochimica Acta*, *Electrochemistry Communications*, *Journal of Electroanalytical Chemistry*, *Materials Science Forum*, *Journal of Applied Electrochemistry*, *Applied Surface Science*, *Materials Research Bulletin*, *Surface and Coatings Technology*, *Langmuir*, *Corrosion Science* and *Journal of Corrosion*.

### Dr. J.M. Briody

- Secretary, Royal Irish Academy, National Committee for Chemistry, 1996-
- Member of the Royal Society of Chemistry, 1975-

### Dr. M.F. Heaney

- Reviewer - *Journals of the Royal Society of Chemistry*.
- Regional representative - Republic of Ireland Section of the Royal Society of Chemistry, 1997-

### Dr. J.P. Lowry

- Committee member Analytical Division of the Royal Society of Chemistry (Republic of Ireland Section).
- Co-organiser of the 2nd Conference on Analytical Sciences in Ireland, Institute of Technology Tallaght, 4–5 April, 2002.
- Co-organiser of the Irish Neuroscience Group Meeting, Tullamore, 15–16 November, 2002.
- Reviewer for the following journals: *Analytical Chemistry*, *Analytica Chimica Acta*, *Analyst*, *Biosensors & Bioelectronics*, *Journal of Neurochemistry*, *Talanta*, *Journal of Neuroscience Methods* and *Bioelectrochemistry*.
- Reviewer of Academic Books: Analytical Chemistry textbooks for Oxford University Press – Higson, *Analytical Chemistry* (2002).
- Member of the Royal Academy of Medicine in Ireland

### Dr. M. McCann

- Referee for *Polyhedron*
- External examiner for undergraduate science courses in Athlone Institute of Technology : 2001-2003
- External examiner for MSc Transfer report in Dublin Institute of Technology December 2002
- Member of The American Chemical Society



**Professor C.M. Quinn**

- Member of the Royal Irish Academy

**Dr. A.D. Rooney**

- Reviewer for *European Journal of Inorganic Chemistry*
- Examiner of PhD thesis for DCU
- Examiner of PhD thesis for TCD
- Examiner of MSc thesis for DCU
- Chartered Chemist, Member of the Royal Society of Chemistry





**Faculty of Science**

**Research Report 2002**

**Computer Science**



# COMPUTER SCIENCE

## ACADEMIC STAFF\*

**Professor R. Reilly**, BSc, PhD Head of Department (2002-)  
**Mr. S. Brown**, BA (Dublin), BAI, MSc (Dublin), MIEI, MIEEE (1995-)  
**Dr. T. Dowling**, BSc (DIT), MSc, PhD (1998-)  
**Dr. P. Gibson**, BSc (Stirling), PhD (Stirling) (1998-)  
**Mr. J.G. Harpur**, BSc, MA (1990-)  
**Dr. J.G. Keating**, BSc, PhD, CPhys, MInstP (1990-)  
**Mr. D. Kelly**, BSc, MSc (1991-)  
**Dr. W.F. Lunnnon**, BA (Manchester), PhD (Manchester) (1989-)  
**Mr. T. Lysaght**, BA, BD, HDipEd, MCompSci (1998-)  
**Mr. J. McDonald**, BSc (1998-)  
**Dr. C. Markham**, BSc (DCU), PhD (DCU), CPhys, MInstP (1999-)  
**Ms. R. Monahan**, BSc, MSc (1999-)  
**Mr. T. Naughton**, BSc (1998-)  
**Mr. D. O'Donoghue**, MSc (1991-)  
**Dr. J. Power**, MSc, PhD (DCU) (1998-)  
**Dr. J. Timoney**, BA (Dublin), BAI (Dublin), MSc (Dublin), PhD (Dublin) (1999-)  
**Dr. A.C. Winstanley**, BA (Cantab), MSc (QUB), PhD (QUB) (1995-)

## CONTRACT LECTURERS

**Mr. D. Delaney**, BE, MSc (2001-)  
**Mr. G. Mitchell**, BSc (2001-)  
**Ms. J. O'Kelly**, BA Management (NCEA), MCompSci (1997-)

## ASSISTANT LECTURERS

**Ms. L. Keyes**, BSc (2001-)  
**Mr. P. Keane**, BA, HDipIT, MCompSci (2001-)

## POSTGRADUATE RESEARCH STUDENTS

**Mr. R. Allen**, BSc (2002-)  
**Ms. B. Annam**, BSc, MSc (Osmania University, India) (2002-)  
**Ms. E. Belso**, BA (2002-)  
**Ms. S. Bergin**, BSc Mgmt (TCD), HDipIT, MCompSci (1999-)  
**Mr. A. Burnett**, BSc (2002-)  
**Mr. B. Busschots**, BSc (2001-)  
**Mr. S. Cleary**, BSc (2001-)  
**Mr. D. Costelloe**, BSc (1999-2002)  
**Mr. A. Delaney**, BSc (2002-)  
**Mr. A. Duffy**, BSc (2002-)  
**Ms. S. Dunne**, BSc (1999-)  
**Mr. R. Finch**, BSc (2002-)  
**Mr. W. Fitzgerald**, BSc (2000-)  
**Mr. P. Gaughran**, BSc (1999-)  
**Mr. J. Ghent**, BSc (2001-)

\* Unless otherwise stated the higher degrees listed are those of the National University of Ireland.

**Ms. S. Jyothi**, BEng (Osmania University, India) (2003-)  
**Mr. M. Hennessy**, BSc (2002-)  
**Mr. A. Jackson**, BSc (2002-)  
**Mr. T. Keane**, BSc (2002-)  
**Mr. A. McHugh**, BSc (2001-)  
**Mr. S. McLoughlin**, BSc (1999-)  
**Ms. J. McQuillan**, BSc (2000-)  
**Ms. A. Mitchell**, BSc (TCD), HDipIT, MCompSci (2002-)  
**Mr. A. Mooney**, BSc (2000-)  
**Mr. L. Mulhare**, BSc (2000-)  
**Mr. B. Salaik**, BSc (Sebha University, Lybia) (2002-)  
**Ms. P. Setola**, BSc (2002-)  
**Ms. A. Shortt**, BSc (1999-)  
**Mr. D. Woods**, BSc (1999-)

## RESEARCH ASSISTANTS

**Dr. D. Martin**, PhD (2002-)  
**Mr. P. Mooney**, BSc (1999-)

## PRINCIPAL TECHNICIAN

**Mr. J. Cotter**, BSc, DipSoftEng (1990-)

## TECHNICIANS

**Mr. P. Marshall**, BSc, Dip. Strategic Management (DIT) (2001-)  
**Mr. M. Monaghan** (1999-)  
**Mr. V. Paturyan**, DipPhys (Yerevan State University, Armenia) (2002-)

## DEPARTMENTAL ADMINISTRATOR

**Mr. D. Noonan**, BSc, MSc (UUJ) (2002-)

## SENIOR EXECUTIVE ASSISTANT

**Ms. A. Murphy** (1983-)

## EXECUTIVE ASSISTANT

**Ms. L. Donohoe**, DipIT (1999-)

## CONTRACT EXECUTIVE ASSISTANT

**Ms. L. Cannon** (2000-)

## INDUSTRIAL PLACEMENT OFFICER

**Ms. P. Murray**, BSc (1980-)

## HEAD OF DEPARTMENT'S REVIEW OF THE YEAR

One of the significant events of 2002 was the graduation of the first cohort of 29 students from the BSc in Computer Science and Software Engineering (CSSE) programme. This four-year denominated entry programme now has its full complement of four years. The first year intake in 2002 was significantly down this year across all programmes, following the national trend. However, based on this year's CAO first preferences it appears as if the decline may have flattened out. The drop in intake to the CSSE programme was, however, offset by students taking up computer science as an Arts subject, with 2002 being the first year when this option was available.

While undergraduate numbers were somewhat depressed, there was an increase in the number of students pursuing both research and taught postgraduate programmes. Research postgraduate numbers in the Department are currently at an all-time high.

On the funding front, the Department was successful in winning a significant amount of funding to put in place a problem-based approach to the teaching of programming. This programme is currently being established, and will be monitored and evaluated over the next few years. The main goal of the initiative is to improve retention rates of first year students.

The Department benefited significantly from postgraduate research funding under the new Embark initiative, with postgraduate students in the Department winning eight scholarships. More recently, the Department had a number of notable successes in winning research funds in 2002/2003. Staff of the Department were awarded two Enterprise Ireland International Collaboration grants, two Enterprise Ireland Basic Research awards, and an SFI Walton Fellowship. Members of the Department are currently actively involved in formulating proposals for submission to the latest call of Science Foundation Ireland's CSET funding scheme.

## RESEARCH INTERESTS OF STAFF

### **Mr. S. Brown**

Embedded systems, performance of networking/communication systems, overloaded systems analysis, development techniques for embedded systems.

### **Mr. D. Delaney**

Computer networks, distributed simulation, and time series analysis.

### **Dr. T. Dowling**

Mathematics of complex analysis and cryptography.

### **Dr. P. Gibson**

Formal methods and object-oriented techniques.

### **Mr. J. Harpur**

Machine intelligence for decision making, soft systems analysis, and culture and software ergonomics.

### **Dr. J. Keating**

Artificial neural networks and their implementation.

### **Mr. D. Kelly**

Distributed systems.

**Dr. F. Lunn**

Computational geometry, symbolic dynamics, combinatorics, and computer graphics.

**Mr. T. Lysaght**

Digital signal processing with application to real-time audio. Sound synthesis. Computer vision.

**Dr. C. Markham**

Medical and industrial imaging. The development of new imaging sensors, such as high speed profiling cameras and computed tomography.

**Mr. G. Mitchell**

Evolutionary Algorithms/Genetic Algorithms with particular attention to the development of improved selection/fitness functions and other genetic operators.

**Ms. R. Monahan**

Object-oriented specification and programming languages. Type theory. Scalability of software systems. Formal methods.

**Mr. J. McDonald**

Computer vision, shape representations for surface registration, object localisation and identification.

**Mr. T. Naughton**

Analogue optical information processing and computational complexity theory.

**Mr. D. O'Donoghue**

Modeling analogical reasoning in creativity, and 3D visualisation of web-search results.

**Ms. J. O'Kelly**

Speech rehabilitation, in particular speech perception and speech analysis.

**Dr. J. Power**

(Meta-)Logical frameworks, formal specification and functional programming.

**Professor R. Reilly**

Cognitive science and computational neuroscience with a specific focus on models of language understanding and vision.

**Dr. J. Timoney**

Digital audio signal processing with an emphasis towards multimedia applications.

**Dr. A.C. Winstanley**

AI and statistical approaches of graphical data, transport information systems, statistical language modeling.

## RESEARCH GRANTS

- 'Statistical algorithms for latency masking in real-time networked environments'. Enterprise Ireland Basic Research Grant, 2002-2005, €80,300 (Mr. D. Delaney).
- 'Point counting on elliptic curve cryptosystems'. Irish Research Council for Science, Engineering and Technology (IRCSET) Embark Initiative MSc Studentship awarded to Mr. Andrew Burnett, 2002, €57,150 (Dr. T. Dowling).
- 'Efficient algorithms for elliptic curves'. Irish Research Council for Science, Engineering and Technology (IRCSET) Embark Initiative MSc Studentship awarded to Mr. Adam Duffy, 2002, €19,050 (Dr. T. Dowling).
- 'Computational models and the turing limit: An investigation of the boundary between discrete and continuous systems'. Irish Research Council for Science, Engineering and Technology (IRCSET) PhD Embark Initiative Studentship awarded to Mr. Damien Woods, 2002-2004, €57,150 (Dr. J. Paul Gibson).
- 'Asperger syndrome, intervention programme, multimedia e-learning'. Intel Ireland, 2002, €20,000 (Mr. J. Harpur).
- 'Asperger syndrome, intervention programme. Multimedia e-learning'. Irish Autism Alliance and North Eastern Autism Alliance, 2002, €5,000 (Mr. J. Harpur).
- 'Asperger syndrome, intervention programme, multimedia, e-learning'. Dept. of the Gaelteacht, Rural and Community Affairs, 2002, €63,000 (Mr. J. Harpur).
- 'Asperger syndrome, computer assisted interviewing, adolescent bullying, social cognitions and theory of mind.' Child and Family Centre, North Eastern Health Board, 2002-2004, €40,000 (Mr. J. Harpur).
- 'Chaos theory', Enterprise Ireland Basic Research Grant, 2000-2003, €35,000 (Dr. J. Keating).
- 'Virtual telescopes in education project'. Enterprise Ireland International Collaboration Grant, 2002, €4,404 (Dr. J. Keating).
- 'Electronic policy project'. NUI Maynooth Research, 2002, €6,000. (Dr. J. Keating).
- 'Development of online student mentoring and quality promotion system'. NUI Maynooth Quality Promotion Office via National Development Plan, 2002, €16,000. (Dr. J. Keating).
- 'Functional brain imaging using diffuse optical tomography'. Higher Education Authority and Media Lab Europe Collaboration, 2002-2005, €177,500 (Dr. C. Markham).
- 'Development of integrated quasi-optical and electromagnetic numerical simulator for the computer aided design and analysis of novel terahertz systems'. Science Foundation Ireland, 2002, €786,000 [Dr. C. Markham in collaboration with Professor J A Murphy (P.I.) Department of Physics].
- 'Automated detection and analysis of pavement distress'. Collaboration with the University of Connecticut. Enterprise Ireland, 2002, €5,650 (Mr. J. McDonald).
- 'The use of types as specifications for modern software components'. National Science Foundation, USA, 2002, €1,000 (Ms. Rosemary Monahan).
- 'Algorithms for digital hologram compression'. Collaboration with the University of Connecticut. Enterprise Ireland, 2002, €6,500 (Mr. T. Naughton).
- 'Specification of an abstract operating system running on a single stack push down automation'. Irish Research Council for Science, Engineering and Technology (IRCSET) Embark Initiative PhD Studentship awarded to Mr. Aidan Delaney, 2002-2005, €57,150 (Dr. J. Gibson and Mr. T. Naughton).
- 'A distributed system and distributed algorithms for bioinformatics applications'. Irish Research Council for Science, Engineering and Technology (IRCSET) Embark Initiative MSc Studentship awarded to Mr. Thomas Keane, 2002-2003, €19,050 (Mr. T. Naughton).
- '3G alarm prediction in conjunction with Ericsson'. ARL Applied Research, Athlone, 2002-2003, €9,000 (Mr. D. O'Donoghue).

'Topographic data analysis and categorisation'. The British Council Research Visits Scheme, 2002-2003, €2,500 (Mr. D. O'Donoghue).

'Explanation based business intelligence systems'. Enterprise Ireland Basic Research Grant, 2002-2005, €125,000 (Mr. D. O'Donoghue).

'2nd International Conference on the Principles and Practice of Programming in Java'. Science Foundation Ireland, 2002-2003, €17,000 (Dr. J. Power).

'Run-time dynamic metrics for Java programs'. Irish Research Council for Science, Engineering and Technology (IRCSET) Embark Initiative PhD Studentship awarded to Ms. Aine Mitchell, 2002-2005, €57,150 (Dr. J. Power).

'Design of parser and compiler front ends using GLR technology'. Irish Research Council for Science, Engineering and Technology (IRCSET) Embark Initiative PhD Studentship awarded to Mr. Mark Hennessy 2002-2005, €57,150 (Dr. J. Power).

'The evaluation and design of benchmark suites for the Java Virtual Machine'. Enterprise Ireland International Collaboration, 2002-2003, €2,700 (Dr. J. Power).

'Study of eye movement behaviour of Thai readers'. Enterprise Ireland with Dr. Sudaporn Lukaneeyanawin of the Centre for Research in speech and Language, Chulalongkorn University, Bangkok, 2002-2003, €5,800 (Professor R. Reilly).

'A connectionist attractor dynamical model of language development'. Irish Research Council for Science, Engineering and Technology (IRCSET) Embark Initiative PhD Studentship awarded to Ms. Eva Belso, 2002-2004, €57,150 (Professor R. Reilly).

'Climate change data integration'. Environmental Protection Agency Environmental Research Development and Innovation Programme. 2002-CCFS4-M4, 2002-2004, €78,750 (Dr. A. Winstanley).

'Automatic recognition and labelling of features on technical drawings'. Enterprise Ireland Innovations Partnership Feasibility Study (with Entropic Ltd, Maynooth), 2002, €8,928.70 (Dr. A. Winstanley).

'Multiple mode and objective travel planning algorithms' (with Department of Civil Engineering, Southampton University and Mott McDonald Transport Consultancy, Chicester), Enterprise Ireland/British Council Research Visits Scheme, 2002-2003, €4,000 (Dr. A. Winstanley).

'Topographic object recognition' (with D.O'Donoghue and Ordnance Survey), Enterprise Ireland/British Council Research Visits Scheme, 2002-2003, €2,500, (Dr. A. Winstanley).

'Multimodal traveller information systems technical exchange network' (with Setec-ITS, Paris), CNRS-Enterprise Ireland *Ulysses Visites de Recherche Scheme*, 2002-2003, €2,400 (Dr. A. Winstanley).

## PUBLICATIONS IN REFEREED JOURNALS

**J.G. Keating**, S. Hoban, M. desJardins, N. Farrell, P. Rathod, J. Sachs, S. Sansare, Y. Yesha, J. Keating, B. Busschots, J. Means, G. Clark, L. Mayo and W. Smith. Virtual Telescopes in Education, *Journal of Digital Information*, **2**, (2002).

**J.G. Keating**, A. Rogers, R. Shorten and D. M. Heffernan. Chaotic maps and pattern recognition - the XOR problem. *Chaos, Solitons and Fractals*, **14**, 57-70 (2002).

**T.J. Naughton**, **J. Mc Donald**, Y. Frauel, and B. Javidi. Efficient compression of digital holograms for Internet transmission of three-dimensional images. *Annual Meeting of the IEEE Lasers and Electro-Optics Society (IEEE LEOS)* **15**, 33-34 (2002).

**T.J. Naughton**, O. Matoba, B. Javidi, T. Shimura and K. Kuroda. Optical reconstruction of three-dimensional objects using phase-only digital holograms, *49th Spring Meeting of The Japan Society of Applied Physics and Related Societies*, **3**, 990 (2002).

- T.J. Naughton**, O. Matoba, E. Tajahuerce, T. Shimura, K. Kuroda and B. Javidi. Secure three-dimensional display using digital holography. *International Workshop on Optical Display and Information Processing*, **1**, 53-67 (2002).
- T.J. Naughton**, Y. Frauel, B. Javidi and E. Tajahuerce. Compression of digital holograms for 3D imaging, *Optics in Information Systems*, **13**, 7 (2002).
- T.J. Naughton** and A. Delaney. Emulation of an unconventional model of computation in Java, *Principles and Practice of Programming in Java*, **1**, 1-6 (2002).
- T.J. Naughton**, T. Keane, R. Allen, J. McInerney, and J. Waldron. Distributed computing for DNA analysis. *Principles and Practice of Programming in Java* **1**, 65-70 (2002).
- T.J. Naughton**, Y. Frauel, B. Javidi and E. Tajahuerce. *Compression of digital holograms for three-dimensional object reconstruction and recognition*. *Applied Optics* **41**, 4124-4132 (2002).
- T.J. Naughton**, O. Matoba, Y. Frauel, N. Bertaux and B. Javidi. Three-dimensional object reconstruction using phase-only information from a digital hologram. *Proc. SPIE Three-Dimensional TV, Video, and Display* **4864**, 122-128 (2002).
- T.J. Naughton**, Y. Frauel, O. Matoba, N. Bertaux, E. Tajahuerce and B. Javidi. Imaging, Compression, and reconstruction of digital holograms. *Proc. SPIE Optical Metrology, Imaging, and Machine Vision* **4877**, 1-11 (2002).
- T.J. Naughton**, O. Matoba, Y. Frauel, N. Bertaux and B. Javidi. Real-time three-dimensional object reconstruction by use of a phase-encoded digital hologram. *Applied Optics* **41**, 6187-6192 (2002).
- T.J. Naughton**, T. Keane, R. Allen, J. McInerney and J. Waldron. Distributed Java platform with programmable MIMD capabilities. *FIDJI International Workshop on Scientific Engineering of Distributed Java Applications* **2**, 153-162 (2002).
- T.J. Naughton**, **J. Mc Donald**, Y. Frauel and B. Javidi. Efficient compression of digital holograms for Internet transmission of three-dimensional images. *Annual Meeting of the IEEE Lasers and Electro-Optics Society (IEEE LEOS)*, **15**, 33-34 (2002).
- J.F. Power**, B.A. Malloy, S.A. Linde and E.B. Duffy. Testing C<sup>++</sup> Compilers for ISO Language Conformance. *Dr. Dobb's Journal* **337**, 71-78 (2002).
- Reilly, R.G.** The relationship between object manipulation and language development in Broca's area: A connectionist simulation of Greenfield's hypothesis. *Behavioral and Brain Sciences*, **25**, 145-153 (2002).

