Applied Mathematics

Dr David Williams
- Head of Applied Mathematics (from October)

Professor Stephen Hyde
- Head of Applied Mathematics (until October)

The Department of Applied Mathematics performs research on fundamental and applied topics in colloid, surface and polymer science, largely in measurement of surface forces; on self-assembly of organic and inorganic structures at mesoscopic scales; and on disordered materials, mostly on micron-scale morphology and transport in porous structures.

http://wwwrsphysse.anu.edu.au/appmaths

Research Summary

After many years of arduous and taxing duty as Head of Department, Stephen Hyde stepped down this year in part to concentrate on his research. Stephen has guided the Department through what could have been a difficult "Post-Ninham" period, in particular through a major review. In fact, in large part due to his efforts, the Department has become significantly stronger and much larger, having approximately doubled in size over the last few years. Our research and funding bases have also broadened considerably.

Early this year we welcomed two new members into the Department, Tomaso Aste and Tiziana di Matteo, who coincidentally celebrated their nuptials at the end of the year. Tomaso has expertise in disordered materials, and in particular in foams and granular media and has a continuing appointment. Tiziana has a background in condensed matter physics, but now concentrates on networks and financial mathematics. Tiziana won a prestigious QEII fellowship in the latest ARC round (one of two awarded to the Department this year). Both researchers were attracted from Italy, and have promised to continue the Department's strong links with the cradle of modern science.

One of the finest strokes of genius of our founder, Barry Ninham, was to create an applied mathematics department that had a strong backbone of experimentalists. In fact, Applied Maths remains first an experimental department but with a number of excellent theoreticians and simulators.

The Department also covers a wide range of research from the very applied and industrial (for instance some of the experimental work done by the paper CRC by Ray Roberts, Tim Senden and Mark Knackstedt), through to the more mathematical and esoteric work on tilings and minimal surfaces done by Stuart Ramsden, Vanessa Robins and Stephen Hyde. In between these two extremes lies the work of much of the Department on surface forces, biophysics colloid science and soft and granular matter. Despite this wide range of activities, our over-riding goal within the Department has always been to carry out curiosity-driven research publishable in high-quality journals.

The Department has a long and proud history of QEII fellowships, starting with Barry Ninham who was the first Australian QEII fellow. This year was probably a first, when the Department won two such fellowships – that of Tiziana di Matteo already mentioned and of Satomi Onishi, who will continue her work on surface forces.

Currently the Department has in fact a large number of ARC fellows, including one Senior Research Fellow, two QEIIs and two Australian Research Fellows.

