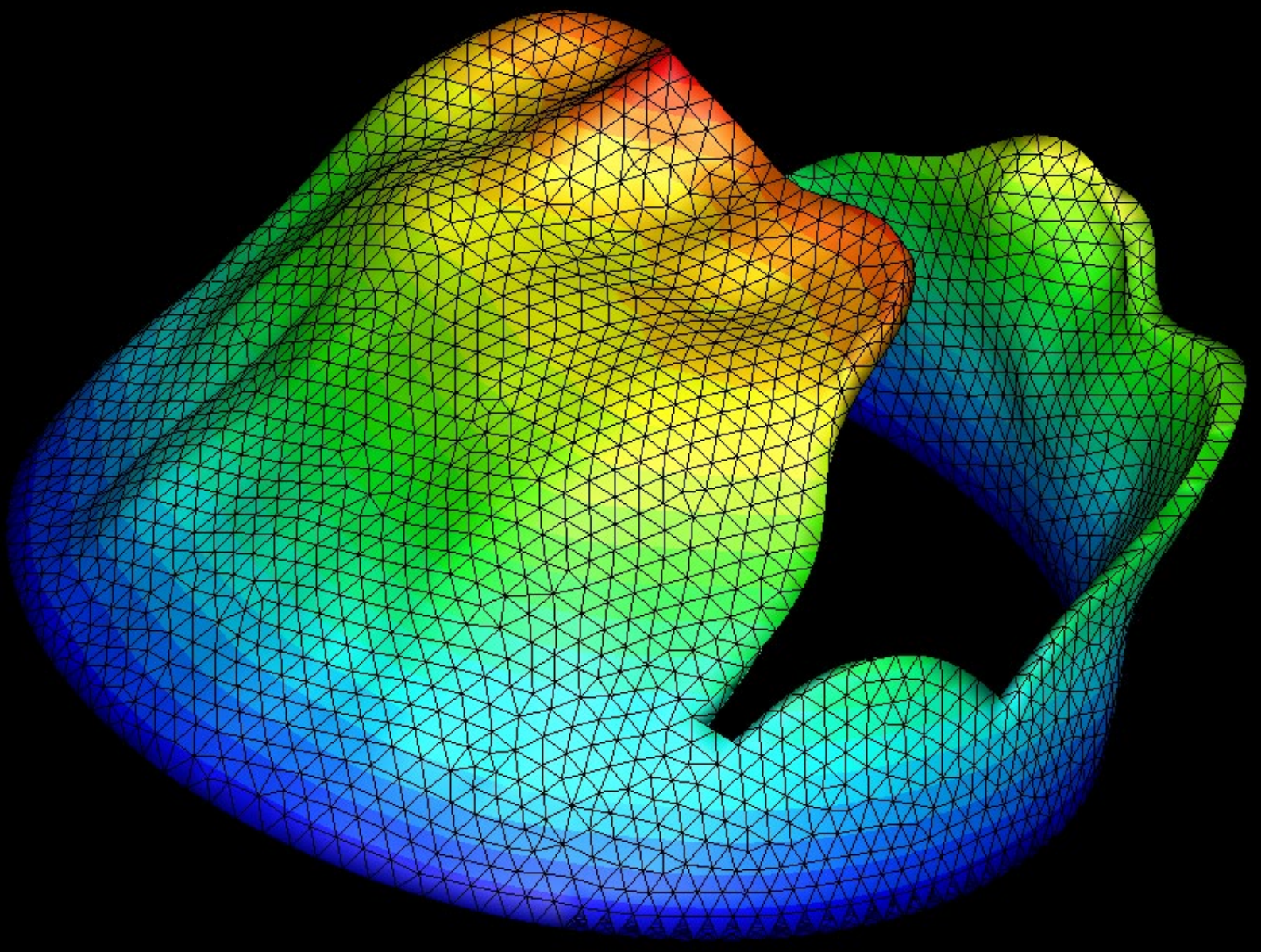
University of Glasgow

Modelling and simulation



Foreword

The University of Glasgow ranks in the top 1% of the world's higher education institutions due to its ongoing focus on research excellence. Within the University, the College of Science and Engineering is home to wide-ranging and high quality modelling and simulation research.