## BOOK, BOOKS, CHAPTERS & REVIEWS

- T. Dowling**. 'Relating Static and Dynamic Measurements for the Java Virtual Machine Instruction Set'. In *Recent Advances in Simulation, Computational Methods and Soft Computing*. WSEAS Press ISBN 960-8052-50-5 (2002).
- T. Dowling**. 'Java implementation of an elliptic curve cryptosystem'. In *Recent Advances in Java Technology: Theory, Application, Implementation*. (eds. J.F. Power and J.T. Waldron). Computer Science Press, Dublin, ISBN 0-9544145-0-0 (2002).
- T.J. Naughton**, Y. Frauel, O. Matoba, B. Javidi, and E. Tajahuerce. 'Compression of digital holograms for three-dimensional video'. In *Three Dimensional Television, Video, and Display Technologies*. (eds. B. Javidi and F. Okano). Springer-Verlag Berlin, pp. 273-295 (2002).
- T.J. Naughton** and A. Delaney. 'Emulation of an unconventional model of computation in Java'. In *Recent Advances in Java Technology: Theory, Application, Implementation*. (eds. J.F. Power and J.T. Waldron). Computer Science Press, Trinity College, Dublin pp. 1-10 (2002).
- T.J. Naughton**, J. McInerney, T. Keane, R. Allen and J. Waldron. 'Distributed computing for DNA analysis'. In *Recent Advances in Java Technology: Theory, Application, Implementation*. (eds. J.F. Power and J.T. Waldron). Computer Science Press, Trinity College, Dublin pp. 99-108 (2002).

**D. O'Donoghue, J.Power**, A. Leddy and J. Waldron, 'Bi-gram analysis of Java bytecode sequences'. In *Recent Advances in Java Technology: Theory, Application, Implementation*. (eds. J.F. Power and J.T. Waldron). Computer Science Press, Trinity College, Dublin pp. 243-288 (2002).

**D. O'Donoghue** and B. Crean 'RADAR: Finding Analogies using Attributes of Structure'. In *Lecture Notes in Artificial Intelligence*, Limerick, ISBN 3540-441840 pp. 20-27 (2002).

**J.F. Power, T. Dowling**, and J. Waldron. 'Relating Static and Dynamic Measurements for the Virtual Machine Instruction Set'. In *Recent Advances in Simulation, Computational Methods and Soft Computing*. ed. N.E. Mastorakis. WSEAS Press, Greece pp. 106-111 (2002).

**J.F. Power**, D. Gregg, and J. Waldron. 'Benchmarking the Java Virtual Architecture - The SPEC JVM98 Benchmark'. In *Java Microarchitectures*. (eds. N. Vijaykrishnan and M. Wolczko). Kluwer Academic, Massachusetts, USA pp. 1-18 (2002).

**J.F. Power** and J.T. Waldron. *Recent Advances in Java Technology*: Computer Science Press, Trinity College Dublin (2002).

**R.G. Reilly** and R. Radach. 'Foundations of an interactive activation model of eye movement control in reading'. In *The mind's eye: Cognitive and applied aspects of eye movement research*. (eds. J. Hyönä, R. Radach and H. Deubel). Elsevier, The Netherlands. (2002).

**R.G. Reilly** and R. Radach. 'Glenmore: An interactive activation model of eye movement control in reading'. In *ICONIP'02: Proceedings of the 9th International Conference on Neural Information Processing*. (eds. L. Wang, J.C. Rajapakse, K. Fukushima, S-Y Lee and X. Yao). Singapore IEEE Neural Network Society pp. 1194-1200 (2002).

**R.G. Reilly** and I. Marian. 'Cortical Software Re-Use: A computational principle for cognitive development in robots'. In *ICONIP'02: Proceedings of the 9th International Conference on Neural Information Processing*. (eds. L. Wang, J.C. Rajapakse, K. Fukushima, S-Y Lee, and X. Yao. Singapore IEEE Neural Network Society pp. 1548-1553 (2002).

**R.G. Reilly**, C. Sas, G.M.P. O'Hare. 'A Connectionist Approach to Modelling Navigation: Trajectory Self Organization and Prediction'. In *Proceedings of 7th ERCIM Workshop, User Interfaces for All* (eds. N. Carbonell and C. Stephanidis). pp. 111-116 (2002).

## CONFERENCE PROCEEDINGS

**J.D. Delaney** and **G.G. Mitchell**, 'PBL applied to software engineering group projects,' *International Conference on Information and Communication in Education (Proceedings of Information and Communication Technologies in Education 2002*, ISBN 84-95251-70-0), 1093-1098, Badajoz, Spain (13-16 November 2002).

A. Delaney and **T.J. Naughton**. Emulation of an unconventional model of computation in Java. *Principles and Practice of Programming in Java*, **1**, 1-6, Trinity College Dublin (13-14 June 2002).

**T. Dowling**, A. Burnett and K.Winters 'A Java implementation of an elliptic curve cryptosystem', *Principles and Practice of Programming in Java conference*, TCD (13-14 June 2002).

**J. Harper**, M. Lawlor, V. Foley and M. Fitzgerald. 'A webs service for Asperger adolescents and their parents'. *Meeting of Irish Autism Alliance*, Mullingar, Co. Westmeath (18 September 2002).

**J. Harper**, M. Lawlor, V. Foley and M. Fitzgerald. 'A comparison of normal and Asperger adolescent as script writers'; *Society of Neuroscience Satellite International Meeting for Autism Research*, Orlando, Florida, USA (1-5 November 2002).

**J. Harper**, M. Lawlor, V. Foley and M. Fitzgerald. 'E-learning social skills with Asperger adolescents'. *Workshop on social Skills Interventions for Able Autistic Children*. Beechpark Centre for Autism Stillorgan, Dublin (11 December 2002).

T. Keane, R. Allen, **T.J. Naughton**, **J. McInerney** and J. Waldron. Distributed computing for DNA analysis. *Principles and Practice of Programming in Java*, **1**, 65-70, Trinity College Dublin (13-14 June 2002).

T. Keane, R. Allen, **T.J. Naughton**, J. McNerney and J. Waldron. Distributed Java platform with programmable MIMD capabilities. *FIDJI International Workshop on Scientific Engineering of Distributed Java Applications*, **2**, 153-162, Luxembourg-Kirchberg, Luxembourg (28-29 November 2002).

**L. Keys** and **A.C. Winstanley**. 'Automatically structuring archaeological features on topographic maps'. *Geographical Information Science Research Conference*, Sheffield, UK (3-5 April 2002). **Best paper award winner**.

**T. Lysaght** and **J. Timoney**, 'Timbre morphing using the Modal distribution', *Digital Audio Effects (DAFX) 2002*, Hamburg, Germany (26-28 September 2002).

**T. Lysaght**, **J. Timoney** and V. Nazarene. 'New SndObj library classes for sinusoidal modeling,' *Digital Audio Effects (DAFX) 2002*, Hamburg, Germany (26-28 September 2002).

O. Matoba, **T.J. Naughton**, B. Javidi, T. Shimura and K. Kuroda. Optical reconstruction of three-dimensional objects using phase-only digital holograms. *49th Spring Meeting of The Japan Society of Applied Physics and Related Societies*, **3**, 990, Tokai University, Hiratsuka, Japan (27-30 March 2002).

O. Matoba, **T.J. Naughton**, E. Tajahuerce, T. Shimura, K. Kuroda and B. Javidi. Secure three-dimensional display using digital holography. *International Workshop on Optical Display and Information Processing*, **1**, 53-67, Gyeononju, Korea (15-16 May 2002). (Invited).

O. Matoba, **T.J. Naughton**, Y. Frauel, N. Bertaux and B. Javidi. Three-dimensional object reconstruction using phase-only information from a digital hologram. *Three-Dimensional TV, Video, and Display, Proceedings of SPIE* **4864**, 122-128, Boston, Massachusetts (29 July - 1 August 2002). (Invited).

**G. Mitchell** and A.M. Rafter. 'The Effect of a General Routing Algorithm Optimisation Function'. *IT&T Conference 2002*, Waterford, Ireland (30-31 October, 2002).

**T.J. Naughton**, T. Keane, R. Allen, J. McNerney and J. Waldron. Distributed Java platform with programmable MIMD capabilities. *FIDJI International Workshop on Scientific Engineering of Distributed Java Applications* **2**, 153-162, Luxembourg-Kirchberg, Luxembourg (28-29 November 2002).

**T.J. Naughton**, **J. Mc Donald**, Y. Frauel and B. Javidi. Efficient compression of digital holograms for Internet transmission of three-dimensional images. *Annual Meeting of the IEEE Lasers and Electro-Optics Society (IEEE LEOS)*, **15**, 33-34 Glasgow, Scotland (10-14 November 2002).

**T.J. Naughton**, Y. Frauel, O. Matoba, N. Bertaux, E. Tajahuerce and B. Javidi. Imaging, compression, and reconstruction of digital holograms. *Optical Metrology, Imaging, and Machine Vision, Proceedings of SPIE* **4877**, 104-114, Galway, Ireland (5-6 September 2002).

**D. O'Donoghue** and B. Crean, 'RADAR: finding analogies using attributes of structure', *13th Irish Conference on Artificial Intelligence & Cognitive Science 2002*, University of Limerick (12-13 September 2002).

**D. O'Donoghue** and B. Crean, 'Searching for serendipitous analogies', *European Conference on Artificial Intelligence ECAI - Workshop on Creative Systems*, Lyon, France (21-26 July 2002).

**D. O'Donoghue**, **A. Winstanley** and L. Mulhare. 'Context-based classification of objects in cartographic data', *Geographical Information Science Research Conference*, Sheffield, UK (3-5 April 2002).

**D. O'Donoghue** and S. Cleary. '3G integration reference points set to replace TMN', *Information Technology & Telecommunications Conference*, IT Waterford, Ireland (30-31 October, 2002).

**D. O'Donoghue**, **J.F. Power**, A. Leddy and J. Waldron, 'Bi-gram analysis of Java bytecode sequences', *Principles and Practice of Programming in Java - Intermediate Representation Engineering for Virtual Machines*, Trinity College Dublin (13-14 June 2002).

**D. O'Donoghue**, and L. Mulhare. 'Context-based classification of objects in cartographic data'. *Geographical Information Science Research Conference*, Sheffield, UK (3-5 April 2002).



**J.F. Power**, 'Program annotation in XML: a parser-based approach' *Working Conference on Reverse Engineering*, Richmond, Virginia, USA (28 October - 1 November 2002).

**J.F. Power** and B.A. Malloy, 'Automated Validation of Class Invariants in C<sup>++</sup> Applications' *17th IEEE International Conference on Automated Software Engineering*, Edinburgh, UK (23-27 September, 2002),

**J.F. Power**, B.A. Malloy and J.T. Waldron, 'Applying Software Engineering Techniques to Parser Design'. *Conference of the South African Institute of Computer Scientists and Information Technologists*, Port Elizabeth, South Africa (16-18 September 2002).

**J.F. Power** and B.A. Malloy, 'Title Program annotation in XML: a parser-based approach', *Working Conference on Reverse Engineering*, Richmond, Virginia, USA (28 October - 1 November 2002).

**J.F. Power**, D. O'Donoghue, A. Leddy and J.T. Waldron. 'Bi-gram analysis of java bytecode sequences'. *Proceedings of the Second Workshop on Intermediate Representation Engineering for the Java Virtual Machine*, Trinity College, Dublin, Ireland (13-14 June 2002).

**J.F. Power**, R. Monahan, B.A. Malloy, S. Matzko, P.J. Clarke and T.H. Gibbs, 'A tool to reverse engineer class diagrams'. *Fortieth International Conference on Technology of Object-Oriented Languages and Systems*, Sydney, Australia (18-21 February, 2002).

**R.G. Reilly** and R. Radach, 'Glenmore: An interactive activation model of eye movement control in reading'. *ICONIP'02: The 9th International Conference on Neural Information Processing*. Singapore (18-20 November, 2002).

**R.G. Reilly** and I. Marian. 'Cortical Software Re-Use: A computational principle for cognitive development in robots'. *ICONIP'02: The 9th International Conference on Neural Information Processing*. Singapore (18-20 November, 2002).

**J. Timoney**, **T. Lysaght**, A. Schwarzbacher and J.P. Silvennoinen, 'Comparison of VLSI implementations of adder circuits', *3rd International Symposium on Communication Systems, Networks and Digital Signal Processing 2002*, Stafford, UK (15-17 July 2002).

**J. Timoney** and A. Schwarzbacher, 'VLSI implementation of an adaptive noise canceller,' *3rd International Symposium on Communication Systems, Networks and Digital Signal Processing*, Stafford, UK (15-17 July 2002).

**J. Timoney**, A. Schwarzbacher, M. Herz and F. David. 'A hardware optimised CMOS adaptive noise canceller implementation'. *Electronic Devices and Systems Conference 2002*, Brno, Czech Republic (September 2002).

**A.C. Winstanley**, D. Costelloe and P. Mooney . 'An evolutionary spatial decision support system'. *Geographical Information Science Research Conference*, Sheffield, UK (3-5 April 2002).

**A.C. Winstanley**, R. Sherlock, J. Husdal and P. Mooney. 'Shortest path computation: A comparative analysis'. *Geographical Information Science Research Conference*, Sheffield, UK (3-5 April 2002).

**A.C. Winstanley** and P. Mooney 'Multi-objective path optimisation in dynamic environments'. *GI Science 2002*, Boulder, USA (25-28 September 2002).

## EXTERNAL ASSIGNMENTS AND PUBLIC SERVICE

### T. Dowling

- Program committee member for Principles and Practice of Programming in Java (PPPJ-2002) international conference, Trinity College, Dublin.
- Session chair at PPPJ-2002 2002.

### J.P. Gibson

- Reviewer for *The Journal of Automated Software Engineering* and *The International Journal of Foundations of Computer Science*.
- Reviewer for Forum on specification and Design Languages (FDL02).
- Reviewer for Principles and Practice of Programming in Java (PPPJ-2002).
- Reviewer for Irish Conference on Artificial Intelligence & Cognitive Science (AICS-2002).
- External examiner for BSc: Applied Computing (Commercial & Industrial) (Waterford Institute of Technology) and BSc: Computing in Commercial Software Development (Waterford Institute of Technology).
- External examiner for MSc thesis at DCU.

### J.G. Harpur

- Book proposal editor for Pearsons.
- Reviewer for *Artificial Intelligence Review*.
- Contributing editor to ACM Crossroads.
- Software development for Cool School anti-bullying programme devised by North Eastern Health Board.

### P. Keane

- Contributor to DOT.IE magazine.

### J. Keating

- External Examiner for MPhil thesis, Dublin Institute of Technology.

### J. McDonald

- Reviewer for *Artificial Intelligence Review*.

### G. Mitchell

- Reviewer for *IEEE Transactions on Evolutionary Computation* and *ACM Crossroads*.
- Reviewer for Principles and Practice of Programming in Java (PPPJ-2002).

### R. Monahan

- Member of the programme committee for Principles and Practice of Programming in Java (PPPJ-2002).
- Reviewer for Principles and Practice of Programming in Java (PPPJ-2002).
- Software Engineering Session Chair and Reviewer for the *ACM Symposium on Applied Computing* (SAC-2002).

**T. Naughton**

- Reviewer for the following journals: *Optics Letters*, *Applied Optics*, *Optics Communications* and *Optical Engineering*.

**D. O'Donoghue**

- Reviewer for ACM Symposium on Applied Computing (SAC-2002), Madrid, Spain.
- Reviewer for Principles and Practice of Programming in Java (PPPJ-2002).
- Reviewer for Irish Conference on Artificial Intelligence & Cognitive Science (AICS-2002).

**J. Power**

- External examiner for Waterford Institute of Technology.
- Program chair for Principles and Practice of Programming in Java (PPPJ-2002).
- Software Engineering Track Chair for the ACM Symposium on Applied Computing (SAC-2002), Madrid, Spain.

**R. Reilly**

- Reviewer for the following journals: *Connection Science*, *Neural Processing Letters* and *Artificial Intelligence Review*.
- Book manuscript reviewer for Kluwer Publishing.
- External examiner for PhD thesis, Department of Computer Science, Trinity College Dublin.
- Project evaluator for the EU FP5 cognitive vision project 'CogVis'.
- External assessor for internal promotions in the School of Computer Applications, Dublin City University.

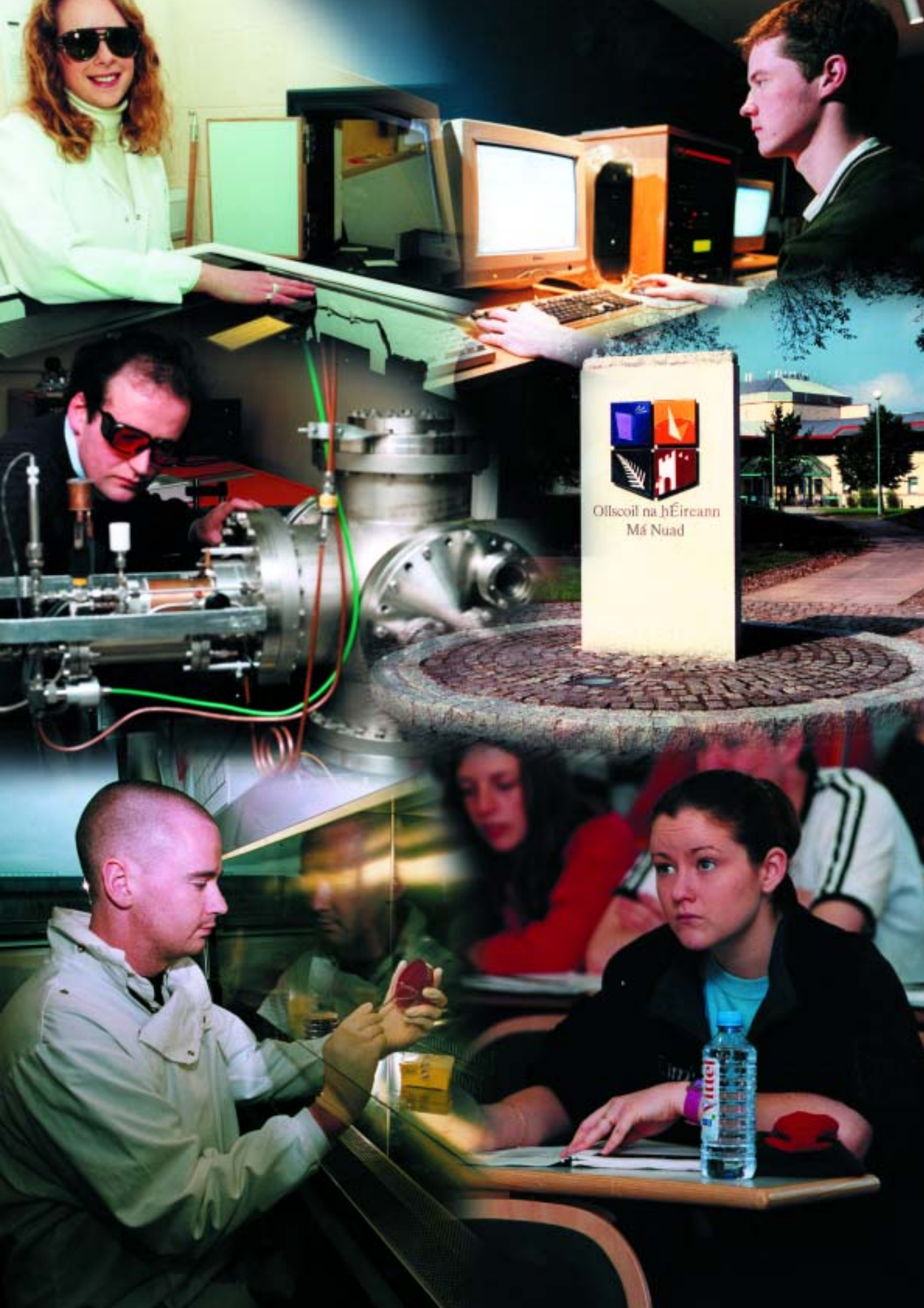
**A. Winstanley**

- Member of technical committee Principles and Practice of Programming in Java (PPPJ-2002).
- Member of technical committee Irish Conference on Artificial Intelligence & Cognitive Science (AICS-2002).