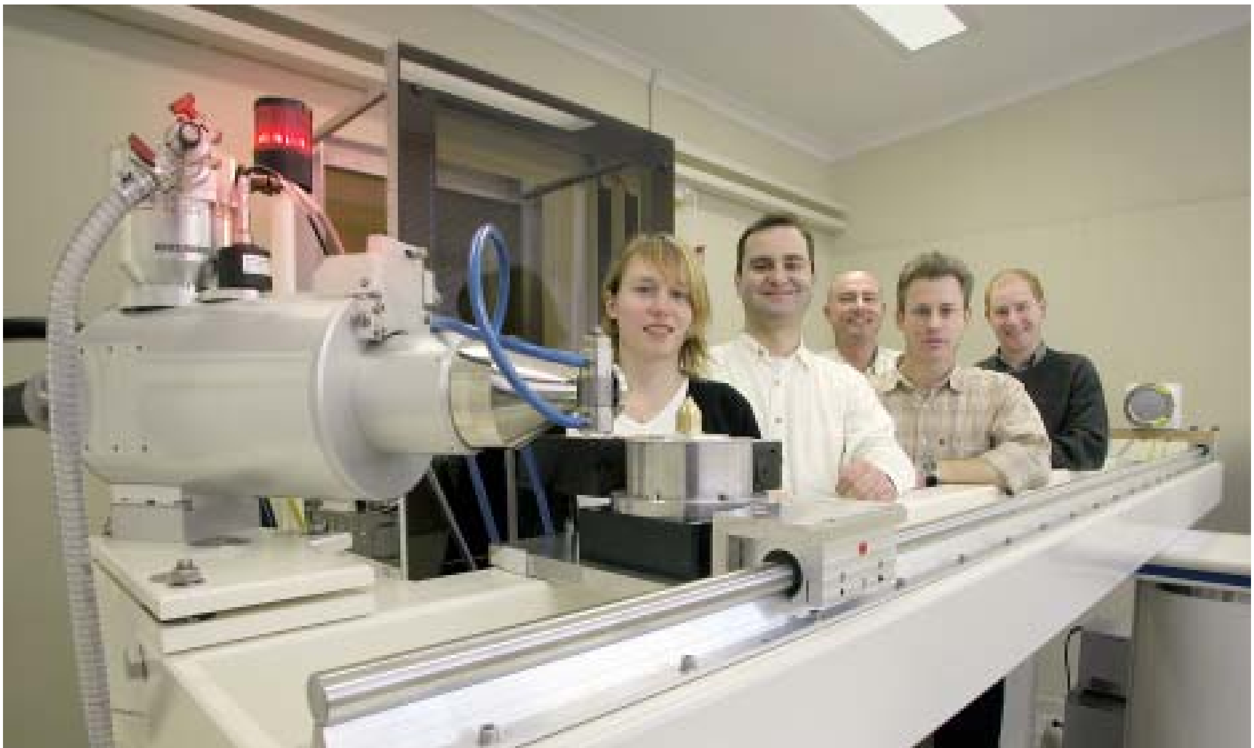
Although the research interests of the Department are broad they almost all fall under the definition of "materials". There are two general streams of research. One is in "soft matter" and the physical chemistry of surfaces. This deals with all kinds of soft materials such as colloids, polymers and liquid crystals, with a significant emphasis on the interaction forces between particles in fluids. This stream in principle underlies all of biology and many industrial processes. The second, more recent and indeed rapidly growing stream deals with disordered materials, such as rocks and sand. The structures of these materials are very poorly understood and one of the major thrusts of the research is in how we can get a reasonably simple description of these complex materials. This stream has many important applications, not the least to the problems of groundwater modelling and oil recovery. Of course there is substantial overlap between the two streams since many soft materials are substantially disordered. Both streams have industrial applications and funding, but both are studied mainly for their fundamental interest.

Tomaso Aste's research interests cover both groups. He has recently completed some very significant work on the structure of granular materials. As their name suggests these are any materials that consist mainly of grains. Some obvious examples are beach sand, breakfast cereals and gravel. The physics of these systems has been investigated at least since the time of Coulomb in the 18th Century, but over the past decade there has been an explosion of research by physicists on these systems as they exhibit many fascinating phenomena that can be demonstrated cheaply on the laboratory scale and are indeed amenable to computer simulation. Despite a vast amount of work they remain very poorly understood compared to simple liquids and both their statics and dynamics are the subject of some debate. Tomaso has recently shown, using a simple model of hard spheres that the large-scale equilibrium dynamical behaviour of these systems can be understood by examining only a few grains. This work combines statistical mechanics with computer enumeration and has significant overlap with the traditional interest in liquid state theory in the Department personified by Stepjan Marcelja who has temporarily left the Department to become Head of the Boscovich Institute in Croatia. Tomaso also has interests in disordered systems generally, particularly networks.

As mentioned previously the Department this year welcomed Tiziana di Matteo, who has recently begun studying "econophysics". This subject seeks to apply the methods of theoretical physics and in particular statistical physics to the empirical analysis of financial markets data (complex data sets). For interest rates data, the study has been mainly focused on the "tail" regions of the fluctuations probability distributions and on the correlations among time series at different maturity dates. The correlations have been analysed through the geometrical and topological properties of their metric graphs. Tiziana also studies complex systems in general by using techniques of statistical physics, non-linear dynamical analyses and numerical computational methods.

Stephen Hyde has a strong overlap of research interests with Tomaso and Tiziana. Despite being Department Head for much of 2002, he made progress in three areas. These are: (1) Euclidean crystalline networks from 2D hyperbolic tilings; (2) Growth of complex self-assembled inorganic materials and (3) Computational geometry and self-assembly. Stephen Hyde, amongst the senior people, is probably the most mathematical, with a special emphasis on geometry, usually on the non-Euclidean kind. However, this does not stop him having a keen interest in, and indeed in performing experiments, particularly those that lead to novel materials.