Modelling and Simulation is an interdisciplinary activity, spanning mathematics, computing science, materials science, engineering, biology and medicine. Models allow us to create mathematical representations of the system under investigation and simulate its properties and behaviour over time and under different conditions. This is an extremely powerful approach in planning and understanding experiments and producing powerful predictions in designing systems. Modelling and simulation techniques are used in all realms of science and engineering and find endless industrial and biomedical applications.

Among the researchers contributing to this brochure are representatives from diverse fields. We trust that this brochure will provide an introduction to the breadth of our activities in this area. Going forward we are looking outward to new partnerships and hope that you will be able to engage with us in the future.

Prof John Chapman
Head of College of Science and Engineering
University of Glasgow

Working with the University of Glasgow

The University of Glasgow has a strong track record of collaborating with industry and other research institutions.

We have successfully helped many organisations to strengthen their capabilities and competitiveness through a range of engagement methods. The University's Knowledge Exchange team are highly experienced in working with collaborators, linking industry to academics who can provide the necessary technical programme and deliver the most appropriate solution. The options outlined below demonstrate our commitment to engaging with external partners.

Vouchers

Awards of up to £5k are available to Scottish based companies to work with academics on activities such as problem solving, proof of concept and technology demonstration. This support helps to create long-term collaborations between SMEs and the University of Glasgow. Priority is given to projects that assess both the feasibility and potential of a new product, process or market and can lead to opportunities to attract follow-on funding.

Student Projects and Industrial Studentships

Student projects are an excellent way for companies to engage with the University to gain access to new ideas, expertise, and capability via the student and their academic supervisor. This approach has the added benefit of allowing the student and the company to consider if there may be future employment opportunities. By sponsoring a studentship the industry partner can specify a PhD topic and work with the student and academic supervisor to access basic research outcomes relevant to their business.

Knowledge Transfer Partnerships (KTP)

KTPs enable businesses to work with the University, bringing knowledge and expertise into your organisation to help solve important technical or business problems.

A KTP Associate, usually a recently qualified graduate, will work within a business to manage the project, apply their own knowledge, and ensure that University expertise is available to the company.

Collaborative research

By collaborating with us companies can benefit from extensive and ongoing input to the research process. They can also gain from access to world-class research expertise and facilities. Jointly we can seek external research funding from organisations such as: Technology Strategy Board, European Commission, Ministry of Defence and Research Councils.

Strategic partnerships

Strategic partnerships deliver research and commercial synergy that neither partner could achieve alone. In many instances, dedicated research laboratories have been established, which significantly extend the capabilities of the industrial partner.

If you would like to engage with the University via any of these routes, please contact us for advice and support to forge new relationships, develop projects and access leading edge research capabilities.

Consultancy

As one of the UK's leading research universities, the University of Glasgow has an outstanding record of achievement in a wide range of subject areas. Our research experts can be relied on to provide substantive opinion and consultancy.

Contract research

The University's expertise and facilities cover a wide range of disciplines allowing us to offer you unique, inter-disciplinary solutions to satisfy your research requirements. Contract research services are tailored to meet the specific needs of individual organisations; projects are well managed and results delivered on time and on budget.

Our wide ranging experience includes working with international blue chip companies from many sectors.

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Arterial dissection

Prof N. A. Hill, Dr S. Roper, Prof X. Luo, Dr N. Tzemos, Prof C. Berry, Dr B. Griffith^ and Dr F. Sutherland*

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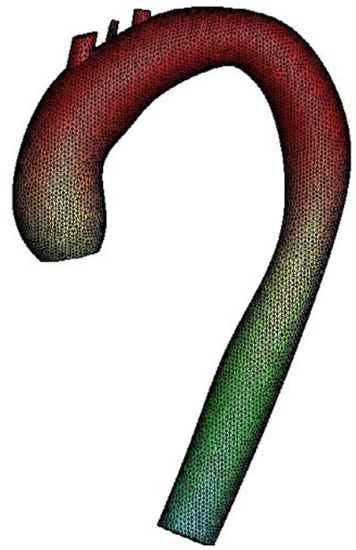

The challenge

An arterial dissection is a tear of the delicate internal lining in the artery. It causes serious damage and is of significant interest to surgeons. When this happens in a coronary artery, it leads to myocardial infarction with a high rate of modality. Although arterial dissection is a frequently occurring phenomenon and a challenging clinical entity, the underlying biomechanics remains largely unclear.