## CONFERENCES HOSTED

**J.P. Gibson, J. Power**, *ACM Symposium on Applied Computing (SAC2002)*, Madrid, Spain (10-14 March, 2002)

**A.C. Winstanley**, *Irish Athens Authentication Workshop*, NUI Maynooth (18 June, 2002).



Ollscoil na hÉireann  
Má Nuad



*Pictured on the occasion of the opening of the Biosciences Research and Electronic Engineering Building by Mr. Noel Dempsey TD, Minister for Education and Science, are (back row left to right) Professor Kay Ohlendieck, Head of the Biology Department, Minister Noel Dempsey, Dr. W.J. Smyth, President NUI Maynooth and Dr. Bernard Mahon, Director Institute of Immunology. With them are Professor John Ringwood, Dean of the Faculty of Engineering (front left), Professor Ann Burnell, Dean of the Faculty of Science and Professor Martin Downes, Director of the Institute of Bioengineering and Agroecology.*



*Minister Noel Dempsey TD looks on as Dr. Tony O'Connor a postdoctoral fellow in the Institute of Immunology genotypes DNA samples from cancer patients. Also pictured is Dr. Bernard Mahon, Institute Director. Dr. O'Connor is carrying out research on a family of immune genes (the killer immunoglobulin-like receptors) which may protect liver cancer patients.*



*Minister Noel Dempsey TD discusses plant biotechnology with Professor Phil Dix in the plant tissue culture facility of the new Biosciences Building.*



*Dr. Paul Gibson, Director of the NUI Maynooth Science Camp (left) with Mr. Fintan Nixen, Manager AIB Maynooth, Ms. Marlene Travers, AIB Student Officer and Dr. Frank Mulligan, Vice-President NUI Maynooth. The AIB Better Ireland Programme was one of the sponsors of the 2003 Maynooth Science Camp. Sponsorship for the Science Camp was also received from Intel, Forfás, Enterprise Ireland, the Finglas Cabra Partnership, the NUI Maynooth Quality Promotions Office and the NUI Maynooth Access Office. This sponsorship provided scholarships that enabled students from disadvantaged backgrounds to attend the camp.*

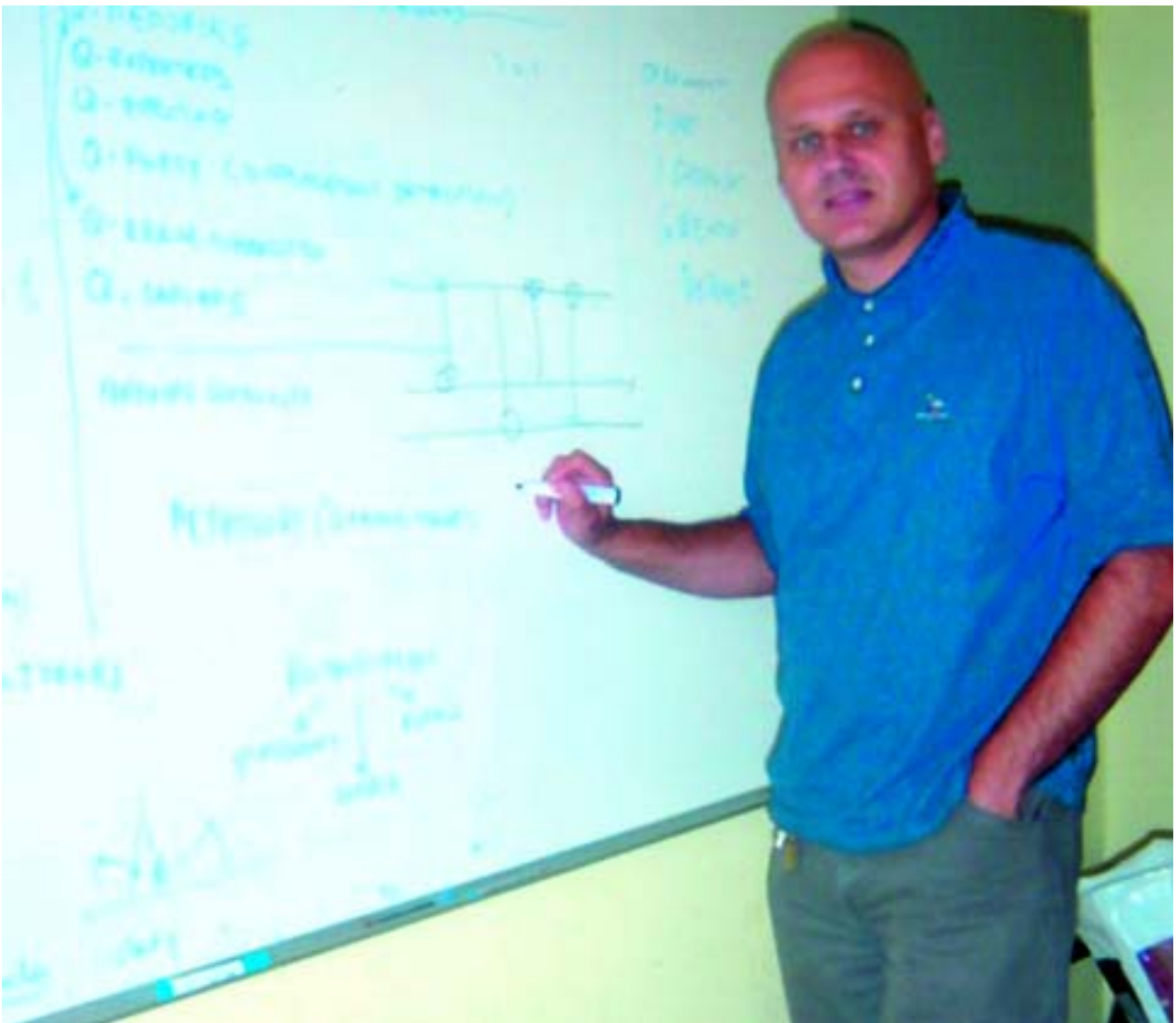


*Ms. Teresa Redmond with some of the Science Camp students at a cell biology workshop in the Biology Department.*

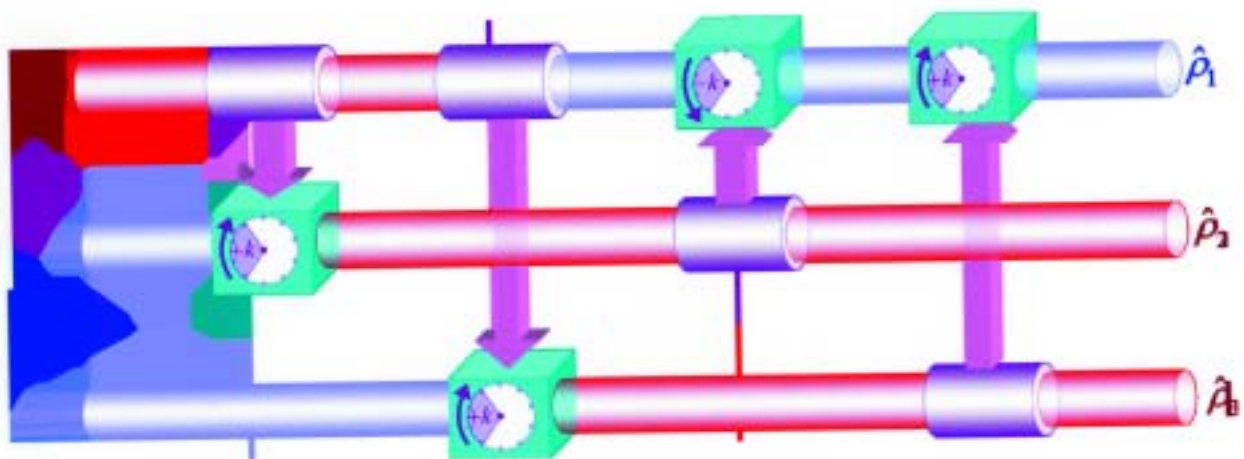


*Professor A.G. O'Farrell addresses the participants at Broombridge on the Quaternion Walk, 16 October 2002. On this day in 1843, the Irish mathematician William Rowan Hamilton created the quaternions in a flash of inspiration while walking along the banks of the Royal Canal in Dublin. Each year the Mathematics Department at NUI Maynooth commemorates the event by retracing Hamilton's steps. The walk begins at Dunsink Observatory and heads south to meet the Royal Canal before going east along the canal to the Broombridge train station in Cabra, where a plaque marks the area where Hamilton scratched his formulas for the quaternions on the bridge.*

*(Photograph courtesy of the Irish Times).*



Professor Vladimír Bužek from the Slovakian Academy of Science, a Science Foundation Ireland ETS Walton Fellow at the Department of Mathematical Physics.



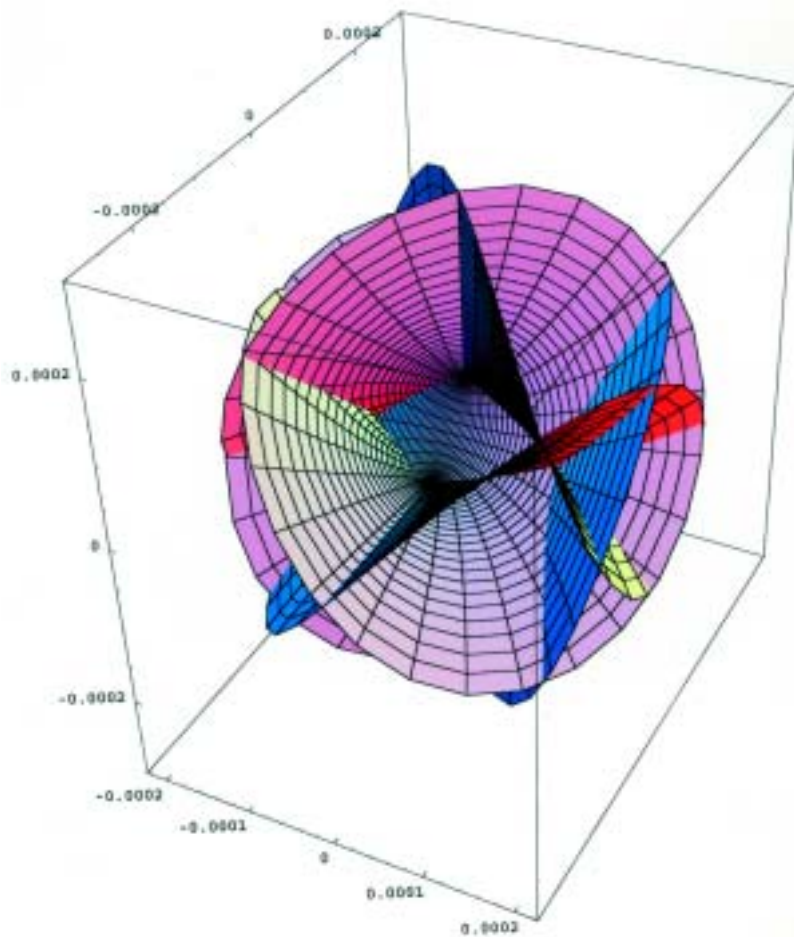
A graphical representation of a universal NOT gate courtesy of Professor Vladimír Bužek. The universal NOT gate is an effort to develop quantum logic circuits with the goal of building a quantum computer. The science of quantum information exploits quantum effects at the level of individual particles. Photon polarization was used for the quantum bits. For any input polarization, the NOT gate (as in conventional electronics) should transmit the opposite - in this case it should produce a photon in the orthogonal polarization state, for example going from vertical to horizontal polarization, or right circular to left circular.



Australian scientist Dr. Peter Doherty, who presented the keynote address at a research symposium in the Institute of Immunology at NUI Maynooth in April 2003 pictured with Dr. Bernard Mahon, Director of the Institute (left) and Dr. Frank Mulligan Vice-President (right). Dr. Doherty was jointly awarded the Nobel Prize in Medicine in 1996 for research that revolutionized the field of immunology by explaining how the immune system recognises virus-infected cells. He is currently Chairman of the Department of Immunology at St. Jude Children's Research Hospital in Memphis, Tennessee.



An Tánaiste Mary Harney TD, making a presentation for the best poster award at the Informations Technology and Telecommunications (IT&T 2002) Conference which took place in Waterford Institute of Technology. The award was made to George Mitchell, Department of Computer Science NUI Maynooth for his poster entitled "The effect of a general routing algorithm optimisation function". Also pictured (right) is Dr. Dirk Pesch, the Conference Chairperson.



*The study of minimal surfaces has played a formative role in the development of mathematics over the last two centuries. Today, minimal surfaces appear in various guises in diverse areas of mathematics, physics, chemistry and computer graphics. Dr. Anthony Small of the Department of Mathematics at NUI Maynooth has been developing techniques which elucidate the global structure of minimal surfaces. By transforming the background space the non-linear equation satisfied by the minimal surface simplifies, enabling the construction of complete minimal surfaces with beautiful Platonic symmetries. This figure illustrates Dr. Small's solution for a minimal surface generated by a charge two monopole.*



*The Department of Computer Science Intelligent Graphical Research Group attended the Geographic Information Science Research Conference in Sheffield in April 2002 where they presented four papers in the fields of automatic cartography and route planning. Postgraduate student Laura Keyes, pictured in the front row, won the conference's young researcher award for her paper on Automatically Structuring Archaeological Features on Topographic Maps.*

# The Encyclopaedia of Ireland



EDITOR

## Three-Dimensional Television, Video, and Display Technologies

Editors: B. Javidi, F. Okano



Proceedings of  
The Twelfth Irish Conference on  
Artificial Intelligence and Cognitive Science



### AICS

Johns Hopkins University  
Baltimore, Maryland, September 2001  
ISBN 0 85201 44 8



## Computational Quantum Chemistry

Charles M Quinn



Proceedings of the Irish Machine Vision  
and Image Processing Conference

University of Ireland Maynooth  
May 2001



NUI MAYNOOTH

## ENTOMOPATHOGENIC NEMATOLOGY



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## Physicists of Ireland

Passion and Precision

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IoP





**Faculty of Science**

**Research Report 2002**

**Experimental Physics**





# EXPERIMENTAL PHYSICS

## ACADEMIC STAFF\*

**Professor J.A. Murphy**, MSc, MS (Caltech), PhD (Cantab), FRAS, CPhys, FInstP, MIEEE (1988-)

**Dr. M.F. Cawley**, MSc, PhD, CPhys, MInstP (1987-)

**Dr. F.J. Mulligan**, BSc, PhD, CPhys, MInstP (1984-)

**Dr. R.W. O'Neill**, BSc, PhD (QUB) CPhys, MInstP (1996-)

**Dr. C. O'Sullivan**, BSc, PhD (Cantab) (1998-)

**Dr. P.J.M. van der Burgt**, MS, PhD (Utrecht), CPhys, MInstP (1993-)

## CONTRACT LECTURERS

**Dr. N. Murphy**, BSc, PhD (2000-)

**Mr. W. Lanigan**, BSc, (Open Univ), MSc, MIIE (1986-)

**Dr. N. Trappe**, BSc, PhD (2002-)

**Mr. G. McMahon**, BSc, MSc (2000-)

## PRINCIPAL TECHNICIAN

**Mr. D. Gleeson**, (1976-)

## TECHNICAL STAFF

**Ms. M. Galligan**, BSc, DipIndInstr (NCEA) (1991-)

**Mr. J. Kelly**, BSc, HDipAppPh (1999-)

**Mr. I. McAuley**, BSc (2000-)

**Dr. N.E. McKeith**, BSc, PhD (QUB) (1978-)

**Mr. D. Watson**, DipMechEng (2000-)

## EXECUTIVE ASSISTANT

**Ms. G. Roche**, BA (1997-)

## RESEARCH FELLOWS

**Dr. V. Yurchenko**, MSc, PhD (Kharkov Polytech), DSc (NAS, Ukraine) (2000-)

**Dr. N. Trappe**, BSc, PhD (2002-)

## POSTGRADUATE RESEARCHERS

**Mr. G. Cahill**, BSc (2001-)

**Mr. M. Cummins**, BSc, HDipAppPh (2002-)

**Ms. C. Delaney**, BSc (2001-)

**Mr. T. Finn**, BSc, (2002-)

**Ms. K. Foley**, BSc, (2002-)

**Ms. E. Gleeson**, BSc, (2001-)

**Mr. M. Gradziel**, BSc (Torun) (2000-)

\* Unless otherwise stated the higher degrees listed are those of the National University of Ireland.

**Mr. J. Lavelle**, BEng (Edinburgh) (2002-)

**Mr. P. McBride**, BSc (2001-)

**Mr. R. Mahon**, BSc (2002-)

**Mr. R. May**, BSc (2002-)

## **PROFESSOR EMERITUS**

**Professor S. McKenna-Lawlor**, MSc, PhD, FRAS, FIBA, CPhys, MInstP, Academician (IAA) (1968-)

## HEAD OF DEPARTMENT'S REVIEW OF THE YEAR

A number of significant events took place in the Department of Experimental Physics during 2002. Dr. Anthony Murphy was appointed as Professor of Experimental Physics and Head of Department in October 2002, taking up the running of the department from Acting Head Dr. Michael Cawley. The department continues to be highly active in research with strong international links in the fields of astrophysics and atomic physics. Dr. Neil Trappe was appointed as a research fellow in February to work on the development of space instrumentation funded under the European Space Agency Prodex programme. Research was funded by grants from a range of funding agencies including Enterprise Ireland, the Irish Research Council for Science Engineering and Technology, the UK Particle Physics and Astronomy Research Council and the European Space Agency. This was significantly boosted with the award of a Science Foundation Ireland Investigator Award in December 2002 along with an ETS Walton Visitor Award to Dr. Stafford Withington of the Cavendish Laboratory, Cambridge, who will visit Maynooth in 2003.