Stephen's work on tilings involves extensive numerical applications as well as recent tiling theory, group theory, surface geometry and topology and non-Euclidean geometry. A complete algorithmic suite is now done and the automatic generation of networks in 3D Euclidean space by projection onto regular triply-periodic minimal surfaces is about to start. The long-term goal is to produce catalogues of networks to study the relative importance of network topology and geometry in their allowed geometrical fluctuations, transport efficiency and general statistical physics. This work is done in collaboration with Stuart Ramsden, Tiziana Di Matteo and Vanessa Robins.



Anna Carnerup, Arthur Sakellariou, Ray Roberts, Tim Sawkins and Tim Senden with the newly built an commissioned X-Ray Computed Tomography Machine. This an in- house piece of equipment allows full 3D images to be made at a resolution of 5 microns

Bubbles levitating by expulsion of carbon dioxide gas . An experiment by Tim Senden and Jean-Marc di Meglio

Stephen Hyde's work on growth of complex self-assembled inorganic materials is in part done in collaboration with Dr Garcia Ruiz in Granada, Spain. It centers on investigations of the structures of carbonate-silica complexes grown in the lab under ambient conditions. The growths are interesting for a number of reasons: they are mimics of purported microfossils; include the oldest known terrestrial "fossils"; they exhibit complex orientational ordering without long-range translational order; and they are interesting model systems to compare with biomineralisation processes in living creatures. Some of this work is done in collaboration with Andy Christy, Anna Carnerup and Ankie Larsson.

Stephen Hyde has long had an interest in computational geometry and self-assembly. Current work in this area includes the work with Gerd Schröder on medial surfaces and medial axes, that will allow rigorous calculations of the relative stability of various morphologies (eg. bicontinuous and mesh mesophases in lyotropic liquid crystals). Apart from her work with Stephen Hyde, Vanessa Robins has worked on a project with Liz Bradley at the University of Colorado, Boulder. They have developed new applications of computational topology in the analysis of data. Specifically, removing noise from chaotic time-series data, and extracting coherent features from scientific images such as cell micrographs and satellite images. Vanessa Robins continues to collaborate with Klaus Mecke in Germany on analysing topological signatures of point-patterns.

Mark Knackstedt leads a large group devoted to the understanding of the structure of disordered materials and also to the properties of fluid flow within such materials, particularly rocks and other porous matter. He also leads one node of the Cooperative Research Center for Functional Communication Surfaces which deals mainly with fundamental problems affecting the paper industry. This node either in whole or part funds several people within the Department. Within this group Ray Roberts has been examining how liquid deposited on a paper surface is imbibed into the bulk of the paper. Using scanning electron microscopy and Raman microscopy, he had previously shown that the rate of liquid imbibition affects the quality of low pressure melamine panels. He also showed that the usual measures used in industry are deeply flawed. More recently, using cryo SEM and two-photon laser confocal microscopy, he has been able to determine the mechanism of liquid imbibition in paper as being film flow in interfiber channels as opposed to piston flow in pores which has been the popular belief/theory for the past 100 years. He is now looking at the structure of paper using the MicroCT and trying to identify how it affects the rate of liquid imbibition and in particular the actual network pathway of an imbibing liquid.

Within the porous materials group Adrian Sheppard has continued his work on the flow of fluids in porous materials, which has applications to the oil industry. The flow of multiple immiscible fluid phases through a porous medium involves numerous factors. Capillary and viscous forces both play a role, while flow occurs in wetting films along the walls of the medium as well as through the bulk of the pore space. An understanding of how the thickness of these films evolves is a critical foundation of any accurate model of this process. We have developed a model that, for the first time, correctly models the dynamics of film flow and film thickening within two- and three-phase flow. Implementation of this new model into our existing network modelling software is well under way.

Also within the group interested in porous and disordered media are two Germans, Lydia Knuefing and Christoph Arns. Lydia has begun to analyse images of porous media. Convinced that a 2D analysis can not capture the nature of connectivity in a 3D structure, Lydia has started to investigate the use of a 3D-Fourier analysis on images we have taken with the Department's MicroCT facility. By using only part of the frequency spectrum when transforming from Fourier-space to real-space, the original image undergoes a process that seems to be similar to a dilation process, i.e. depending on the cut-off small-scaled features of the original image vanish, thus revealing areas of close- or loose-packed material. Whether these are truly responsible for most of the fluid flow has still to be investigated.