How it is solved

In this project, we will address a particular situation of aortic dissection associated with patients with congenitally bicuspid aortic valve. A congenitally bicuspid aortic valve has two functional leaflets instead of three leaflets. Bicuspid aortic valve is often observed with other left-sided obstructive lesions such as coarctation of the aorta or interrupted aortic arch, and dilated aortic root. This dilatation has some similarities to the dilatation of the aorta seen in Marfan syndrome. The dilatation may involve the ascending aorta (most commonly) but may also involve the aortic root or transverse aortic arch. It is presumably due to the weakened aorta, patients with bicuspid aortic valve are particularly prone to artery dissection.

We will derive analytical solutions for simplified artery dissection models using a novel (cohesive zone) approach to resolve the crack (dissection) propagation in the arterial wall embedded in fluid (blood). The simplified models will be used to develop more realistic physiological models using numerical methods and MRI, and results will be compared with Glasgow clinical database of patients with congenitally bicuspid aortic valve. The project will identify the key factors contributing to the higher rate of arterial dissection in this patient group.

Why it is important

Aortic dissection is life threatening. The condition can be managed with surgery before the aorta ruptures. Unfortunately only less than half of patients with ruptured aorta usually survive.

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Multi-scale modelling of the human heart

Prof X. Y. Luo, Prof C. Berry, Dr B. Griffith^, Prof R. W. Ogden, Dr R. Simitev, Prof J. Soraghan*, Dr F. Burton, Prof G. Smith, Prof N. A. Hill, and Dr J. Going

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The challenge

Improved approaches are urgently needed to identify the extent of heart muscle injury involved in heart conditions and potentially predict future outcomes, including treatment response. Multi-scale modelling of human heart combined with MRI can be used to develop a clinically-useful framework to combat diseases and to improve our understanding of both physiological and pathological behaviours of human heart.

How it is solved

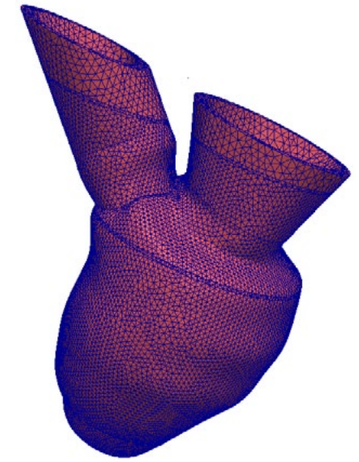
Our work embraces this problem by bringing together imaging, mathematics and medicine. We use magnetic resonance imaging (MRI) and mathematics to construct 3D multi-scale modelling of the heart to explore acute myocardial infarction (MI) in experimental animals and humans. The cardiac MRI scans provide information on structure, function and pathology in a single scan. The mathematical methods use MRI data to recreate geometric models of the heart, including fibre structure, and make use of structure-based constitutive models and bi-domain based active contraction. The parameters of the constitutive models will be identified using an inverse approach from the dynamic strain field measured by the 3D displacement. These data will be encoded with stimulated-echos (DENSE) MRI from human subjects taken at the University of Glasgow British Heart Foundation Centre.

Since MRI is safe and scans can be repeated without adverse effects in the patient, heart models can be developed serially and so evolve in response to changes in the heart post-MI.

For the mechanical modelling of the heart, we use the finite-element immersed boundary method (IBAMR) modelling to study the 3D finite strain with fluid-structure interaction. IBAMR combines the strength of the conventional immersed boundary methods and the finite element methods, and enables both the fluid-structure interaction, and the complicated nonlinear finite strain solid mechanics to be modelled accurately and effectively.

Why it is important

Heart attack is a leading cause of premature ill health and death and places a significant burden on the NHS. Consequently, improved approaches are urgently needed to identify the extent of heart muscle injury and potentially predict future outcomes, including treatment response.