Both staff and students attended a number of international conferences during the year and presentations were made on research work carried out in the department. These conferences included the *25th European Space Agency Antenna Workshop on Satellite Antenna Technology*, at the European Space Agency Technology Centre in the Netherlands, the *SPIE Optoelectronics, Photonics and Imaging Conference*, in Galway, and the *Tenth Terahertz Electronics Symposium*, in Cambridge. Other notable events included the selection for publication in the *Virtual Journal of Ultrafast Science* of the paper by Shortt, van der Burgt, Giammanco, Slevin and Lanigan in *Physical Review E* 'Wavelength-dependent collective effects in the multiphoton ionization of atomic deuterium'. In the atomic collisions group 2002 saw the fruition of a three year project to measure all three coherence parameters that completely describe electron impact excitation of the H(2p) state.

In October 2002 the continuing popularity of the *Physics with Astrophysics* degree programme was underlined by the entry of a large second cohort of bright students with high CAO points. In line with the full implementation of the course the departmental telescope facilities were expanded during the year with the development of radio and cosmic ray telescopes as undergraduate projects, and field trips were organized to Dunsink Observatory and to Lord Rosse's famous observatory and museum in Birr Castle Demesne.

The department continues to have a strong commitment to the promotion of physics in schools with a very popular and successful laboratory class initiative for senior cycle students. A special series of experiments have been developed, which are compulsory on the new Leaving Certificate Curriculum and are difficult for schools to mount. Over 700 students from 30 schools visited the department, and not just from the local catchment area (East-midlands-Dublin) but even from as far afield as Galway, Wexford and Monaghan. This develops an extremely positive impression of science at Maynooth, builds a close relationship with physics teachers in schools and by extension with career guidance teachers, parents and the wider community. The popularity of the programme is such that this year it has been extended to run through from October to the end of May.

## RESEARCH INTERESTS OF STAFF

### Professor J.A. Murphy

In 2002 we continued our involvement in a number of international collaborative projects in far-infrared astronomical instrumentation. In terms of space projects we are primarily concerned with the development of two satellite systems. The first of these, the European Space Agency PLANCK Surveyor, will make detailed maps of the cosmic microwave background radiation, while the second, the Herschel Space Observatory, will enable wide-ranging astronomical observations of far-infrared sources in the sky. The two satellites are due to be launched in 2007 and will probe the cosmos from deep space orbits. Our main contribution to both projects is in the optical design and the detailed simulations necessary to predict and calibrate the performance of hyper-sensitive instruments on board the satellites. This research work is undertaken in close collaboration with the ESTEC (the European Space Agency Technology Centre), the Institute d'Astrophysique Spatiale (Paris), the Space Research Organisation of the Netherlands (SRON) and Cardiff University.

During 2002 we also continued our involvement in the QUEST ground based telescope development in collaboration with Stanford and Cardiff Universities, and also involving Caltech/JPL. QUEST is being built in Chile and is optimized for mapping the polarization characteristics of the cosmic microwave background. Such observations are vital to unambiguously determine fundamental cosmological parameters and distinguish between theories of the early universe. At Maynooth we played a key role in the development of the focal plane array of horn antennas as well as diffraction analysis of the optical design. We will also be testing some of these components at Maynooth during 2003.

Terahertz (T-ray) optics is a fast developing field of applied physics. Since 1998 we have been involved in a contract with the European Space Agency concerned with the verification of software tools for the terahertz waveband. As a result of this work and its importance for the future development of T-rays in biotechnology, we were fortunate to be awarded a significant grant under the Science Foundation Ireland Investigator Award scheme in 2002. This award will fund the development of CAD tools for terahertz optics and also the construction of a prototype far-infrared brain imager.

#### **Dr. M.F. Cawley**

Work continued during 2002 on the study of free convection in water in the vicinity of its density maximum at 4°C. The majority of fluids (liquids and gases) expand on heating over wide ranges of temperature and pressure – this behaviour is in accordance with our understanding of the behaviour of matter at a microscopic level (kinetic theory). The behaviour of water is anomalous in many respects; in particular, it exhibits a density maximum at 4°C at a pressure of one atmosphere ( $\sim 10^5$ Pa). Between 0°C and 4°C, water contracts when heated; above 4°C it expands on heating in the normal manner. Although the effect is small (0.01% density change between 0°C and 4°C) compared to the anomalous expansion of water upon solidification (8% volume increase in going from liquid to solid H<sub>2</sub>O at 0°C) its consequences may be readily detected in its influence on free convective flows. In a vertical cylinder of water with a horizontal temperature gradient, cooled from 8°C to 0°C (i.e. encompassing the non-linear density region), we expect that the free convective cycle will reverse in direction, which will have profound effects on the shape of the cooling curve as recorded along the central vertical axis of the cylinder. Experimental techniques used to date involve continuous recording of the temperature at several positions along the central axis during cooling and warming through the non-linear density region, combined with flow visualization using particle image velocimetry, in order to explain the changes in the cooling curves as the convective flow reversal is achieved. Computer simulations of the convective flow are also used to explore the effects of changing such parameters as the container geometry, and the degree of non-linearity of the water density as a function of temperature.

#### **Dr. P.J.M. van der Burgt**

Research on electron- and photon-impact fragmentation processes is focussing on molecules and clusters that are of interest to plasma physics, atmospheric physics and other fields, in particular metal-embedded rare-gas clusters. The experiment consists of a differentially pumped vacuum system, with an expansion chamber to generate a pulsed supersonic beam of molecules or clusters, and a collision chamber where the molecules or clusters are fragmented. In the collision chamber the supersonic beam is crossed with an electron beam or a laser beam (or both) and the reaction products are detected. Ions are detected with a reflectron time-of-flight mass spectrometer, and neutral metastable atoms are detected with a metastable detector. Several mass spectra have been measured, showing that the reflectron in combination with the pulsing and data acquisition electronics is working very well, and presently work is done on the computer interfacing (LabView) of the apparatus. A metastable atom detector is presently under construction.

Several years of work on transient plasmas produced by multiphoton ionisation of deuterium atoms culminated with the publication of two papers in research journals. A major publication covering the PhD research of Dr. Brian Shortt's work appeared in *Physical Review E*. This publication was selected for the November 2002 issue of the *Virtual Journal of Ultrafast Science* ([www.vjulfrafast.org](http://www.vjulfrafast.org)), which is a multi-journal compilation of links to articles covering frontier research on ultrafast phenomena in physics, optics, chemistry, and biology. In the experiment, a pulsed laser beam is crossed with a beam of deuterium atoms, and atoms that simultaneously absorb two photons are excited to their metastable 2s state which is ionised by a third photon. Collective effects

occurring in the transient plasma of electrons and ions produced by the multiphoton ionization are observed in the yield and the time-of-flight profiles of the ions measured as a function of laser intensity. We are collaborating with Professor F. Giammanco from the University of Pisa, Italy, who is simulating the collective effects based on a numerical plasma model.

#### **Dr. R.W. O'Neill**

In 2002 our research programme on electron scattering from atomic targets has made excellent progress. This process is important in a variety of fields including plasma physics, astrophysics, atmospheric physics (planetary and stellar atmospheres, interstellar clouds) and the physics of lasers. We are making electron-photon coincidence measurements of electron scattering from hydrogen using a “double rotation” vacuum ultraviolet polarisation analyser. This device allows simultaneous determination of both the linear and circular polarisation properties of the light emitted in the decay of the excited 2p state of atomic hydrogen and thus provides a more complete and detailed description of the excited state than has previously been possible. We have completed measurements up to 40° electron scattering angle and found that current theories provide an accurate description over most of this range. This work is detailed and each measurement takes several months to complete; results have been submitted for publication to *Journal of Physics B*.

Work is also ongoing in the area of Quantum Information. A pair of entangled particles is described by a single wave function that dictates the mutual properties of the pair. Any measurement carried out on one particle will instantaneously influence the other member of the pair regardless of the distance separating the particles. This physics of entanglement is central to possible schemes for novel technologies such as quantum computation and quantum cryptography. We are working to construct a bright source of polarisation entangled photons at 883.2nm, using parametric down conversion of 441.6nm light from a Helium-Cadmium laser. Our medium term goals are to undertake experiments in cryptography using these entangled particles, and also experiments aimed at further elucidating the fundamental aspects of quantum mechanics.

#### **Dr. C. O'Sullivan**

Dr. O'Sullivan's research interests are in the fields of astrophysics and astronomical instrumentation. As part of the NUIM Far-Infrared and Submillimetre Space Astrophysics group Dr. O'Sullivan has worked on a number of international research programmes. These include a collaboration to investigate optical design tools for far-infrared astronomical systems for which standard optical design techniques are inappropriate, and telescopes to image faint temperature and polarisation anisotropies in the cosmic microwave background radiation.

Adaptive optics is a technique by which adjustments are made to the shape of a telescope's mirror in order to correct for aberrations introduced into observations by the atmosphere. A guide star is used to sample the atmospheric turbulence, and the most promising method creates this guide star by using the backscatter of sodium laser light from the upper atmosphere. Dr. O'Sullivan has worked with NUI Galway as part of a European collaboration co-ordinating efforts to produce a set of theoretical and experimental studies necessary for the implementation of laser guide star adaptive optics on large ground-based optical telescopes.

#### **Mr. W. Lanigan**

Mr. W. Lanigan's research interests are in the field of Terahertz instrumentation for astronomy and medical imaging. As part of the NUIM Far-Infrared and Submillimetre Space Astrophysics group Mr. Lanigan carries out measurement and verification of quasi-optical components for space based astronomical instruments. His other area of research is in the field of using Terahertz radiation for medical imaging. Terahertz radiation is much less damaging to biological tissue than conventional x-rays and while it does not provide the same penetration or resolution as X-rays there are many potential applications where it will be well suited.

## RESEARCH GRANTS

'Very energetic radiation imaging telescope array system'. Enterprise Ireland Basic Research Grant, 2000-2002, €5,700 (Dr. M.F. Cawley).

'Terahertz optics and technology'. ETS Walton Visitor Award 2002, (Dr. Stafford Withington, Cavendish Laboratory, to visit NUIM Summer 2003) Science Foundation Ireland, 2002, €36,143 (Professor J.A. Murphy).

'Optical design of the HFI instrument on ESA PLANCK satellite to map the cosmic microwave background'. Enterprise Ireland Basic Research Grant, 2001-2003, €127,000 (Professor J.A. Murphy).

'Study of systematic effects for PLANCK HFI project'. Enterprise-Ireland Ulysses France-Ireland Exchange Research Visitor Award, 2002, €2,400 (Professor J.A. Murphy).

'Optical design of HiFi instrument on the FIRST space telescope.' Grant from PRODEX Fund (European Space Agency), 1999-2003, €75,000 (Professor J.A. Murphy).

'Optical design of the QUEST telescope to map the polarisation properties of the cosmic microwave background'. IRCSET Basic Research Grant, 2002-2005, €152,800 (Professor J.A. Murphy and Dr. C. O'Sullivan)

'Far infrared optical design and verification.' Research Contract, European Space Agency, 1998-2003, €50,000 (Professor J.A. Murphy and Dr. C. O'Sullivan).

'Optical design support for instrumentation development on James Clerk Maxwell Telescope.' Rolling Travel Grant from UK PPARC (Particle Physics and Astronomy Research Council), 2002-2004, €15,000 (Professor J.A. Murphy).

'The development of an integrated quasi-optical and electromagnetic numerical simulator for the computer aided design and analysis of novel terahertz systems'. Science Foundation Ireland Investigator Award, 2003-2006, €786,000 (Professor J.A. Murphy, Mr. W. Lanigan, Dr. C. O'Sullivan and Dr. V. Yurchenko).

'Experimental electron impact excitation of H(2p)'. Enterprise Ireland Basic Research Grant, 1999-2002, €51,000 (Dr. R.W. O'Neill).

## PUBLICATIONS IN REFEREED JOURNALS

A. Benoît, P. Ade, A. Amblard, R. Ansari, É. Aubourg, S. Bargout, J.G. Bartlett, J.-Ph. Bernard, R.S. Bhatia, A. Blanchard, J.J. Bock, A. Boscaleri, F.R. Bouchet, A. Bourrachot, P. Camus, F. Couchot, P. de Bernardis, J. Delabrouille, F.-X. Désert, O. Doré, M. Douspis, L. Dumoulin, X. Dupac, P. Filliatre, P. Fosalba, K. Ganga, F. Gannaway, B. Gautier, M. Giard, Y. Giraud-Héraud, R. Gispert, L. Guglielmi, J.-Ch. Hamilton, S. Hanany, S. Henrot-Versillé, J. Kaplan, G. Lagache, J.-M. Lamarre, A.E. Lange, J.F. Macías-Pérez, K. Madet, B. Maffei, Ch. Magneville, D.P. Marrone, S. Masi, F. Mayet, **J.A. Murphy**, F. Naraghi, F. Nati, G. Patanchon, G. Perrin, M. Piat, N. Ponthieu, S. Prunet, J.-L. Puget, C. Renault, C. Rosset, D. Santos, A. Starobinsky, I. Strukov, R.V. Sudiwala, R. Teyssier, M. Tristram, C. Tucker, J.-C. Vanel, D. Vibert, E. Wakui and D. Yvon. The cosmic microwave background anisotropy power spectrum measured by Archeops. *Astronomy and Astrophysics* **399**, L19-23. (2003).

A. Benoît, P. Ade, A. Amblard, R. Ansari, É. Aubourg, S. Bargout, J.G. Bartlett, J.-Ph. Bernard, R.S. Bhatia, A. Blanchard, J.J. Bock, A. Boscaleri, F.R. Bouchet, A. Bourrachot, P. Camus, F. Couchot, P. de Bernardis, J. Delabrouille, F.-X. Désert, O. Doré, M. Douspis, L. Dumoulin, X. Dupac, P. Filliatre, P. Fosalba, K. Ganga, F. Gannaway, B. Gautier, M. Giard, Y. Giraud-Héraud, R. Gispert, L. Guglielmi, J.-Ch. Hamilton, S. Hanany, S. Henrot-Versillé, J. Kaplan, G. Lagache, J.-M. Lamarre, A.E. Lange, J.F. Macías-Pérez, K. Madet, B. Maffei, Ch. Magneville, D.P. Marrone, S. Masi, F. Mayet, **J.A. Murphy**, F. Naraghi, F. Nati, G. Patanchon, G. Perrin, M. Piat, N. Ponthieu, S. Prunet, J.-L. Puget, C. Renault, C. Rosset, D. Santos, A. Starobinsky, I. Strukov, R.V. Sudiwala, R. Teyssier, M. Tristram, C. Tucker, J.-C. Vanel, D. Vibert, E. Wakui and D. Yvon. Cosmological constraints from Archeops. *Astronomy and Astrophysics* **399**, L25-30. (2003).

A. Benoit, P Ade, A. Amblard, R. Ansari, E. Aubourg, J. Bartlett, J.P. Bernard, R.S. Batia, A. Blanchard, J.J. Bock, A. Boscaleri, F.R. Bouchet, A. Bourrachot, P. Camus, P. deBernardis, J. Delabrouille, F.X. Desert, O. Dore, M. Douspis, L. Dumoulin, X. Dupac, P. Filliatre, K. Ganga, F. Gannaway, B. Gautier, M. Giard, Y. Giraud-Heraud, R. Gispert, L. Guglielmi, J.C. Hamilton, S. Hanany, S. Henrot-Versille, V.V. Hristov, J. Kaplan, G. Lagache, J.M. Lamarre, A.E. Lange, K. Madet, B. Maffei, D. Marrone, S. Masi, **J.A. Murphy**, F. Naraghi, F. Nati, G. Perrin, M. Piat, J.L. Puget, D. Santos, R.V. Sudiwala, J.C. Vanel, D. Vibert, E. Wakui and D. Yvon. Archeops: A high resolution large sky coverage balloon experiment for mapping CMB anisotropies. *Astroparticle Physics* **17**, 101-124 (2002).

**E. Gleeson, J.A. Murphy** and B. Maffei. Phase centers of far infrared multi-moded horn antennas. *International Journal of Infrared and Millimeter Waves*, **23**, 711-730, (2002).

**J.A. Murphy, N. Trappe** and S. Withington. Gaussian beam mode analysis of partial reflections in simple quasi-optical systems fed by horn antennas. *Infrared Physics and Technology* (in press).

**C. O'Sullivan, J.A. Murphy**, S. Withington, G. Yassin, E. Atad-Ettdogui, W. Duncan, D. Henry, W. Jellema and H. van de Stadt. Far-Infra red optics design and verification. *International Journal of Infrared and Millimeter Waves*, **23**, 1029-1045, (2002).

B.J. Shortt, **P.J.M. van der Burgt**, F. Giammanco, J.A. Slevin and **W. Lanigan**. Wavelength-dependent collective effects in the multiphoton ionization of atomic deuterium. *Physical Review E* **66** (2002) 046411 - 1-10. This paper was selected for publication in the *Virtual Journal of Ultrafast Science* ([www.vjulfast.org](http://www.vjulfast.org)), **1**, (2002).

B.J. Shortt, **P.J.M. van der Burgt** and F. Giammanco. Resonant three-photon ionization of atomic hydrogen in a finite-bandwidth laser field and a static electric field. *Laser Physics* **12**, 1402-1409. (2002).

**N. Trappe, J.A. Murphy** and S. Withington. The Gaussian beam mode analysis of classical phase aberrations in diffraction limited optical systems. *European Journal of Physics* (in press).

## CONFERENCE PROCEEDINGS

**G. Cahill, C. O'Sullivan** and **J.A. Murphy**. 'The Quest experiment to measure the polarisation properties of the Cosmic Microwave Background,' *Astronomical Science Group of Ireland Spring Meeting*, TCD, Dublin (22 March 2002).

**G. Curran, R Hennessy, J.A. Murphy, C. O'Sullivan** and **W. Lanigan**. 'Quasi-optical systems for space telescopes', *Astronomical Science Group of Ireland Spring Meeting*, TCD, Dublin (22 March 2002).

**E. Gleeson**. 'Optical design of the PLANCK surveyor for mapping the cosmic microwave background,' *Institute of Physics Spring Meeting*, Cork (22-24 March 2002).

**E. Gleeson, J.A. Murphy**, B. Maffei, J-M Lamarre and R. J. Wylde. 'Definition of the multi-mode horns for the HFI instrument on PLANCK,' *Proceedings of the 25th ESA Antenna Workshop on Satellite Antenna Technology (ESTEC)* Noordwijk, The Netherlands, (18-20 September, 2002)

J.M. Lamarre, J.L. Puget, M. Piat, P.A.R. Ade, A. Lange, A. Benoit, P. de Bernardis, F.R. Bouchet, J. Bock, F.X. Desert, R. Emery, M. Giard, B. Maffei, **J.A. Murphy**, J.P. Torre, R. Bhatia, R. Sudiwala, and **V. Yourchenko**. 'The Planck high frequency instrument, a third generation CMB probe and the first submillimeter surveyor,' *Astronomical Telescopes and Instrumentation*, Waikoloa, Hawaii SPIE Conference, pp. 5840, 2002. (22-28 August, 2002).

J.M. Lamarre, M. Piat, P.A.R. Ade, J. Bock, P. de Bernardis, M. Giard, A. Lange, **J.A. Murphy**, J.P. Torre, A. Benoit, R. Bhatia, F.R. Bouchet, B. Maffei, J.L. Puget, R. Sudiwala and **V. Yourchenko**. 'Use of high sensitivity bolometers for astronomy: Planck high frequency instrument,' *Low Temperature Detectors (LTD9)*, Madison (WI), USA, *AIP Conference Proceedings*, 605, 571-576, 2002 (22-27 July 2001).