Christoph Arns has started a new collaboration with Professor D. Stoyan, University of Freiberg, Germany, carrying out a geostatistical analysis of tomographic data. He also continued his work with Mark Knackstedt and extended the physical properties they calculate for tomographic data sets of rocks to NMR relaxation. Here in particular they looked at the inversion of NMR relaxation curves, which is an ill-conditioned problem and involves the inversion of a Laplace-transform. For this one needs regularisation techniques and Christoph implemented several different ones.

The Department has long had an interest in, and in fact been one of the world leaders in the field of colloid science, and physical chemistry in general. This field deals with interactions between solute particles, from molecules to proteins and polymers in solution, to suspensions of colloidal particles, and these in turn determine the properties of most real world systems. Examples include self assembly of biomembranes, reactivity in biotechnologies and biochemistry, chemical synthesis, and a host of chemical engineering applications, from minerals processing, oil recovery to soil science and detergent formulation and drug delivery. The entire theoretical framework of physical chemistry that underpins such applications is so well established that it is hardly ever questioned. A naive observer might therefore expect to call on an array of theories that offer some quantitative guide to developments in industry and the biosciences. The truth alas lies in the opposite direction. We take as an example what ought to be the most applicable field, colloid science. A perusal of the standard textbooks and monographs in this area reveals a degree of triumphalism, but contains not a hint of its current embarrassing state. While there are many accurate and detailed experimental measurements almost no results are known where theory and experiment agree. In some cases there is a limited understanding, but no predictability. Almost the whole field is empirical. It abounds with fitting parameters and phenomenological rules. One strong thrust of research in the Department is to address these problems. This is being done from a theoretical viewpoint by Mathias Boström, David Williams and Barry Ninham. There are also experiments in this area being conducted by Vince Craig and Vassili Yaminsky.

The major problem with current theories is that they almost all assume that electrostatics dominates all the interactions. In fact for many systems, and indeed for almost all biological systems, the salt concentration is high and the electrostatic

Spirula shell imaged by the department's X-ray Computed Tomography Machine interaction is strongly screened. This means that other forces become dominant and the classic example which we have focussed on is dispersion forces.

The team of Boström, Williams and Ninham has recently applied these ideas to a number of systems of interest to the physical and biophysical community. In particular we have revamped the old "DLVO" theory of the interaction between charged colloids to show that it is invalid at reasonable salt concentrations. We have also examined the behaviour of ions near membranes and DNA. In general, our major result is that almost the whole of colloid science and molecular biophysics needs to be re-examined since the fundamental assumption that electrostatics dominates is wrong. In particular, almost all molecular simulations of biological systems must be called into question.

The Department has had a long history of using the Surface Forces Apparatus to measure molecular forces. One project which was recently undertaken by Vassili Yaminsky and Andrew Stewart was the first direct high-resolution measurements of dispersion force against distance between crossed cylindrical mica surfaces in air with a surface force apparatus that detects displacement by means of a capacitor with a resolution of 0.1 nm. The surface forces apparatus has also been used by Satomi Onishi and Andrew Stewart to measure frictional forces at low humidity. In this regime the surfaces slide without shearing. The dynamic shear stress decreased with increasing humidity and a mechanism based on capillary condensation is proposed to explain the role of humidity on friction by adsorption of water layers on the free mica surfaces, and at the contact.

Vince Craig has continued and extended his work on nanorheology and in particular the effect of slip between a fluid and a solid interface. In classical fluid dynamics it is usually assumed that there is no slip between a liquid flowing in a pipe and the walls of the pipe, i.e. the liquid is at rest at the walls. This however is only an approximation and there has been a growing body of evidence that slip occurs at walls. In large pipes, such as those used for the transport of domestic water this slip is of no consequence. However for very small systems with length scales of order 1000 Å this slip has dramatic effects. In particular Vince Craig and Chiara Netto have shown experimentally using an atomic force microscope that slip can substantially change the force between a small sphere moving towards a fixed plane. This, apart from being of fundamental importance, will be crucial in understanding the lubrication of nano-machines. Vince also spent a few months towards the end of the year at the YKI in Sweden where he collaborated in several projects of importance to the paper industry.