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Dynamic modelling of bioprosthetic and human mitral valves

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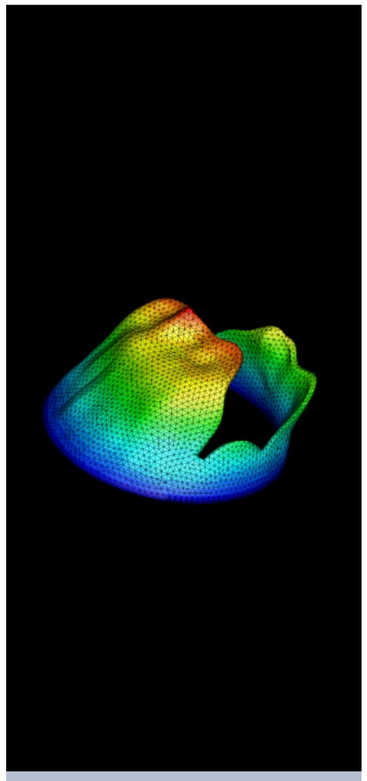

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The challenge

In humans, the mitral valve is a complex anatomical structure consisting of two leaflets, an annulus, chordae tendineae, and papillary muscles. Different to the aortic valve, the leaflets of the mitral valve are asymmetric and are attached to the left ventricle through a bundle of chordae tendineae. These differences have a significant effect on its function.

To handle the dynamic modelling, we use the immersed boundary method, modelling the 3D dynamic fluid-structure interactions. The immersed boundary method is a practical and effective way to simulate certain types of fluid-structure interaction (FSI) problems, which use the elastic fibres to represent the elastic body (heart valve) immersed in a viscous incompressible fluid (blood). Its effective dynamic capability has been used to model blood flow patterns in the heart, and to assist prosthetic valve design.

How it is solved

To investigate the mechanical behaviour of the mitral design under physiological flow conditions without having to model the left ventricle, we make use of in vivo magnetic resonance images of the left ventricle. The relative motion of the mitral annulus and the papillary muscle regions of the ventricle determined from these MRI images are then used as a prescribed boundary condition for the chorded mitral valve in a dynamic cycle. Results show that without the proper functioning of the papillary muscle, the mitral prosthesis can suffer from an intolerable over-stretch during systole compared with laboratory tests in which the mitral chordae are fixed in space. This turns out to be the key weakness of the current design.

Why it is important

A diseased mitral valve is usually repaired by various surgical means such as the replacement or transfer of the damaged chordae. When a mitral valve is too severely diseased for repair to be effective, it is generally replaced with a mechanical or bioprosthetic valve. Understanding native mitral valve dynamic behaviour is thus highly important for developing more efficient repair techniques, and perhaps even more so to aid the design of artificial mitral valves. With improved cardiopulmonary bypass, myocardial protection, and surgical techniques, the mortality rate from aortic valve replacement has decreased substantially, whereas the mortality rate from mitral valve replacement remains high (around 50% at 10 years), largely because of the low cardiac output syndrome.

Numerical study of flow in collapsible tubes

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The challenge

Cylindrical tube deforms in a strongly nonlinear fashion when subject to large external pressure, a problem that frequently appear in many biological applications. Engineering approaches to this problem often use linear deformation, which can give very inaccurate predictions.

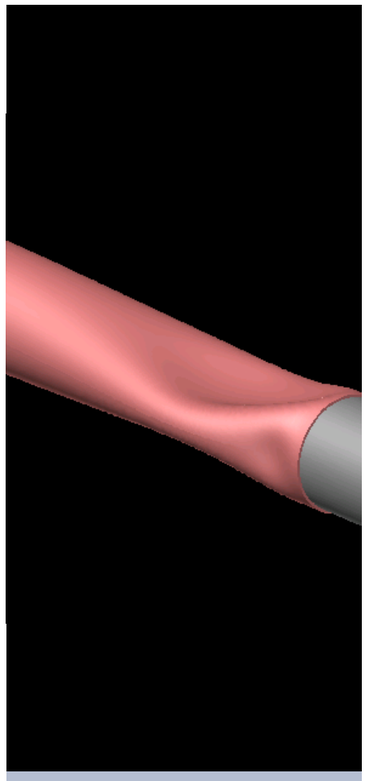
How it is solved

In this project a totally nonlinear analysis is conducted for an axisymmetricly deformed thick-walled cylindrical tube which is subject to external pressure. The results are then compared to those obtained with linear predictions.

For small deformations, both linear and nonlinear models give very similar results. However, cylindrical tubes behave very differently under large external pressure with the dominant features being the corner bulging and higher modes. This is the first time that a totally nonlinear analysis is carried out for thick walled tubes, and the results may have significant implications to many physiological applications involving soft vessels undergoing large deformation.