**C. O'Sullivan**. 'Far-infrared optics design and verification', *European Space Agency*, Noordwijk, The Netherlands (27 November 2002).

**C. O'Sullivan.** 'The big bang and the background radiation', *Astronomy Ireland*, DCU (10 June 2002).

**N. Trappe** and **J.A. Murphy.** 'The Quasi-optical analysis of the HIFI front-end optical system'. *Proceedings of the 25th ESA Antenna Workshop on Satellite Antenna Technology, 2, ESTEC*, Noordwijk, The Netherlands (18-20 September, 2002).

**N. Trappe** and **J.A. Murphy.** 'The HIFI instrument for the Herschel space observatory'. *Astronomical Science Group of Ireland Autumn Meeting*, NUI, Galway (18 October 2002).

**N. Trappe, J.A. Murphy,** B. Kruizinga, H. Visser, W. Jellema, K. Wildeman and H. van de Stadt. 'Quasi-Optical analysis of the front-end optical system of the HIFI instrument for the Herschel space observatory', *Proceedings of the 25th Antenna Workshop on Satellite Antenna Technology*, ESA, Noordwijk, Holland (20 September 2002).

**N. Trappe, J.A. Murphy,** B. Kruizinga, H. Visser, W. Jellema, K. Wildeman and H. van de Stadt. 'Quasi-Optical analysis of the HIFI instrument for the Herschel space observatory', *SPIE Proceedings Optoelectronics, Photonics and Imaging*, Galway (5 September 2002).

**P.J.M. van der Burgt.** 'Collective effects in the multiphoton ionisation of atomic deuterium'. *Département de Physique, Université Catholique de Louvain, Louvain-la-Neuve, Belgium* (18 July 2002).

V. Yassin, S. Withington, **C. O'Sullivan, J.A. Murphy,** T. Peacocke, W. Jellema and P. Wesselius. 'Electromagnetic modelling of submillimetre-wave systems'. *Proceedings of the 13th International Symposium on Space Terahertz Technology*, Harvard, USA (26-28 March 2002).

**V. Yurchenko, J.A. Murphy,** and J.M. Lamarre. 'PLANCK HFI beam simulations for polarized and multi-moded horns.' *Proceeding of the 25th ESA Antenna Workshop on Satellite Antenna Technology* (eds. K. van't Klooster and L. Fanchi), ESTEC, Noordwijk, The Netherlands, 18-20 September, 2002, pp. 281-286 (2002).

## EXTERNAL ASSIGNMENTS AND PUBLIC SERVICE

### Dr. N. McKeith

- Curator, National Science Museum, St. Patrick's College, Maynooth
- Member, Radiological Protection Institute of Ireland.

### Professor J.A. Murphy

- Member, Royal Irish Academy Sub-committee for Physics
- External Examiner for PhD Thesis at Physics Department, Cambridge University, September 2002.

### Dr. F.J. Mulligan

- Chairman of the Radiological Protection Institute of Ireland (2000-2005)
- Member of the Board, Radiological Protection Institute of Ireland (April 1997 – present).

### Dr. R.W. O'Neill

- Member of the Institute of Physics
- Member of the American Physical Society.

### Dr. C. O'Sullivan

- Member, National Committee for Astronomy and Space Research, Royal Irish Academy.

### Dr. P. van der Burgt

- Honorary Secretary, Institute of Physics in Ireland
- Member, National Committee for Physics, Royal Irish Academy.



**Faculty of Science**

**Research Report 2002**

**Mathematics**



# MATHEMATICS

## ACADEMIC STAFF\*

**Professor A.G. O'Farrell**, MSc, PhD (Brown), MRIA, FIMA, CMath (1975-)  
**Dr. S.M. Buckley**, MSc, PhD (Chicago) (1993-)  
**Dr. C.M. Comiskey**, BA (Mod), MSc, PhD (DCU) FIMA, C Math(1998-)  
**Dr. D.Dickinson**, BSc DPhil (York) (2001-)  
**Dr. C.B. Hurley**, BSc, PhD (Washington) (1995-)  
**Dr. P. McCarthy**, MSc, PhD (1994-)  
**Dr. G. McGuire**, MSc, PhD (Caltech) (1998-)  
**Dr. J. Murray**, BEng, DipMathSc, MSc, PhD (Illinois) (2001-)  
**Dr. F. Ó Cairbre**, MSc, PhD (Berkeley) (1990-)  
**Dr. A. O'Shea**, MA, MS (Notre Dame), PhD (Notre Dame) (1992-)  
**Dr. D. Redmond**, MSc, PhD (Illinois) (1977-)  
**Dr. A. Small**, BA (Warwick), PhD (Warwick) (1995-)  
**Dr. D. Walsh**, MSc, PhD (Swansea) (1972-)  
**Dr. R.O. Watson**, MSc, BD, MPhil (Warwick), PhD (1973-)  
**Dr. D. Wraith**, BA (Cambridge), PhD (Notre Dame) (1997-)

## CONTRACT LECTURERS

**Dr. S. Breen**, BSc (DCU), PhD (DCU) (1999-)  
**Dr. J. Foy**, MSc, PhD (Yale) (2001-2002)  
**Dr. G. Crispino-O'Connell**, BSc (Bocconi), PhD (IT Tallaght) (2002)  
**Dr. D. O'Keefe**, PhD (2001-2002)  
**Dr. D. Ryan**, PhD (2001-2002)

## POST-DOCTORAL FELLOWS

**Dr. A. Diatta**, PhD (Montpellier) (2001-2002)  
**Dr. E. Byrne**, MSc, PhD (2001-)

## TECHNICAL STAFF

**Ms. J. Love**, Technical Support Officer. MSc (1994-) Secondment (2002-2003)  
**Mr. C. List**, Technical Support Officer. DipMath (Tübingen), MA (2002-2003)

## POSTGRADUATE RESEARCH STUDENTS

**Mr. C. Bracken**, BSc (2001-)  
**Mr. S. Brannick**, BSc, HDipMa (2001-)  
**Ms. M. Gannon**, BSc, HDipMa (2000-)  
**Ms. P. Howard**, BSc, MSc (Reading) (2000-)  
**Mr. M. Kerin**, BSc (2001-)  
**Mr. C. List**, DiplMath (Tübingen), MA (1996-)  
**Mr. C. Mac an Bhaird**, BA, MSc (1998-)  
**Ms. S Mac Donald**, BA, MA, PGDipCompSc (Keele) (2002-)  
**Mr. O. Mason**, BA (Mod), MSc (Dublin) (2001-)

\* Unless otherwise stated the higher degrees listed are those of the National University of Ireland.

**Ms. K. O'Flaherty**, BSc (1999-)

**Mr. D. Walsh**, BSc (DCU) (2000-)

**Mr. M. Walsh**, BSc, HDipAppPh, HDipMa (2000-)

## **RESEARCH ASSISTANTS**

**Ms. E. McGovern**, Bachelors of Business Studies – Marketing (IT Tallaght) (2002-)

## **VISITING FELLOW**

**Dr. V. Chrastinova**, BA, MA, PhD (Masaryk University, Brno) (2001-)

## **EXECUTIVE ASSISTANTS**

**Ms. D. Keenan**, (1999-)

**Ms. G. O'Rourke**, BA (2000-)

## HEAD OF DEPARTMENT'S REVIEW OF THE YEAR

There were no changes in the permanent staff of the Department during the year (apart from the usual advance in age). Two senior members, Richard Watson and David Redmond, continued to serve in senior University positions, as Dean of Arts and Registrar, respectively. Sinéad Breen continued as Richard's substitute. Stephen Buckley and Anthony Small returned from Sabbatical Leave, and their replacements left, John Foy for the Hamilton Institute across campus, and Declan O'Keeffe for Austria and a new career. Postdoc André Diatta left for a position with Giblin at Liverpool. New postdoctoral researchers arrived. Eimear Byrne came from Fitzpatrick's group in Cork to work with Gary McGuire and our Coding Theory group. Veronika Chrastinova came on an eighteen-month visit from Brno. Her work is on differential equations. The ROSIE Project got under way towards the end of the year, and Gloria Crispino and Elaine McGovern arrived from IT Tallaght as the first of two postdoctoral workers and three students. This project results from a successful tender to the National Advisory Committee on Drugs by Catherine Comiskey, and involves a study of drug-abuse treatment regimes in Ireland.

Janice Love, our Software Support Officer, was seconded to the Quality Promotions Office for a year, and replaced in the interim by Christoph List.

The regular hebdomadal Colloquia and instructional Seminars continued, as well as the specialised seminar on Coding Theory and 'scheduled conversations' (informal interdisciplinary working groups). Members of the Department continued joint research with members of the Hamilton Institute, the National Institute for Regional and Spatial Analysis, and the Department of Education.

The Department reviewed its postgraduate lecture course programme and revised it with a view to facilitating a US-style structure for its research students' studies (with coursework assisting their preliminary reading), and facilitating multi-year forward planning.

## RESEARCH INTERESTS OF STAFF

### **Dr. Sinéad Breen**

Sinéad Breen's research interests are in asymptotic analysis, resurgent analysis and perturbation theory. In the past much of her work has involved determining asymptotic estimates of integrals which can arise, for instance, in the solution of various differential equations. Of particular interest to her are functions that can be represented as integrals containing saddlepoints. More recently she has been interested in the application of resurgence theory to problems in asymptotic analysis - such an approach has proved useful in obtaining hyperasymptotic (exponentially-improved) estimates in certain cases. Recently, she has also become interested in the use of queueing theory in modelling waiting lists.

### **Dr. Stephen Buckley**

Stephen Buckley is interested in many areas of analysis, including harmonic analysis, partial differential equations, potential theory, quasiconformal mappings, and hyperbolic geometry. This year, he finished work on relative solidity for holomorphic spaces, on quasiconformal images of Hölder domains, and joint work with Alex Stanoyevitch (Guam) on weak slice conditions. He continued research with Alex Stanoyevitch and André Diatta on weak slice conditions, and began work on Orlicz-Hardy inequalities with Pekka Koskela (Jyväskylä). He made research visits to U. Chicago, U. Illinois (Urbana), Cincinnati, Helsinki, Jyväskylä, Bern, gave invited talks in Chicago, Urbana, Cincinnati, Helsinki, Bern, UCD, Limerick, IT Tallaght, and Michigan (three times), plus at an AMS regional meeting in Ann Arbor. He also attended AMS meetings in Ann Arbor and Lexington, and the IMS meeting in Cork. He availed of sabbatical leave to spend the 2001-2002 academic year at the University of Michigan, Ann Arbor for a Special Year in Complex Analysis.

**Dr. Eimear Byrne**

Symbolic Computation: Gröbner bases, finite chain rings, key equations, linear feedback shift registers. Algebraic Coding Theory: Z<sub>4</sub>-codes, codes over finite chain rings, alternant, cyclic and negacyclic codes, Lee-metric codes, codes and lattices, decoding algorithms, constructions of low-density parity check codes (LDPCs), algebraic codes on graphs. Designs and Geometries: Steiner systems, partial geometries, designs and codes, LDPCs from designs, incidence structures over Galois rings, coloured designs.

**Dr. Veronika Chrastinova**

Veronika Chrastinova works on modules of differential forms, especially the use of such modules to classify and simplify systems of differential equations, particularly those arising from variational problems.

**Dr. Catherine Comiskey**

Catherine Comiskey has been working in the area of the dynamics of mathematical modeling of epidemics since 1985 and has published in Ireland, Europe and Australia on HIV and AIDS in drug users. Dr. Comiskey was invited to become the Irish representative on the European Monitoring Centre of Drugs and Drug Addiction's expert group in dynamic modeling of drug related problems. She is also the Irish representative on the EMCDDA's network of researchers looking at local and national prevalence and geographical spread of drug use.

**Dr. Detta Dickinson**

Detta Dickinson's research interests lie in the areas of measure theory and metric Diophantine approximation. In particular, Diophantine approximation on manifolds. Classically, Diophantine approximation is the study of how well real numbers can be approximated by rationals. This can be extended to higher dimensions by asking how well real points in n-dimensional Euclidean space can be approximated by rational points or by rational hyperplanes. Results in this area are very delicate as shown in Khintchine's theorem, where the set of well approximable points has either zero or full measure depending on the convergence or divergence of a certain volume sum. This leads to further questions - those of Hausdorff dimension in the case of measure zero and those of asymptotic number of solutions in the case of full measure. Both of the above questions become more difficult when the set under investigation is restricted to a manifold embedded in Euclidean space and this is Detta's current area of interest.

**Dr. John Foy**

John Foy has research interests in logic, theoretical computer science and the foundations and interpretation of quantum mechanics.

**Dr. Catherine Hurley**

Catherine Hurley's research interests are in statistical computing, graphics and data analysis. At present, she and her PhD student, Mr. Christoph List, are interested in developing statistical graphics tools based on JAVA. Dr. Hurley attended the Conference for Applied Statistics in Ireland (CASI) in May 2002 where she presented her work on 'Clustering Visualizations of Multidimensional Data'. In August, she gave a talk on a related topic 'Clustering Graphics' at the CompStat 2002 meeting in Berlin. She also participated in a workshop on Data Visualization at the University of Augsburg in October 2002.

**Dr. Pat McCarthy**

Pat McCarthy is interested in the interplay between real and complex analysis and in particular in the study of interpolation operators and maximal summation operators. He is also interested in analytic and algebraic number theory, especially in cyclotomic number fields and Gaussian sums. His current MSc student Shane Brannick, is working on symbolic integration and differential fields.

**Dr. Gary McGuire**

Algebra and discrete mathematics, error-correcting codes, combinatorial designs, finite geometries, algebraic number theory.

**Dr. John Murray**

John Murray's area of research is the representation theory of finite groups. This is a subject that has strong connections with group theory and linear algebra, and has applications to all areas of mathematics (for instance the theory of Galois representations was crucial to the proof of Fermat's Last Theorem) and mathematical physics (including quantum theory and string theory). The most important and exciting problem in this area is known as 'Alperin's weight conjecture'. This was formulated by J. Alperin in 1986, and has since been generalised in a number of complex ways, notably by the abelian defect conjecture of M. Broue, and the alternating sum conjectures of E. Dade and G. Robinson. What makes these conjectures so interesting is that they hint at connections between representation theory and other areas of mathematics such as algebraic topology and the theory of Lie algebras and Quantum groups.

**Dr. Fiacre Ó Cairbre**

F. Ó Cairbre's main research interests lie in the general area of Dynamical Systems and in applications to electronic engineering. He worked with Robert Shorten (Hamilton Institute, Maynooth) in the area of 'switching dynamical systems' in control theory. Control theory involves the study of control systems and some examples of applied control systems are flight control systems and robotic systems. There are many fundamental problems in the area of switching systems that remain unsolved. In particular, many important questions concerning the stability of switching systems are still unanswered. They worked on stability problems for various classes of switching systems.

**Professor Anthony G. O'Farrell**

Anthony G. O'Farrell continues to be interested in approximation problems involving holomorphic functions of one and several variables, harmonic functions, smooth real-valued functions, polynomials and rational functions, and related problems about geometric, measure-theoretic, potential-theoretic, dynamical, and functional analytic matters. He tried to learn some new things during the year, in conversation with André Diatta, Veronika Chrastinova, and other colleagues on the permanent staff. He finished two books of mathematics, mainly intended for young people. The first, an Olympiad Training Manual, was written jointly with Gary McGuire, David Redmond, Richard Watson and David Wraith. The second is in Irish.

**Dr. Ann O'Shea**

Ann O'Shea's recent research has been in the area of Financial Mathematics. She has focused on the problem of pricing exotic derivatives, especially energy derivatives. She is also interested in Mathematics Education and gave a talk at the Undergraduate Mathematics Education Symposium held in TCD in December.

**Dr. David Redmond**

David Redmond's area of specialisation is Group Theory and Permutation Groups. He has been working with Professor Quinn (Maynooth) and Dr. P.W. Fowler (Exeter) on the application of group theory in Chemistry and in particular on the recent developments in the chemistry and geometry of Fullerenes.

**Dr. Dermot Ryan**

Algebraic K-theory, homological algebra, algebraic geometry and error-correcting codes.

#### **Dr. Anthony J. Small**

Anthony Small is working on problems in algebraic/differential geometry, in particular, the construction and study of differential geometric objects of variational origin, via ‘transforms’ that convert the data into more tractable algebro-geometric objects, e.g. Minimal surfaces (soap films), Constant mean curvature surfaces (soap bubbles) and Monopoles.

#### **Dr. David Walsh**

David Walsh’s research interests are in Classical and Functional Analysis especially in the theory of function spaces (analytic and otherwise) and in Hankel and Toeplitz Operators. There is a close interplay between these topics. He continues to work on Besov spaces, Mean Lipschitz Classes and related spaces. A problem of particular interest at the moment is that of best analytic approximation of functions in a variety of spaces and the properties of the best approximation operator.

#### **Dr. Richard Watson**

Richard Watson is interested in algebraic number theory, algebraic K-theory, and algebras of smooth functions. He continues to work with Susan MacDonald (Waterford Institute of Technology) on matters related to Irish secondary school geometry syllabi.

#### **Dr. David Wraith**

The main focus of David Wraith’s research concerns existence questions for Riemannian metrics with prescribed curvature characteristics.

## **RESEARCH GRANTS**

‘Aspects of geometric measure theory and harmonic analysis’. Enterprise Ireland Basic Research Grant, 1998-2002, €48,758 (Dr. S. Buckley).

‘Gromov hyperbolicity and geometry of domains’. NUI Maynooth Research Enhancement Fund, 2002-2004, €5,079 (Dr. S. Buckley).

‘A longitudinal study evaluating the treatment provided for opiate use in Ireland’. National Advisory Committee on Drugs, 2002-2005, €640,000 (Dr. C.M. Comiskey).

‘A network analysis study of opiate use in Ireland’. National Advisory Committee on Drugs, 2002–2003, €140,000 (Dr. C.M. Comiskey with Dr. J. Saris, Department of Anthropology, NUI Maynooth).

‘Modelling the spread and cost of Hepatitis C in Irish drug users’. The Health Research Board, 2000-2003, €55,000 (Dr. C.M. Comiskey).

‘P-adic Diophantine approximation’. Enterprise Ireland International Collaboration Programme with Northwest University, Xian P.R., China, 2002–2003, €3,800 (Dr. D. Dickinson).

Awarded funding for a one week visit to the University of Augsburg by the Department of Education under European Cultural Agreements 2002, €800 (Dr. C. Hurley).

‘Constructions of new error-correcting codes’. Enterprise Ireland Basic Research Grant, 2000-2002, £23,500 (Dr. G. McGuire).

‘Coding theory collaboration’. NUI Maynooth Research Enhancement Fund, 2002-2004, £2,000 (Dr. G. McGuire).

‘Multi-Agent control’. European Commission Research Training Network, 200-2004, €200,000 (Dr. F. Ó Cairbre).

‘Network on analysis and operators’. European Union DG XII 2000-2003, €1.5 million (Professor A.G.O’ Farrell, Dr. D. Walsh, Dr. A. O’ Shea, Dr. P. McCarthy).

'The existence of metrics with positive Ricci curvature.' New Researcher Award, NUI Maynooth, 2001, £4,000 (Dr. D. Wraith).

'Contact manifolds in Riemannian geometry.' Enterprise Ireland International Collaboration Grant, 2002, €1,000 (Dr. D. Wraith).

'Surgery and the topology of 5-manifolds.' Cultural Agreement Award, in association with the Irish and German governments 2002, €1,000 (Dr. D. Wraith).