Ira Cooke and David Williams have investigated the collapse of semiflexible polymers. In the past year our work on the collapse of copolymers has been extended to include chains with varying degrees of stiffness. Many important polymers are stiff over length scales of several subunits. These include biological polymers such as DNA and Actin and synthetic polymers such as those that conduct electricity. By modelling the collapse of polymers with various stiffness properties we have observed a wide variety of collapsed structures at the nanometer length scale including rods, toroids, striped toroids and networks.

This year also saw a large amount of equipment installed within the Department, much of it carried out by Tim Senden with the help of technicians Anthony Hyde and Tim Sawkins, both of whom were awarded well-deserved medals for General Staff Excellence in 2002.

The minimal surface formed by a soap film on a wire frame, draped over the corresponding solid surface

The equipment highlight was the building of our X-Ray CT machine which allows full 3D images of materials with resolution down to the micron scale. This will greatly enhance the research capabilities of the porous media group. An Imaging Ellipsometer was installed which allows detailed examination of thin surface layers. A new Atomic Force Microscope was installed with total-internal-reflectance fluorescence microscopy capabilities. This will allow detailed examination of surfaces and a number of experiments involving the manipulation of individual molecules. Tim Senden also continued his applied biological work with Vimed Biosciences and signed a five-year research agreement to develop to the clinical stage a medical diagnostic agent for the detection of blood clots.

As a final point, in November this year the Department held the second annual Kiola conference, which allowed everyone in the Department to present a slice of their work. This meeting also involves a few honoured outside guests and presents the work of the Department in a primitive but relaxed environment.

STAFF

Professor and Head of Department
Stephen Hyde, BSc PhD Monash (until October)

Senior Fellow and Head of Department
David Williams, BSc Sydney, PhD Cambridge (ARC Fellowship, University of Sydney) (from October)

Professors
Stephen Hyde, BSc PhD Monash (from October)
Barry Ninham, MSc WA, PhD Maryland, DTech (hon causa) KTH Stockholm, D Phil (hon causa) Lund, FAA (Visiting Professor, University Florence, Italy, April – December)

Senior Fellows
Andrew Stewart, MA ScD Cambridge, AM Harvard, EE Col, DIC PhD London, FAIP
Vasili Yaminsky, DipHons PhD Moscow

Fellow
Tomaso Aste, DipHons Genova, PhD Milan
Mark Knackstedt, BSc Columbia, PhD Rice (jointly with School Pet. Eng., UNSW) (ARC QEII Fellowship)

Research Fellows
Andy Christy, MA PhD Cambridge
Vince Craig, BSc PhD (ARC Fellowship)
Satomi Ohnishi, BSc SUT, PhD Saitama
Tim Senden, BSc PhD (ARC Fellowship)
Adrian Sheppard, BSc Adel, PhD

Adjunct Fellows
Rob Sok, BSc PhD Gronigen

Post-Doctoral Fellows
Christoph Arns, Dipl-Phys Aachen, PhD UNSW
Armin Bauer, Dipl-Chem Dr.Rer.Nat Regensburg
Tiziana Di Matteo, BSc PhD Universita' di Salerno
Ann-Kristin Larsson, MSc Lic PhD Lund, Doc Stockholm
Vanessa Robins, BSc MSc, PhD Colorado
Arthur Sakellariou, BSc PhD Melbourne

Computational & Visualisation Consultants
Stuart Ramsden, GradDip Film & Television Swinburne
Ray Roberts, BSc (CRC Administrator)
Adam Stone

Visiting Fellows
Mattias Boström, MSc PhD Linkoping
Anna Carnerup, BSc Malmo (from February)
Georges Debrégeas, PhD Paris VI
Jean-Marc di Meglio, PhD Paris VI
Eugene Gamaly, PhD DSc Moscow
Bruce Hyde, BSc Bristol, PhD DSc
Siewert-Jan Marrink, PhD Groningen
Yoshinori Nagai, DSc Waseda
James Quirk, DSc WA, AO, FTS, FAA
Nicholas Welham, BEng Leeds, PhD Imperial College

Senior Technical Officers
Anthony Hyde, Assoc IE Aust
Tim Sawkins

Departmental Administrators
Vicki Beissner (part-time) (until May)
Cindy Bradley (part-time)