Why it is important

The collapse of compressed elastic tubes conveying a flow occurs in several physiological applications and clinical devices. Examples are arteries collapsing during sphygmomanometry and large bronchi collapsing during forced expiration. Experiments on such a system have revealed a rich variety of self-excited oscillations that exist in such flows, demonstrating that the system is a nonlinear dynamical system of great complexity. Several one-dimensional and lumped-parameter theoretical models have been proposed, revealing different mechanisms by which oscillations can be generated or maintained. However, due to the crude approximations that have to be used in such models, there is as yet no complete theoretical description of the oscillations in any realisable experimental conditions.



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Mathematical modelling of the cornea

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The challenge

The cornea has a unique shape in that its curvature is steeper centrally than on the periphery. Any change in the curvature of the cornea will affect the refractive status of the eye profoundly. In a condition called keratoconus (KC), which usually affects young people, the corneal curvature becomes conical and the central corneal curvature becomes steeper.

This results in poor image formation on the retina. Patients affected by this condition require a corneal transplant. This procedure is carried out in a circular shape and the central 8 mm of the cornea is removed and replaced with a donor cornea. However, KC is not always central and it can involve the periphery of the cornea. Current surgical practice still adopt a central corneal graft leaving the peripheral corneal uncorrected.

How it is solved

We will develop a mathematical modelling of the curvature of the cornea in KC, with the objective of designing the best fit shape graft. This could be extremely useful in surgical planning for diseased eyes, or in the Emergency Department for dealing with eyes that have collapsed due to perforation.

Why it is important

KC is a degenerative condition that affects the front of the eye causing severe visual impairment. The casues of KC are not clear but there is a suggestion that the disease might be already in the patient at birth. It is generally diagnosed in young people and although it is not very well known, it is not rare, with an incidence in the general population of 1 to 430/2000.

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Understanding human gallbladder pain

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The challenge

The most common cause of gallbladder disease is the presence of gallstones. However, it is not uncommon to have stones in the gallbladder that cause no symptoms. On the other hand, a proportion of people do suffer from severe acalculous (i.e. without gallstones) biliary pain. The decision to surgically remove the gallbladder is based on the patients symptoms (pain) and not on the presence of gallstones.

Of a major concern is that not all patients benefit from the cholestectomy, and the symptoms can continue even though the gallbladder has been removed. The fundamental issue is to understand the underlying mechanisms of gallbladder pain, which remains a challenge.

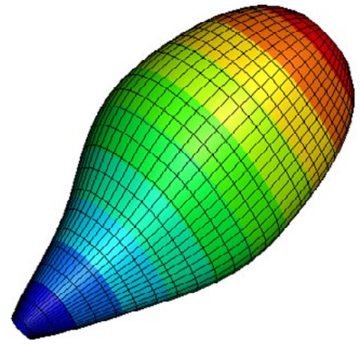
How it is solved

This project aims to develop mechanical models and to identify the mechanisms of gallbladder pain. Initial investigations predicted that the peak total stress in the gallbladder wall has a strong correlation with the pain.

The biliary system consists of pliable tubes and various valves into which bile and pancreatic juices are secreted under pressure. The gallbladder receives diluted bile from the liver, stores and concentrates it during the inter-digestive period and evacuates the more viscous gallbladder bile in response to a meal-stimulated contraction. The bi-directional flow is controlled by the cystic duct, commonly known as the Heister valve or the spiral valve. Extensive clinical and in vitro studies at the Sheffield Gallstone Centre have strongly suggested that the critical unknown in the normal and pathophysiology of the biliary system is in the filling and evacuation of the gallbladder and the flow through the cystic duct.

Why it is important

Gallstones and other biliary diseases affect about 10% of the adult population of the UK. Up to 60,000 operations to remove the gallbladder are being performed in the UK each year, at a cost of about £40 million to the NHS. Understanding of the pathogenesis of gallstone disease and pain production mechanism is key to improve diagnosis and patient outcome and prevent complications of gallstones such as acute pancreatitis and obstructive jaundice, which can be fatal.