## PUBLICATIONS IN REFERRED JOURNALS

Z. Balogh and **S. Buckley**. 'Geometric characterizations of Gromov hyperbolicity'. *Inventiones Mathematicae* (in press).

**S. Buckley**. 'Relative solidity for spaces of holomorphic functions'. *Proceedings of the Royal Irish Academy* (in press).

**E. Byrne** and P. Fitzpatrick. 'Hamming metric decoding of alternant codes over Galois rings'. *IEEE Transactions on Information Theory* **48**, 683-694 (2002).

**E. Byrne**. 'Decoding a class of Lee metric codes over a Galois ring'. *IEEE Transactions on Information Theory* **48**, 966-975 (2002).

A. Carroll, T. Mattison, and **C.M. Comiskey**. 'An audit of a new system of self referral in the management of patients with multiple sclerosis'. *International Journal of MS Care* **4**, 1-5, (2002).

Y.H. Choi and **C.M. Comiskey**. 'Modelling Ross River virus transmission in Western Australia'. *Mathematics Applied in Medicine and Biology* **18**, 61-74 (2002).

**V. Chrastinova**. 'On the Mayer Problem - I. General Principles'. *Mathematica Slovaca* **52**, 555-570 (2002).

**V. Chrastinova**. 'On the Mayer Problem - II. Examples'. *Mathematica Slovaca* **52**, 571-590 (2002).

**C.M. Comiskey**. 'Young people, drug use and early school leaving - estimating the prevalence, assessing the impact and assisting policy and planning'. *Education, Prevention and Policy* (in press).

**D. Dickinson**, T. Gramchev and M. Yoshino. 'Perturbations of vector fields on tori : resonant normal forms and Diophantine phenomena'. *Proceedings of the Edinburgh Mathematical Society* **45**, 731-759 (2002).

**G. McGuire** and W. Broughton. 'On the non-existence of quasi-3 designs'. *Discrete Mathematics* (in press).

**J. Murray**. 'Squares in the centre of the modular group algebra of a finite symmetric group'. *Bulletin of the London Mathematical Society* **34**, 155-164 (2002).

**J. Murray**. 'Generators for the centre of the group algebra of a symmetric group'. *Journal of Algebra* (in press).

**A.G. O'Farrell** and M.A. Sanabria-García. 'De Paepe's disc has nontrivial polynomial hull'. *Bulletin of the London Mathematical Society* **34**, 1-5 (2002).

R. Shorten and **F. Ó Cairbre**. 'A new methodology for the stability analysis of pairwise triangularisable and related switching systems'. *Institute of Mathematics and its Applications: Journal of Applied Mathematics* **67**, 441-457 (2002).

**A. Small**. 'The spectral lines of the charge 2 axially symmetric monopole'. *Journal of Physics A: Mathematical and General*, **35**, 5763-66 (2002).

**A. Small**. 'Remarks on a construction of Duistermaat'. *Mathematica Scandinavica* (in press).

**A. Small**. 'Algebraic minimal surfaces in  $3\mathbb{4}$ '. *Mathematica Scandinavica* (in press).

**D. Walsh**. 'Criteria for membership of the mean Lipschitz spaces'. *Zeitschrift für Analysis und ihre Anwendungen* (in press).

**D. Wraith**. 'Deforming Ricci positive metrics'. *Tokyo Mathematics Journal* **25**, 181-189 (2002).

## BOOKS, BOOK CHAPTERS AND REVIEWS

**S.M. Buckley.** 'On pseudospheres that are quasispheres' by J Lewis and A. Vogel, *Mathematical Reviews* (in press).

**S.M. Buckley.** 'Invariance properties of  $L_1(\mu)$  - averaging domains under some mappings' by G. Bao and S. Ding. *Mathematical Reviews*, 2002d:30026 (2002).

**S.M. Buckley.** 'Analytic properties of locally quasisymmetric mappings from Euclidean domains' by J.T. Tyson. *Mathematical Reviews*, 2002b:30025 (2002).

**S.M. Buckley.** 'A counterexample theorem in quasiconformal mapping theory' by Y. Shen. *Mathematical Reviews* 2002a:30035 (2002).

**G. McGuire, A.G. O'Farrell, D.B. Redmond, R. O. Watson and D. Wraith,** *Maynooth Mathematical Olympiad Manual*. Logic Press, Kildare (2002).

**A.G. O'Farrell.** *Nótaí an Bhráthar MacCraith*. Marino Institute of Education, Dublin (2002).

## CONFERENCE PROCEEDINGS

**S.M. Buckley.** 'Geometric characterizations of Gromov hyperbolicity'. *AMS Mid-west Regional Meeting*, Ann Arbor (3 March 2002).

**D. Dickinson.** 'Simultaneous Diophantine approximation on manifolds'. *B(A)MC Warwick* (April 2002).

**D. Dickinson.** 'P-adic Diophantine approximation', Seminar Presentation, Northwest University, Xi'an, China (9 August 2003).

**D. Dickinson.** 'Diophantine approximation on translated polynomial surfaces'. *Workshop on Differential Operator Theory*, Cagliari, Italy (June 2002).

**C.B. Hurley.** 'Clustering Graphics'. *CompStat 2002 Proceedings - Short Communications and Posters* (2002). Berlin (26 August 2002).

**C.B. Hurley.** 'Clustering visualizations of multidimensional data'. *Proceedings of Conference of Applied Statistics in Ireland*. Antrim (16 May 2002).

T. Laffey, R. Shorten, and **F. Ó Cairbre,** 'On the stability of convex sums of rank-1 perturbed matrices'. *Proceedings of the American Control Conference*, Anchorage, Alaska (8 May, 2002).

**P. McCarthy.** 'The geometry of reproducing kernels'. *Irish Mathematical Society Meeting*, University College Cork (7 September, 2002).

**A. O'Shea.** 'Addressing declining standards in Mathematics'. *Undergraduate Mathematics Education Symposium*, TCD (7 December, 2002).

**D. Walsh.** 'Criteria for membership of the mean Lipschitz classes'. *Irish Mathematical Society Conference*, University College Cork (7 September, 2002).

## EXTERNAL ASSIGNMENTS AND PUBLIC SERVICE

### Dr. Stephen M. Buckley

- Opponent for the PhD defence of Petteri Harjulehto (University of Helsinki).
- Reviewer for *Mathematical Reviews*.
- Referee for the *Journal of the London Mathematical Society* and for *Proceedings of the American Mathematical Society*.
- Member of the Irish Mathematical Olympiad training team.

**Dr. Catherine Comiskey**

- External Examiner for MSc research thesis at the School of Mathematical Sciences, DCU.
- External Examiner for PhD thesis, Mathematics Department, Edith Cowan University, Western Australia.
- Evaluator on the Mathematics and Computer Science Panel for Enterprise Ireland Basic Research Grants Programme.
- Member of the Operational Committee of NIRSA, National Institute of Regional and Spatial Analysis, NUIM

**Dr. Detta Dickinson**

- Reviewer for *Mathematical Reviews*.
- External examiner for PhD thesis, University of Strasbourg.

**Dr. Catherine Hurley**

- Associate editor for *Statistics and Computing*.
- Referee for *Computational Statistics*.
- Representative of the Irish Pattern Recognition and Classification Society to the International Federation of Classification Societies.
- Secretary on the Executive Committee of the Irish Statistical Association.
- Maintains Irish Statistical Association website.

**Dr. Patrick McCarthy**

- Referee for London Mathematical Society
- External examiner for MSc thesis at Trinity College, Dublin.

**Dr. Gary McGuire**

- External Examiner for PhD thesis at University of Exeter.
- External Examiner for MSc thesis at Trinity College Dublin.
- Referee for *Designs, Codes and Cryptography* and *IEEE Transactions on Information Theory*.
- Member of the Irish Mathematical Olympiad training team.

**Dr. John Murray**

- Member of the Irish Mathematical Olympiad training team.

**Dr. Fiacre Ó Cairbre**

- Member of the Royal Irish Academy's National Sub-Commission for Mathematical Instruction.
- Book review for the *Ríocht na Midhe*.
- Media interviews for the Quaternion walk in October 2002.

**Professor Anthony G. O'Farrell**

- Member of the Irish Mathematical Olympiad training team.
- Advisor, Teacher Registration Council.
- Research Associate, DIAS.
- RIA Library Committee.

**Dr. Ann O'Shea**

- Reviewer for *Zentralblatt MATH*.
- Committee member of the Irish Mathematical Society.

**Dr. Anthony Small**

- Referee for *Tohoku Journal of Mathematics*.

**Dr. Richard Watson**

- Irish delegate at the General Assembly of the International Mathematical Union, Shanghai, China.
- Chair of the National Committee for Mathematics of the Royal Irish Academy.
- Member of the Board of Science of the Royal Irish Academy.
- Member of the Irish Mathematical Olympiad training team.
- Member of the Academic Liaison Board, National Distance Education Centre.
- Member of the NUI Publication Committee.

**Dr. David Wraith**

- Treasurer of the Irish Mathematical Society.
- Reviewer for *Mathematical Reviews*.
- Referee for *The London Mathematical Society Bulletin* and *Compositio Mathematica*.
- Member of the Irish Mathematical Olympiad training team.



**Faculty of Science**

**Research Report 2002**

**Mathematical Physics**





# MATHEMATICAL PHYSICS

## ACADEMIC STAFF\*

**Professor D.M. Heffernan**, MA (Dublin), MS, PhD (Cornell) (Head of Department) (1993-)

**Professor D.H. Tchrakian**, BSc (Lond), ARCS, PhD (Edinburgh) (1971-)

**Professor C. Nash**, BA (Mod) (Dublin), PhD (Cantab) (1979-)

**Dr. B.P. Dolan**, BSc (Edinburgh), PhD (Durham) (1986-)

**Dr. J. Twamley**, BA (Mod) (Dublin), PhD (Alberta) (1997-)

## CONTRACT LECTURER

**Dr. D. Grigoriev**, MSc, PhD (Moscow) (2003-)

## PART-TIME LECTURERS

**Mr. W. Hanan**, BSc (DCU) (2001-)

**Mr. D. Stynes**, BA (Mod) (Dublin), MSc (DCU) (2001-)

## E.T.S. WALTON FELLOW

**Professor V. Buzek**, MSc, PhD (Moscow) (2002-2003)

## RESEARCH FELLOWS

**Dr. A. Cummings**, BSc, PhD (2001-)

**Dr. D. Grigoriev**, MSc, PhD (Moscow) (2003-)

**Dr. M. Feng**, MSc, PhD (Hefei, China) (2003-)

## POSTGRADUATE RESEARCH STUDENTS

**Ms. D. Kilbane**, BSc (1999-)

**Mr. D. McHugh**, BA (Mod) (Dublin), MSc (2000-)

**Mr. G. Kells**, BSc (2001-)

**Mr. A Rogers**, BE, MEng (2001-)

**Mr. V. Paturyan**, DipSc (2000-)

**Mr. M. Howard**, BSc (2003-)

## TUTORS

**Mr. B. Fagan**, BSc (DCU), HDipMaSc (1999-)

## EXECUTIVE ASSISTANT

**Ms. M. Harte**, (1993-)

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\* Unless otherwise stated the higher degrees are those of the National University of Ireland.

## HEAD OF DEPARTMENT'S REVIEW OF THE YEAR

The study of Mathematical Physics at Maynooth has a long and distinguished tradition. Modern theoretical physics and applied mathematics are exciting and dynamic and that excitement is reflected in the research projects which are pursued in the Department. Each permanent member of the Department holds a Research Associateship at the School of Theoretical Physics of the Dublin Institute of Advanced Studies, in whose scientific work they participate actively. In addition, the Department maintains strong, international contacts with major academic centres abroad.

The main areas of research are nonlinear physics, at both the macroscopic and microscopic level, and the study of the fundamental forces of nature. Detailed studies are undertaken to understand the dynamical behaviour of fundamental physical systems far from equilibrium and in quantum computing and information processing. A major research effort within the Department is to develop a better understanding of the fundamental forces of nature. There are four basic forces: Gravity, Electromagnetism and the two nuclear forces, the Strong and the Weak nuclear forces. The last three are believed to be well described by the mathematical framework of Relativistic Quantum Field Theory, while Gravity is so far understood only at the level of classical physics. Both the gravitational force and the other three forces are described in terms of Gauge Field Models. Most prominent amongst these is the Yang-Mills model with its rich geometrical and topological features, and plays a central role in current understanding of these forces.

It has been a busy year for the Department. Here are some of the events worthy of note. The Department has approval for a new Honours Degree in Theoretical Physics. A new phase in the Department's development is the teaching of mathematics to the Electronic Engineering programme. Professor Buzek of the Slovakian Academy of Sciences joined the Department as a Science Foundation Ireland E.T.S. Walton Fellow. Dr. Twamley secured funding for and leads a major EU project worth €1.7m entitled 'Quantum Information Processing using Doped Fullerenes and the Readout of Single Electron Spin (ROSES)'. The Department has continued to support the International Irish Quantum Field Theory Conference. The ninth conference was held in May 2002 at the Dublin Institute for Advanced Studies and was organized by Professor Nash of this department (in association with C. Houghton and I. Sachs of TCD).

## RESEARCH INTERESTS OF STAFF

### **Professor Vladimír Buzek**

The research interests of Professor V. Buzek can be divided into several mutually related groups:

- 1) quantum information processing - universal optimal manipulations with quantum information (e.g. universal quantum machines such as quantum cloners, or universal NOT gates)
- 2) quantum state reconstruction - reconstruction of states of quantum systems from incomplete data (e.g. application of the principle of maximum entropy and the Bayesian quantum inference)
- 3) dynamics of open quantum systems - stochastic quantization, quantum decoherence, nonclassical effects in quantum optics, reconstruction of Liouvillian superoperators, description of dynamics of open systems from the point of view of quantum information theory.
- 4) quantum entanglement in multi-partite systems - generation of entanglement (non-classical correlations) in many body systems, utilization of multi-partite entanglement to communication protocols (e.g. quantum secret sharing).
- 5) theoretical quantum optics - various aspects of matter-light interactions and generation of non-classical states of light.

### **Dr. Anthony Cummings**

The research interests of Dr. Cummings are theoretical and experimental photoabsorption/emission spectra of atoms and ions, with particular interest in giant dipole resonances and the effects of radial wave function contraction. He is working with Professor Heffernan on the Quantum Signatures of Chaos in atomic spectra and structure.

**Dr. Brian Dolan**

Research interests: relativistic quantum field theory, general relativity, quantum gravity and condensed matter. From a theoretical point of view geometry has always provided an immensely fertile bridge between physics and mathematics, many mathematical concepts being motivated by physical considerations and vice versa. All four of the fundamental forces of Nature (Gravity, Electro-magnetism and two nuclear forces-the Strong and Weak nuclear forces) fit nicely into the mathematical framework of the geometry of curved spaces and gauge field theories. A quantum mechanical analysis of these theories however reveals profound differences, in particular between Gravity and the three forces studied in modern Particle Physics - the Electro-magnetic, the Strong and the Weak forces. The aim of my research programme is to develop a deeper understanding of these fundamental physical theories and of the unifying role played by geometry and symmetry, both in classical and in quantum physics but especially in the latter. The physical and mathematical techniques involved are applicable to many other areas of physics too, such as solid state, low temperature physics and the theory of condensed matter.

*Current research includes:*

- i) Duality symmetries. Physical phenomena change under variations in scale (the renormalisation group), for example the parameters that determine the strength of the fundamental forces change with the energy scale at which they are measured. Discrete symmetries, sometimes called duality, can play a very important role here, for example they can be used to obtain information on the different possible phases of supersymmetric Yang-Mills theories and in the quantum Hall effect - two apparently very different phenomena which show a remarkable similarity in terms of the structure of their different phases and their renormalisation group flow. Symmetries can be used to gain deep insights into the way in which parameters change under changes in energy scale and this is one aspect of research.
- ii) Non-commutative geometry. A new technique for analysing quantum field theories is under investigation, that of non-commutative geometry in which the space-time continuum is replaced by a discrete set of points in an abstract 'fuzzy' space in a way specially designed to preserve all of the symmetries of the theory. This has applications in renormalisation group theory and to the problem of quantum gravity.
- iii) Chaotic renormalisation group flow. In some circumstances the parameters of a physical theory change in a chaotic manner when the length scale or the energy scale is changed and this phenomenon is also currently under investigation.

*Scientific Visits*

Centro de Investigación y de Estudios Avanzados del IPN (CINVESTAV), Mexico, July 2002.

Dept. of Physics, University of Erlangen, Erlangen, Germany, August 2002.

Dept. of Physics, ETH, Zurich, Switzerland, August 2002.

Dept. of Physics, University of Syracuse, Syracuse, USA, November 2002.

**Dr. Dmitri Grigoriev**

The general research interests of Dr. Grigoriev include the role and out-of-equilibrium kinetics of topological objects in field theory. In the year 2002 his work was concentrated on three main projects related to proton decay, fermion localisation in higher dimensions and magnetic monopoles.

Monopole catalysis of proton decay is a striking demonstration of quantum nature of matter and also an important basis for current experimental limit on relic magnetic monopoles which has deep cosmological implications. Last year it has been shown that a study of this process on semiclassical level in Skyrme-monopole system can provide a deep insight into nontrivial topological phenomena taking place during the Skyrmion decay, while estimating their actual effect onto the decay rate involves full out-of-equilibrium dynamics of the model. A detailed numerical study of the decay dynamics is now in progress.

Although the fermion localisation in higher dimensions is a more academic subject, the general results proven within this particular study can be of importance for wide spectrum of problems involving fermions in external backgrounds. In particular, it has been proven that no localised solutions are possible in any background for 3 and more additional dimensions, while for 2 dimensions the presence of solutions depends on the boundary conditions for background profiles. A general proof of existence was given for sigma-model profiles which are nonzero both at the origin and infinity, and also for Goldstone model profiles which vanish at the origin. In the latter case, it has been proven that the solutions exist only for backgrounds which change their sign at some intermediate point(s).

New results were obtained in simulated annealing study of magnetic monopoles. It has been proven numerically that the boundary conditions previously used for obtaining Platonic and axially-symmetric monopoles are in fact gauge equivalent, so within the general approach used the Platonic monopole is in fact a saddle point at the path to the true minimum. A detailed study of annealing dynamics near the minimum shows the true minimum to be consistent with the axially-symmetric monopole solution.

In March 2002 Dr. Grigoriev made scientific visits to several German universities and research institutes. He presented research seminars at the University of Bonn (19 March), the University of Dortmund (20 March), the University of Oldenburg (21 March), Max-Planck-Institut für Physik Munich (25 March), the University of Bielefeld (26 March) and Deutsches Elektronen Synchrotron (DESY), Hamburg (27 March).

#### **Professor Daniel M. Heffernan**

The main area of research is nonlinear science. Detailed work is being undertaken to quantify and characterize the fractal structures that occur in nature and in the phase space of dynamical systems. The problem is a fundamental and universal one underlying many areas of physics, such as diffusion limited aggregation, percolating clusters, neural networks and turbulence in fluids. The question of the existence of a quantum analogue of classical chaos is fundamental and is a major preoccupation of our research group. Computational and theoretical techniques have been developed and applied to obtain an understanding of the physics of these systems. Some of the projects under study by the group in 2002 were:

- a) The development and utilization of generalised dimensional and  $f(\alpha)$  spectral techniques for the study of the dynamics of physical systems. Detailed studies were completed of the formation and evolution of multifractal structures in some simple nonlinear dynamical systems. This is part of a major programme to develop a statistical-thermodynamic approach to the characterization and elucidation of the structural and dynamical properties of nonlinear systems, particularly spatio-temporal chaos.
- b) The detailed study of the classical and quantum chaos. In particular a fundamental and detailed programme is underway to study the nonlinear dynamics of low dimensional mesoscopic systems and the study of chaos in atomic spectra and structure. The application of chaos theory for nonlinear control and pattern recognition was systematically investigated.
- c) The physics, both classical and quantum, of external cavity lasers and low dimensional systems.

#### **Professor Charles Nash**

Professor Nash carries out research into quantum field theories using both analytical and topological techniques.

Of interest on the analytical side is the renormalisation of quantum field theories and the relation of this to quark confinement and QCD. The topological investigations centre on the properties of Yang-Mills gauge theories and the relation of these to quantum field theories in dimensions 2, 3 and 4. These involve investigations of classical solutions representing instantons, solitons and monopoles and relate to chiral anomalies, Donaldson invariants and Witten-Turaev-Viro invariants. The analytical and topological aspects can be combined in a geometric study of the renormalisation group and this is also under study.

A key recent topic is an investigation of quantum field theory models on the lattice in order to shed insight into suitable approximation methods which may be tractable for basic calculations. This has resulted so far in results relating the topology of the continuum quantum field situation with the lattice combinatorial one. This rather like the relation between the combinatorial formulation of cohomology and the continuum de Rham formulation using calculus (i.e. differential forms). There are interesting new, and calculable, features of the energy momentum tensors of such models and links with the modular invariance of string theory.

A development closely related to the above is that of the discovery by Witten of an Abelian monopole description of the 4-manifold polynomial invariants of Donaldson. This is also related to the new equations of Seiberg and Witten and this is under study at present. In particular some new results on the three dimensional Seiberg-Witten equations have been derived recently and are under active development.

Other separate work is a new project on non-commutative matrix models of Quantum field theories.

**Professor T. Tchrakian**

Professor Tchrakian's main research areas are Gauged Higgs and Skyrme field theories, and Gravitation.

*Individual projects:*

1. Continued the numerical analysis of 3 dimensional  $SO(3)$  Higgs models (featuring Skyrme like terms) to verify that like charged monopoles were attractive. The main purpose of the study was to discover whether (the lowest energy) bound states with higher charge than 2 were axially symmetric, or whether they exhibit Platonic symmetries.
2. The same results as above were arrived at when studying the higher charge monopoles of the 3 dimensional  $O(4)$  Sigma model with a symmetry breaking potential. (This work is in progress and has not been reported yet).
3. Continued the investigation of  $SO(3)_L \times SO(3)_R$  gauged Skyrme model supporting monopole solutions, for the purpose of demonstrating monopole catalysis of Baryon decay. Devised improved model featuring an additional  $(2, 2)$  Higgs field designed to enable only one (physical) electromagnetism. The results confirm the disappearing of the Skyrmion, namely the nucleon, when it approaches the monopole core. The time dependent analysis subject to spherical symmetry was carried out analytically, but the numerical analysis is pending.
4. Continued the study, both analytically and numerically, of the system consisting of the first two members of the Einstein-Hilbert and the Yang-Mills hierarchies. (This model has some relevance to the low energy effective action of string theory.) The results differ appreciably from those of Bartnik and McKinnon for the usual Einstein-Yang-Mills system. We carried out this analysis for spacetime dimensions  $d=6,7,8$  and separately (for technical reasons)  $d=5$ . The results indicate that solutions exist only for limited ranges of the gravitational constant, like when Higgs field are present.
5. Started the study of a family of fermionic models, where the Fermion is localized to the brane. These generalize the case of 1 extra dimension to that of  $d$  extra dimensions. Restricting to the models at hand, it turns out that such solutions exist only for extra dimension  $d=2$ .

*Scientific Visits for research collaborations*

Centre de Physique Théorique, Ecole Polytechnique, April 2002.

Department of Mathematical Sciences, University of Durham, May and December 2002.

Institut für Theoretische Physik, University of Bonn, June 2002.

Fachbereich Physik, University of Kaiserslautern, June 2002.

Fachbereich Physik, University of Oldenburg, July 2002.

Institut für Theoretische Physik, University of Hannover, July 2002.

**Dr. Jason Twamley**

Dr. Twamley is primarily interested in the whole area of Quantum Technology and Information Science. This is a new emerging area of science which examines the issues relating to the control of quantum systems and the use of controlled quantum systems to perform certain tasks such as quantum information processing. The field is highly multi-disciplinary and encompasses quantum theory, computer science, atomic physics, condensed matter physics, chemistry, photonics etc. Issues that are of particular interest to Dr. Twamley are: new quantum computer architectures, decoherence and decoherence repair techniques, new uses for quantum computers such as simulating other quantum systems. He has pioneered the potential use of doped Buckyballs (C60), molecules as ingredients in a solid-state quantum computer and he also has interests in trapped-ion quantum computer designs.

## RESEARCH GRANTS

Alexander von Humboldt visiting fellowship, University of Nuremberg-Erlangen, Germany, August 2002, €2,300 (Dr. B. Dolan).

'Quantum signatures of chaos in atomic spectra and structure'. Enterprise Ireland Basic Science Research Grant, 1999-2002, £75,000 (Professor D.M. Heffernan).

'Chaos based system identification and pattern recognition'. Enterprise Ireland Basic Science Research Grant, 2000-2004, £35,000 (Professor D.M. Heffernan).

'Semiclassical dynamics of gauged Skyrmed systems: monopole catalysis of Baryon-number decay'. Enterprise Ireland Basic Science Research Grant, 2000-2003, £75,000 (Professor D.H. Tchrakian).

'Solitons in gauged Higgs and Skyrme theories'. Enterprise Ireland International Collaboration Grant, 2001-2002, £3,500 (Professor D.H. Tchrakian).

'Monopole catalysis of Baryon-number decay'. Enterprise Ireland International Collaboration Grant 2002-2003, €5,600 (Professor D.H. Tchrakian).

'Integrability in statistical physics and quantum field theories'. Contractor in INTAS project INTAS-00-00561, 2000-2003, €9,000 (Professor D.H. Tchrakian).

'Quantum information processing and communication'. EU IST FET Network of Excellence, 2000-2003, Funds: Variable – average £1000/year (Dr. J. Twamley).

'Quantum computing - entanglement and algorithms'. Enterprise-Ireland Basic Research Grant, 1999-2002, £30,000 (Dr. J. Twamley).

European Science Foundation Programme in Quantum Information Theory and Quantum Computation, 1999-2003, Funds: Variable-average £2000/year (Dr. J. Twamley).

## PUBLICATIONS IN REFEREED JOURNALS

J. Bouda and **V. Buzek**. Purification and correlated measurements of bipartite mixed states. *Physics Review A* **65**, 034304-1-4 (2002).

Y. Brihaye, J. Burclaff, V. Paturyan and **D.H. Tchrakian**. The 1-soliton in the  $SO(3)$  gauged Skyrme model with mass term. *Nonlinearity* **15**, 385-392 (2002).

A. Chakrabarti and **D.H. Tchrakian**. Gravitation with superposed Gauss-Bonnet terms in higher dimensions: Black hole metrics and maximal extensions. *Physics Review D* **65**, 024029 (2002).

F. DeMartini, **V. Buzek**, F. Sciarrino and C. Sias. Experimental realization of the quantum universal NOT gate. *Nature* **419**, 815-819 (2002).

**B.P. Dolan** and C.P. Burgess. Duality and non-linear response for quantum Hall systems. *Physics Review B* **65**, 155323 (2002).

**B.P. Dolan**, A.P. Balachandran, J. Lee, X. Martin and D. O'Connor. Fuzzy complex projective spaces and their star products. *Journal of Geometry and Physics* **43**, 184-204 (2002).

**B.P. Dolan** and **C. Nash**. The standard model fermion spectrum from complex projective spaces. *Journal of High Energy Physics* **10**, 041 (2002).

**B.P. Dolan** and **C. Nash**. Chiral fermions and  $\text{spin}^c$  structures on matrix approximations to manifolds. *Journal of High Energy Physics* **07**, 057 (2002).

**B.P. Dolan**, D. O'Connor and P. Presnajder. Matrix  $\phi^4$  models on the fuzzy sphere and their continuum limits. *Journal of High Energy Physics* **03**, 013 (2002).

- B.P. Dolan**, D.A. Johnston and R. Kenna. The information geometry of the one-dimensional Potts model. *Journal of Physics. A* **35**, 9025-9035 (2002).
- B.P. Dolan** and D.A. Johnston. One-dimensional Potts model, Yang-Lee edges and chaos. *Physics Review E* **65**, 057103 (2002).
- B.P. Dolan** and O. Jahn. Fuzzy complex Grassmannian spaces and their star products. *International Journal of Modern Physics A* (in press).
- G. Drobny and **V. Buzek**, Reconstruction of motional states of neutral atoms via MaxEnt principle. *Physics Review A* **65**, 053410 (2002).
- M. Dusek and **V. Buzek**. Quantum multimeters: A programmable state discriminator. *Physics Review A* **66**, 022112, 1-5 (2002).
- D. Yu. Grigoriev**, P. M. Sutcliffe and **D. H. Tchrakian**. Skyrmed monopoles. *Physics Letters, B* **540**, 146-152 (2002).
- D. Yu. Grigoriev**, Y. Brihaye, V.A. Rubakov and **D.H. Tchrakian**. An extended model for monopole catalysis of nucleon decay. *Physics Review D* (in press).
- W. Harneit, C. Meyer, A. Weidinger, D. Suter and **J. Twamley**. Architectures for a spin quantum computer based on endohedral fullerenes. *Physica Status Solidi (B)* **233**, 453 (2002).
- M. Hillery, **V. Buzek** and M. Ziman. Probabilistic implementation of universal quantum processors. *Physics Review A* **65**, 022301-1-7 (2002).
- M. Hillery, M. Ziman, and **V. Buzek**. Implementation of quantum maps by programmable quantum processors. *Physics Review A* **66**, 042302-1-9 (2002).
- D. Kilbane**, **A. Cummings**, C. McGuinness, N. Murphy and G. O'Sullivan. '4f collapse and level density inflation and the emergence of 'compound like' atomic states in rare earth ions'. *Journal of Physics B : Atomic, Molecular and Optical Physics*, **35**, 309-321 (2002).
- M.S. Kim, W. Son, **V. Buzek** and P.L. Knight. Entanglement by a beam splitter: Nonclassicality as a prerequisite for entanglement. *Physics Review A* **65**, 032323-1-7 (2002).
- D. Nagaj, P. Stelmachovic, **V. Buzek** and M.S. Kim. Quantum homogenization for continuous variables: Realization with linear optical elements. *Physics Review A* **66**, 062307-1-11 (2002).
- C. Nash**, C. Adam and B. Muratori. Chern-Simons action for zero-mode supporting gauge fields in three dimensions. *Physics Review D* (in press).
- M. Plesch and **V. Buzek**. Entangled graphs. *Quantum Information and Computing* **2**, 530-539 (2002).
- A. Rogers, J. Keating, R. Shorten and **D.M. Heffernan**. Chaotic maps and pattern recognition - the XOR problem. *Chaos, Solitons and Fractals* **14**, 57-70 (2002).
- M. Sasura and **V. Buzek**. A tutorial review: Cold trapped ions as quantum information processors. *Journal of Modern Optics*, **49**, 1593-1647 (2002).
- V. Scarani, M. Ziman, P. Stelmachovic, N. Gisin and **V. Buzek**. Thermalizing quantum machines: Dissipation and entanglement. *Physics Review Letters* **88**, 097905 (2002).
- D. Stynes** and **D. Heffernan**. Universality and scaling in chaotic attractor to chaotic attractor transitions. *Chaos, Solitons and Fractals* **13**, 1195-1204 (2002).
- J. Twamley**. Quantum cellular automata quantum computing with endohedral fullerenes. *Physics Review A* (in press).
- M. Ziman, P. Stelmachovic, **V. Buzek**, M. Hillery, V. Scarani and N. Gisin. Diluting quantum information: An analysis of information transfer in system-reservoir interactions. *Physics Review A* **65**, art. no. 042105-1-11 (2002).

## CONFERENCE PROCEEDINGS

- V. Buzek.** 'Diluting of quantum information'. *IV Adriatic Conference on Quantum Interferometry*, Trieste, Italy, (14 March, 2002).
- V. Buzek.** 'An analysis of information transfer in open systems'. *Workshop on Quantum Decoherence in Quantum Information Processing*, Durham, England (12 April, 2002).
- V. Buzek.** 'Diluting of quantum information: An analysis of information transfer in open systems'. *9th Central European Workshop on Quantum Optics*, Szeged, Hungary (4 May, 2002).
- V. Buzek.** 'Quantum cloning and no-signaling constraint'. *Quantum Physics and Communication*, Dubna, Russia (16 May, 2002).
- V. Buzek.** 'Optimal manipulations with quantum information I & II'. *NATO Advanced Study Institute on Quantum Communication and Information Technologies*, Antalya, Turkey (11-12 June, 2002).
- V. Buzek.** 'Programmable quantum processors'. *11th International Laser Physics Workshop*, Bratislava, Slovakia (4 July, 2002).
- V. Buzek.** 'Programmable quantum processors: Implementation of quantum maps'. *3rd European QIPC Workshop - QUIPROCONE*, Dublin, Ireland (16 September, 2002).
- B. Dolan.** 'Non-commutative geometry as a regularisation technique in quantum field theory'. Seminar presentation, Dept. of Physics, University of Erlangen, Erlangen, Germany (22 August 2002).
- B. Dolan.** 'Non-commutative geometry as a regularisation technique in quantum field theory'. Seminar presentation, Dept. of Physics, ETH, Zurich, Switzerland (27 August, 2002).
- D. Grigoriev.** 'Simulated annealing for monopoles'. *Department of Physics Seminar Series*, TCD, Dublin (4 March, 2002)
- D. Grigoriev.** 'Proton decay in Skyrme-monopole system'. *Ninth Irish Quantum Field Theory Meeting*, Dublin Institute of Advanced Studies (19 May, 2002)
- D. Grigoriev.** 'Proton decay in Skyrme-monopole system'. *Quarks-2002*, Novgorod, Russia (3 June, 2002)
- D. Grigoriev.** 'Resonant amplification of electroweak baryogenesis', *Quarks-2002*, Novgorod, Russia (4 June, 2002)
- D. Grigoriev.** 'Proton decay in Skyrme-monopole system'. *Channel Meeting on Theoretical Particle Physics*, University of Plymouth UK (23 August, 2002).
- D.H. Tchrakian.** 'Gauge field systems in higher dimensions'. Invited presentation at *Quarks 2002*, Novgorod, Russia (3 June, 2002).
- D.H. Tchrakian.** 'Regular solutions in Einstein-Yang Mills systems in higher dimensions'. Seminar Presentation, Fachbereich Physik, University of Oldenburg (17 July, 2002).
- D.H. Tchrakian.** 'Gauging sphere-valued sigma models in all dimensions'. Seminar Presentation, Institut für Theoretische Physik, University of Hannover (18 July 2002).
- J. Twamley.** 'Quantum computing with endohedral fullerenes'. Plenary Speaker at *the Annual Meeting of the Spezial Forschungs Bereich (SFB) Austrian National Priority Research Programme on Control and Measurement of Coherent Quantum Systems*, Vienna, Austria (10-11 December 2002).
- J. Twamley.** 'Molecular quantum computing using endohedral fullerenes'. Invited presentation at the *NANO-7/ECOSS-21 conference*, Malmo, Sweden (24-28 June 2002).
- J. Twamley.** 'A Molecular Quantum Computer using Endohedral Fullerenes'. *6th International Conference on Quantum Communication, Measurement and Computing*, MIT, Boston, U.S.A. (22-26 July 2002).
- J. Twamley.** 'Quantum cellular automata quantum computing using endohedral fullerenes'. Invited presentation at the *CNRI Quantum Information Theory Workshop*, Dublin (21-23 March 2002).

## EXTERNAL ASSIGNMENTS AND PUBLIC SERVICE

### Professor V. Buzek

- Served as an evaluator for INTAS (International Association of the EC).
- Served as an expert for FET (Future and Emerging Technologies) IST (Information Society Technologies) of the EU 5th Framework Programme.
- Served as a member of editorial boards of the following journals: *Journal of Modern Optics*, *Journal of Optics B: Semiclassical* and *Quantum Central European Journal of Physics*.

### Professor D.M. Heffernan

- External Examiner for PhD Degree, University of Limerick.
- External Examiner for MSc Research Degree, University of Limerick.
- External Examiner for MSc Research Degree, Dublin City University.

### Professor C. Nash

- Organiser (with C. Houghton and I. Sachs of TCD) the Ninth International Irish Quantum Field Theory Conference in May 2002 held at the School of Theoretical Physics, Dublin Institute for Advanced Studies, Dublin.

### Professor T. Tchrakian

- External examiner for MSc Research Degree (by dissertation), University of Cape Town, Rondebosch, South Africa.

### Dr. J. Twamley

- Reviewer for the following Journals: *Physical Review A*, *Institute of Physics Journal in Nanotechnology* and *Physical Review Letters*.

## CONFERENCES HOSTED

**Dr. J. Twamley**, 3rd European Union Workshop in Quantum Information Processing and Communication, Dublin, (15-18 September 2002).





**Faculty of Science**

**Research Report 2002**

**Research Institutes**



## HAMILTON INSTITUTE

Following an international competition in 2001, Science Foundation Ireland awarded an initial seed grant of €6.3m to establish the Hamilton Institute at NUI Maynooth. In addition to this seed grant from SFI, the Institute is currently also supported by substantial funding from Enterprise Ireland and the European Commission. The Institute provides an environment with state of the art facilities within which a team of inter-disciplinary researchers can closely interact.

## RESEARCH OVERVIEW

The trend is increasingly toward not only large-scale interconnected or networked systems, but also moving software off the desktop and into the environment, such as to embedded systems in which software interacts directly with the physical world. Examples range from cars that are packed full of software to mobile devices and the intelligent network infrastructures required to support broadband-wireless data services. The research programme at the Hamilton Institute is tackling the fundamental issues underlying such systems.

**Hybrid Systems:** Many forms of software system (including nearly all embedded systems) can be considered as hybrid systems i.e. systems involving both logic-based behaviour and dynamic/physical behaviour. The Hamilton Institute is involved in creating the basic theoretical tools needed to enable us to analyse and understand hybrid systems.

**Reconfigurable Systems:** One of the most attractive features of modular, inter-connected architectures is the possibility of automatically reconfiguring the system in response to changes in operating requirements.

**Communication Networks:** Reliable communication among sub-systems is of key importance in information sharing environments. The software protocols such as TCP that implement the Internet have provided a communications medium of remarkable scalability but the limits of existing protocols are starting to be reached. New protocols will be needed in next generation networks and staff at the Hamilton Institute are in the forefront of research in this area.

**Human-Computer Interaction:** In modern software systems the trend is away from structured keyboard/screen interactions and increasingly towards continuous interaction with humans. Modern cars are an everyday example, where the steering controls are becoming an interface to a computer. Gesture-Driven interfaces for next generation mobile handsets are another example.