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Multi-physics modelling of gravitational wave pendulum suspensions

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The challenge

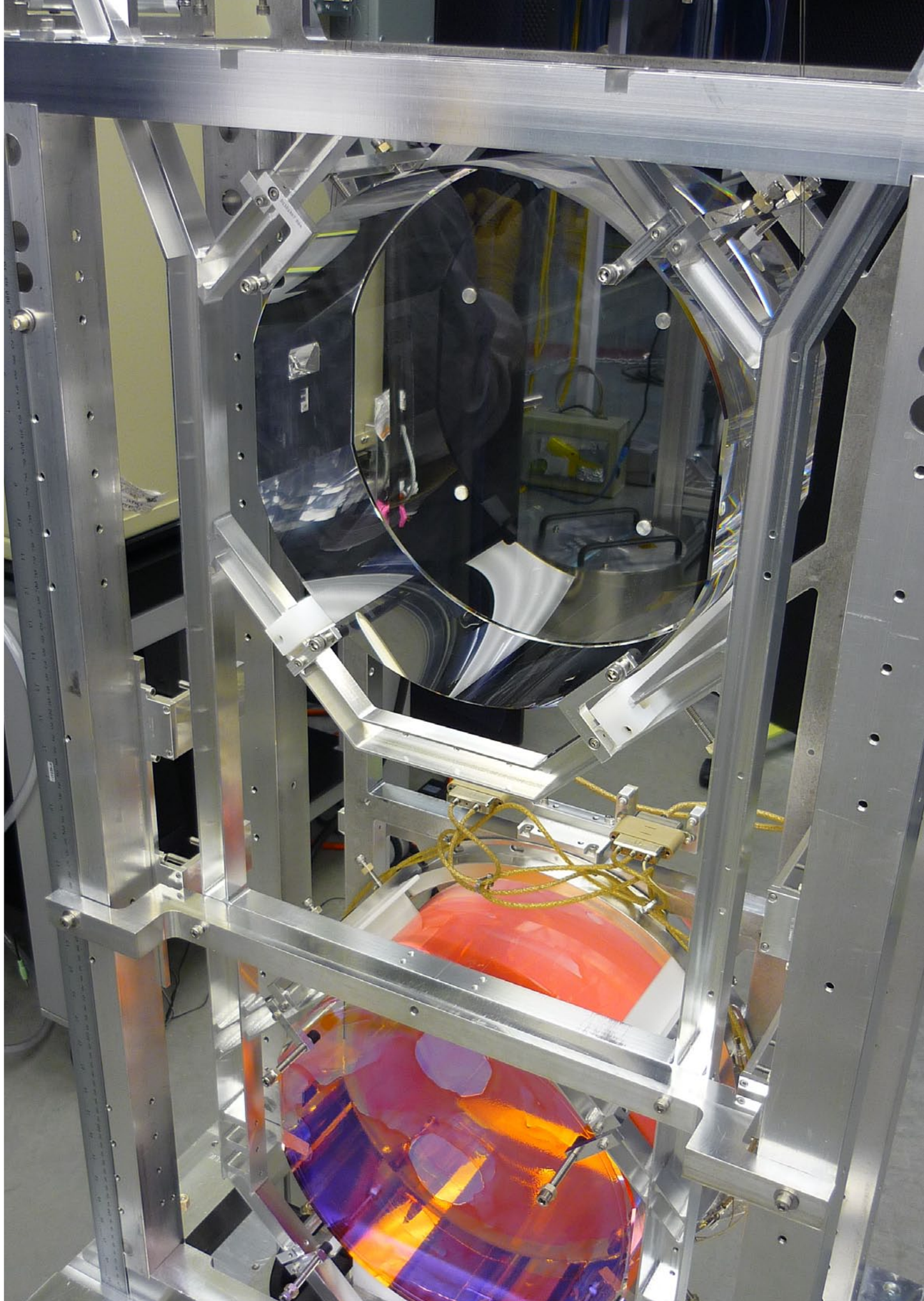
Gravitational wave interferometers are the most sensitive length measuring instruments in the world, able to sense changes at the level of 10^{-18}m over baselines of 4km. This is achieved by attaching the interferometer mirrors to multi-stage pendulum suspensions to isolate from seismic noise and by fabricating the final pendulum stage from ultra-low mechanical loss fused silica to lower thermal noise. The challenge is to design and fabricate suspensions that meet the target sensitivity and thus allow the first detection of gravitational waves from astrophysical sources.