## INSTITUTE PERSONNEL

### *Faculty*

Professor Jens Kalkkuhl  
Professor Douglas Leith (Director)  
Professor William Leithead  
Dr. Roderick Murray-Smith  
Professor Barak Pearlmutter  
Dr. Robert Shorten  
Professor Peter Wellstead

### *Research Fellows*

Dr. Zhendong Sun  
Dr. Miguel Vilaplana

### *Research Students*

Mr. Santiago Jaramillo  
Mr. Robert Kilduff  
Mr. Ollie Mason  
Mr. Vamsi Potluru  
Mr. Emanuele Ragnoli  
Mr. Kai Wulff

### *Scientific Advisors*

Professor Kumpati Narendra

### *Associate Members*

Professor Daniel Heffernan  
Professor Ronan Reilly  
Professor John Ringwood

### *Research Affiliates*

Dr. Tom Dowling  
Dr. John Keating  
Dr. Charles Markham  
Mr. John McDonald  
Dr. Fiacre O'Cairbre  
Professor Li Ping  
Dr. Alan Rogers

### *Visitors*

Dr. John Foy  
Ms. Sommer Gentry (MIT)  
Mr. Bojan Likar (Jozef Stefan Institute, Slovenia)

### *Information & Enquiries:*

Professor Doug Leith  
Director  
Hamilton Institute,  
National University of  
Ireland Maynooth,  
Maynooth  
Co. Kildare.

*Tel:* +353 1 7086100  
*Email:* Hamilton@may.ie  
*Website:* <http://hamilton.may.ie>

### *Administrator*

Ms. Rosemary Hunt

## RESEARCH GRANTS

'Off-equilibrium linearisation: A new paradigm for divide and conquer identification'. Engineering and Physical Sciences Research Council, Grant no. GR/R15863, 2001-2004, UK£186,485 (Professor D.J. Leith, Professor W.E. Leithead and R. Murray-Smith)

'Modern methods for data intensive modelling of nonlinear dynamic systems'. Engineering and Physical Sciences Research Council 2002, UK£14,000 (Professor D.J. Leith and Dr. S. McLoone).

'Centre for computer controlled systems'. Science Foundation Ireland, Grant No. 00/PI.1/C067, 2001-2006, €6.3m (Professor D.J. Leith & Dr. R.N. Shorten)

'Multi-Agent control'. European Union Research Training Network, 2000-2004, €1.2 million (Professor D.J. Leith, Dr. R.N. Shorten and Dr. R. Murray-Smith).

'Audioclouds: Three-dimensional audio and gestural interfaces for mobile and wearable computers'. The Engineering and Physical Sciences Research Council, 2002-2005, UK£237,000 (Dr. R. Murray-Smith).

'Matrix pencil stability criteria'. Enterprise Ireland Basic Research Grant, 2001-2004, €46,980 (Dr. R.N. Shorten).

'Chaos based pattern recognition and systems identification'. Enterprise Ireland Basic Research Grant, 2001-2004, £43,170 [Dr. R.N. Shorten, Professor D. Heffernan (PI) and Dr. J. Keating].

## PUBLICATIONS IN REFEREED JOURNALS

S.C. Jun, **B.A. Pearlmutter** and G. Nolte. Fast accurate MEG source localization using a MLP trained with real brain noise. *Physics in Medicine and Biology*, **47**, 2547-2560 (2002).

**J. Kalkkuhl**, T.A. Johansen and J. Lüdemann. Improved transient performance of nonlinear adaptive backstepping using estimator resetting based on multiple models. *The Institute of Electrical and Electronics Engineers, Transactions on Automatic Control*, **47**, 136-140 (2002).

M.L. Ni, M.J. Er, **W.E. Leithead** and **D.J. Leith**. New approach to the design of robust tracking and model following controllers for uncertain delay systems. *IEE Proceedings*. **46(D)**, 472-475 (2002).

L. Parra, C. Alvino, A. Tang, **B.A. Pearlmutter**, N. Yeung, A. Osman, and P. Sajda. Linear spatial integration for single trial detection in encephalography. *NeuroImage*, **17**, 223-230 (2002).

**B.A. Pearlmutter**, A.C. Tang, N.A. Malaszenko and D.B. Phung. Independent components of magnetoencephalography: single-trial response time estimation. *NeuroImage* (in press).

A. Rogers, J. Keating and **R.N. Shorten**. A novel classification scheme using the Baker's map *Neurocomputing* (in press).

A. Rogers, J. Keating, **R.N. Shorten** and D.H. Heffernan. Chaotic maps and pattern recognition: the XOR problem. *Chaos Solitons and Fractals*, **14**, 57-70 (2002).

**R.N. Shorten** and K.S. Narendra. Necessary and sufficient conditions for the existence of a CQLF for a finite number of stable LTI systems. *International Journal of Adaptive Control and Signal Processing*, **16**, 709-728 (2002).

**R.N. Shorten** and F. O'Cairbre. A new methodology for the stability analysis of pairwise triangularisable and related switching systems. *Institute of Mathematics and its Applications: Journal of Applied Mathematics*, **67**, 441-457 (2002).

**Z. Sun**, S.S. Ge and T.H. Lee. Controllability and reachability criteria for switched linear systems. *Automatica*, **38**, 775-786 (2002).

A.C. Tang, **B.A. Pearlmutter**, N.A. Malaszenko, D.B. Phung and B.C. Reeb. Independent components of magnetoencephalography: localization. *Neural Computation*, **14**, 1827-1858 (2002).

K. Wulff, **R.N. Shorten** and P. Curran. On the 45 degree region and the uniform asymptotic stability of classes of second order parameter varying and switched systems. *International Journal of Control*, **75**, 812-823 (2002).

M.I. Zibulevsky, P. Kisilev, Y.Y. Zeevi and **B.A. Pearlmutter**. Blind source separation via multinode sparse representation. *Advances in Neural Information Processing Systems* **14**, 1049-1056 (2002).

## BOOKS, BOOK CHAPTERS AND REVIEWS

S.C. Jun, **B.A. Pearlmutter** and G. Nolte. 'Fast Subject Independent Magnetoencephalographic (MEG) Source Localization using an Artificial Neural Network'. *Society for Neuroscience Abstracts* 28 (2002).

**J. Kalkkuhl**, T.A. Johansen and J. Lüdemann. 'Nonlinear adaptive backstepping with estimator resetting using multiple observers'. *Nonlinear and Hybrid Control in Automotive Applications*. (eds. R. Johansson and A. Rantzer). Springer-Verlag, **2034**, p.p. 319-324 (2002).

I. Petersen, T.A. Johansen, **J. Kalkkuhl** and J. Lüdemann. 'Wheel slip control in ABS brakes using gain scheduled constrained LQR'. In *Nonlinear and Hybrid Control in Automotive Applications*. (eds. R. Johansson and A. Rantzer). Springer-Verlag, Germany (2002).

E. Solak, **R. Murray-Smith**, **W.E. Leithead**, **D.J. Leith** and C. Rasmussen. 'Derivative observations in Gaussian process models of dynamical systems'. *Advances in Neural Information Processing Systems*, CD Rom (2002).

A.C. Tang and **B.A. Pearlmutter**. Chapter 7 – 'Independent Components of Magnetoencephalography: Localization'. In *Exploratory Analysis and Data Modelling in Functional Neuroimaging* (eds. F.T. Sommer and A. Wichert). MIT Press, p.p. 129-162 (2002).

## CONFERENCE PROCEEDINGS

C. Girard, J. Rasmussen, C. Quinonero and **R. Murray-Smith**. 'Gaussian Process priors with uncertain inputs – application to multiple-step ahead time series forecasting'. *Neural Information Processing Systems 16*, Vancouver, Canada (11-13 December, 2002).

S.C. Jun, **B.A. Pearlmutter** and G. Nolte. 'Fast robust MEG source localization using MLPs'. *BIOMAG-2002*, Jena, Germany (10-14 August, 2002).

T. Laffey, **R.N. Shorten** and F. O'Cairbre. 'On the stability of convex sums of matrices: New results and a conjecture on the simultaneous stability of pairs of matrices'. *Proceedings of the American Control Conference*, **2**, 1246-1247 (2002).

**D.J. Leith**. 'Determining nonlinear structure in time series data'. *Workshop on Modern Methods for Data Intensive Modelling*, NUI Maynooth (12-13 September, 2002).

**D.J. Leith** and **W.E. Leithead**. 'Global reconstruction of nonlinear systems from families of linear systems'. *International Federation of Automatic Control World Congress (IFAC)*, Barcelona, Spain (22-26 July, 2002).

**D.J. Leith**, **W.E. Leithead** and **R. Murray-Smith**. 'Divide and conquer identification using Gaussian process priors'. *Workshop on Non-linear and Non-Gaussian Signal Processing*, Peebles, UK (16-17 December, 2002).

**D.J. Leith**, **W.E. Leithead**, O. Mason and **R.N. Shorten**. 'A wind turbine benchmark for hybrid system analysis and design'. *International Federation of Automatic Control World Congress (IFAC)*, Barcelona, Spain (22-26 July, 2002).

**D.J. Leith**, **W. Leithead**, O. Mason and **R.N. Shorten**. 'A benchmark study for the design of switching systems'. *Proceedings of the IFAC World Congress*, CD Rom, (2002).

**D.J. Leith**, **W.E. Leithead**, E. Solak and **R. Murray-Smith**. 'Divide and conquer identification: using Gaussian process priors to combine derivative and non-derivative observations in a consistent manner'. *Conference on Decision and Control*, Las Vegas (10-13 December, 2002).

**R. Murray-Smith** and D. Sbarbaro. 'Nonlinear adaptive control using non-parametric Gaussian process prior models'. *International Federation of Automatic Control, 15th IFAC Triennial World Congress, Barcelona, Spain* (22-26 July, 2002).

**R. Murray-Smith**, J.Q. Shi and **D.J. Leith**. 'Engineering applications of Gaussian process priors'. *International Conference on Current Advances and Trends in Nonparametric Statistics, Crete* (15-19 July, 2002).

**R. Murray-Smith**, **R. Shorten** and **D.J. Leith**. 'Nonparametric models of nonlinear dynamics', *IEE Workshop on Nonlinear, non-Gaussian Signal Processing, Peebles Hydro*, (9-10 July, 2002).

**R. Murray-Smith**, J. Williamson, J. Borland, P. Gray. 'Supporting early intervention programmes for special-needs children with personal digital assistants'. *Experimental Analysis of Behaviour Group Conference, London* (12-13 February, 2002).

G. Nolte, T. Sander, A. Lueschow and **B.A. Pearlmutter**. 'Nonlinear time series analysis of human alpha rhythm'. *BIOMAG-2002. Jena, Germany* (10-14 August, 2002).

**B.A. Pearlmutter**. 'Algorithmic differentiation, functional programming, and iterate to fixed point'. *The Learning Workshop. Utah, USA* (2-5 April, 2002).

**R. Shorten**. 'How to translate circle into German without using a dictionary'. Seminar Presentation, Department of Electronic Engineering, NUI Maynooth (14 November 2002).

**R. Shorten**. 'Something new about 2'. Seminar Presentation, Department of Electronic Engineering, NUI Maynooth (27 March 2002).

**R.N. Shorten**, K.S. Narendra and O. Mason. 'A comment on the existence of a common quadratic Lyapunov function'. *Proceedings of the Conference on Decision and Control*, **3**, 2780-2785 (2002).

E. Solak, **R. Murray-Smith**, **W.E. Leithead**, **D.J. Leith** and C.E. Rasmussen. 'Derivative observations in Gaussian Process models of dynamic systems'. *Neural Information Processing Systems 16, Vancouver, Canada* (11-13 December, 2002).

K. Wulff, **R.N. Shorten** and P. Curran. 'On the relationship between matrix pencil eigenvalue criteria and the choice of Lyapunov function for the analysis of second order switching systems'. *Proceedings of the American Control Conference*, **2**, 1248-1253 (2002).

K. Wulff, **R. Shorten** and P. Curran. 'On the relationship between matrix pencil eigenvalue criteria and the choice of Lyapunov function for the analysis of second order switching systems'. *American Control Conference, Anchorage, Alaska* (8-10 May, 2002).

## EXTERNAL ASSIGNMENTS & PUBLIC SERVICE

### Professor D.J. Leith,

- Reviewer of research proposals for the following: Enterprise Ireland, European Commission, UK Engineering and Physical Sciences Research Council.
- Reviewer for: *Automatica*, *International Journal of Control*, *IEE Proceedings* and *Control Engineering Practice*.

### Professor W.E. Leithead,

- Project reviewer for UK Engineering & Physical Sciences Research Council.
- Reviewer for: *Automatica*, *International Journal of Control*, *IEE Proceedings* and *Control Engineering Practice*.
- Consultant to Renewable Energy Systems Ltd., UK; BAE Systems, UK and Neg-Micon, Denmark.
- External Examiner for Dept. of Electronic and Electrical Engineering at Loughborough University.

**Dr. R. Murray-Smith,**

- Reviewer for Enterprise Irelands Basic Research Grants programme.

**Professor B.A. Pearlmutter,**

- Reviewer/panel member for US NSF, Research Grants Council of Hong Kong.
- Co-Chair of NIPS 2002 Workshops (Neural Information Processing Systems: Natural and Synthetic).

**Dr. R.N. Shorten,**

- External examiner for PhD thesis, University of Glasgow.
- Project reviewer, European Union.

**CONFERENCES HOSTED**

**D.J. Leith** and S. McLoone, *Workshop on Modern Methods for Data Intensive Modelling of Nonlinear Dynamic Systems*, Hamilton Institute, NUIM (12-13 September, 2002).

## INSTITUTE OF BIOENGINEERING AND AGROECOLOGY

The Institute for Bioengineering and Agroecology (IBA) has been set up with public and private support under Cycle 1 of the Irish Higher Education Authority PRTL initiative, building on a pre-existing consortium of six academic laboratories at NUI Maynooth. Its overall concern is the benign manipulation of organisms for field use in pursuit of food security, human health, environmental enhancement, and novel materials.

The IBA conducts research in the following areas: genetics, development, behaviour and ecology of biological control organisms, developmental biology, stress physiology and genetic modification of plants, and the management requirements of genes inserted in plants or biocontrol organisms.

### INSTITUTE PERSONNEL

#### *Principal Investigators*

Professor Martin Downes, Director  
Dr. Christine Griffin, Deputy Director  
Professor Ann Burnell  
Professor Phil Dix  
Dr. Jackie Nugent  
Dr. Conor Meade (Senior Research Fellow)

#### *Research Fellows*

Dr. Killian Brady  
Dr. John Browne  
Dr. Catherine Dempsey  
Dr. Ica Dix  
Dr. Katharine Dolan  
Dr. Eugene Kane  
Dr. Matt McCabe  
Dr. Greg Nugent  
Dr. Noreen McGrath Curran  
Dr. Declan Roche  
Dr. Jonathan Ryder  
Dr. Mary Sekiya

#### *Postgraduate*

Ms. Susan Cloney  
Ms. Aoife Dillon  
Mr. Roy Enright  
Ms. Eleanor Fitzgibbon  
Ms. Beverly Henley  
Ms. Theodora Lola-Luz  
Mr. Ian McEvoy  
Ms. Mary Moran  
Mr. Hilton McWeeney  
Ms. Kathryn O'Callaghan  
Mr. Damien O'Halloran  
Ms. Mary Poage  
Mr. Wesley Reardon  
Ms. Sassia Omar Regeai  
Mr. Alec Rolston  
Mr. Adam Shannon  
Ms. Karen Shiel  
Ms. Nguyen Thi Thanh  
Mr. Trevor Tyson  
Ms. Deborah Vicuna

#### *Administrative Staff*

Ms. R. Bradshaw  
Dr. R. Dempsey  
Ms. N. Travers

#### *Information and enquiries\*:*

Professor Martin Downes, Director,  
Institute for Bioengineering and Agroecology,  
Department of Biology,  
National University of Ireland  
Maynooth,  
Maynooth, Co. Kildare.

*Tel:* +353-1-7083837

*Email:* martin.downes@may.ie

*Website:* <http://www.may.ie/academic/biology/iba.shtml>

\* The research grants, publications and external assignments of Institute members are listed with the Biology Department entries.

## INSTITUTE OF IMMUNOLOGY

Immunology is a core discipline to the emerging technologies that are revolutionising biology. The science is recognised as central to Ireland's biomedical sector. The immune response protects the body from attack by foreign organisms but is also implicated in diseases as diverse as asthma and cancer. The overriding aim of the Institute for Immunology at NUI Maynooth is to conduct internationally competitive research of the highest standard in the discipline of immunology and to train individuals at undergraduate, postgraduate and postdoctoral level to become future leaders in this area.

The Institute was established in 1999 following recognition of Centres of research excellence at the University and the award of major funding under the Irish Higher Education Authority (HEA) Programme for Research in Third-Level Institutions (PRTL). In December 2002 the Institute relocated to its purpose built laboratories within the new Bioscience & Engineering Research Building. These facilities have been described as among the finest in Europe. In particular the core facilities are ideally suited to advanced immunological research. These include a digital imaging facility, real-time quantitative PCR equipment, and a specialist histology laboratory. Access to these facilities is not restricted to Institute members, but is available to others through strategic collaboration. Specialist facilities for working with category III pathogens will come on stream in 2003.

A unique feature of the Institute is the attempt to build a career structure for Irish Scientists. 2002 saw this policy bear fruit, with two scientists working under this scheme attracting significant funding. Dr. Shirley O'Dea was obtained a prestigious SFI fellowship and Dr. Patricia Johnson an EU award amounting to over €1.3 million in total. The policy of support and mentoring fostered by the Institute for emerging researchers is proving an excellent mechanism to retain the brightest young scientists in Ireland. In fact the Institute has a strong commitment to education at all levels. This is clearly seen in the numbers of postgraduate and postdoctoral fellows starting their careers at Maynooth and the contribution to new teaching courses at undergraduate level. In 2002 this was extended to second level students by organizing an essay competition on Immunology for transition year students. This essay was designed to help secondary school teachers introduce the Immunology elements of the new leaving certificate syllabus in Biology and has proved very popular.

NUI Maynooth has built a solid foundation in immunological research over the past nine years and currently has several internationally recognised Scientific Investigators, with substantial research funding from The Wellcome Trust, SFI, The European Commission, The Health Research Board, Enterprise Ireland and Industry. Further recognition of excellence in research can be judged by a large number of peer-reviewed papers in high impact research journals that achieve the widest possible dissemination. International recognition of expertise in the field of Immunology is also recognised through inclusion on Grant review boards, Working groups, Invitations to speak at International scientific conferences, and serving on editorial board and peer review panels for leading International Scientific Journals.

## CURRENT AND FUTURE RESEARCH AREAS

- Understanding asthma
- Immunity to infectious diseases - pertussis, mumps, influenza, hepatitis C and HIV
- New vaccines and mucosal adjuvants
- Mucosal immunology of the respiratory tract
- Lymphocytes with restricted recognition
- Immunomodulation of Th1/Th2 cells
- Mucosal immunity of the gut

## INSTITUTE PERSONNEL

### *Principal Investigators*

Dr. Bernard Mahon, Director  
Dr. Shirley O'Dea  
Dr. Derek Doherty  
Dr. Patricia Johnson

### *Postdoctoral Fellows*

Dr. David Casey  
Dr. Tony O'Connor  
Dr. Laura Madrigal-Estebas

### *Postgraduate Fellows*

Ms. Mary O'Gorman  
Mr. Tony Kenna  
Mr. Darren Ennis  
Ms. Marion Flynn  
Ms. Jane Kelly Rogers  
Ms. Claire Brady  
Ms. Cariosa Noonan  
Ms. Hamed Astrafel  
Mr. Omeiros Zachariadis

### *Research Assistants*

Ms. Ellen Lewis

### *Information and enquires\*:*

Dr. Bernard P. Mahon, Director,  
Institute for Immunology,  
Department of Biology,  
National University of Ireland  
Maynooth, Co. Kildare

*Tel:* +353-1-708 3835

*Email:* bpmahon@may.ie

### *Website:*

<http://www.may.ie/academic/biology/mim.shtml>

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\* The research grants, publications and external assignments of Institute members are listed with the Biology Department entries.