How it is solved

We use the ANSYS finite element package to perform a variety of multi-physics simulations including mechanical, electromagnetic and thermal. Static structural and modal analyses are used to infer the strain energy and resonant frequencies of the suspensions elements which, combined with imported mechanical loss terms, can be used to provide the most robust thermal noise estimates. An electromagnetic solver is used to design damping coils which have high linearity, sufficient control authority and low viscous eddy current damping. Thermal analysis is used to model the fused silica suspensions and infer the thermal stress frozen into the material during fabrication. This utilises the radiative solver and the thermo-mechanical properties of fused silica in the temperature range 20^0C-2000^0C.

Why it is important

These modelling techniques allow us to analyse and design the next generation of gravitational wave detector suspensions which will enhance the sensitivity by a factor of 10 and provide the first detection of gravitational waves. A combined modelling and measurement campaign on test suspensions has shown these techniques to be extremely accurate and thus allows the study of upgrade scenarios. This includes the use of crystalline materials at cryogenic temperature such as silicon and sapphire to further lower thermal noise. There are also a number of applications in industry including the design of the ultra-sensitive fused silica borehole gravity meters.



Hardware acceleration of high-performance computing using GPUs and FPGAs

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The challenge

Hardware accelerators such as GPUs and FPGAs have great potential for speeding up computations and can result in huge power savings for High-Performance Computing systems. However, obtaining good performance on GPUs and FPGAs with the current tools is difficult. Our research aims to lower the barrier to adoption by developing tools and methodologies to facilitate the use of hardware accelerators.

How it is solved

Dr Vanderbauwhede works on accelerating High-Performance Computing applications using Field-Programmable Gate Arrays (FPGAs) and Graphical Processing Units (GPUs).

These novel hardware platforms have the potential to speed up many types of HPC applications by exploiting the latent parallelism in the algorithms.

Highlights of this work include:

- The MORA technology which allows to develop high performance FPGA applications using C++. This work was recently featured in the press as the "1000-core FPGA processor".
- The Greener Search work which demonstrated a 20- fold speed up of Information Retrieval algorithm implemented on FPGA, at a fraction of the power consumption of a CPU implementation.
- Acceleration of climate simulations on GPU platforms, which will allow more accurate models to be simulated.
- Acceleration of Markov-Chain Monte-Carlo methods for modelling nuclear physics.

Why it is important

The benefits of hardware acceleration are not only in getting results faster, or enabling more complex simulations, but also in a considerable reduction in energy consumption per task. In particular FPGA platforms are therefore very attractive for reducing energy and cooling costs in data centres.

StatDes project: statistical design and verification of analogue systems

Prof A. Asenov

The challenge

With decades of research, manufacturing efforts and successes of transistor miniaturisation by the leading Semiconductor Industries and research groups comes the "cramming" of large-scale transistors into a single chip, which results in more and more powerful chips. However, smaller transistors are far more variable and less reliable. This is one of the major challenges to the design, development and manufacturing of such advanced chips, to which there is no easy solution. This problem is exacerbated by a strong demand for smaller devices with more functionality from consumer electronics companies, which is reflected by the surge of great popularity of, for example, iPhones, iPods, iPads and other digital media products.

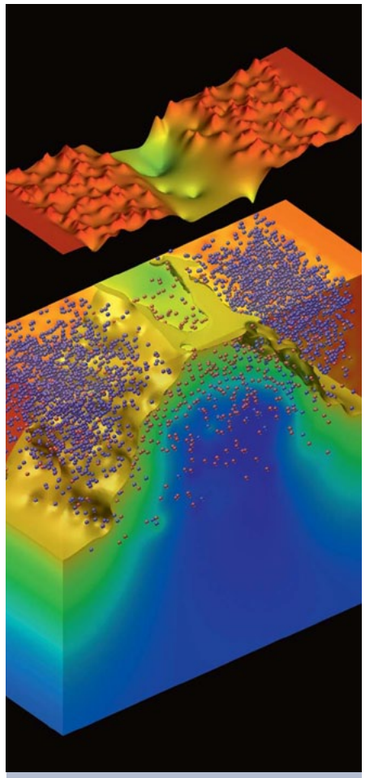
How it is solved

Over the last 10 years Prof Asen Asenov's group has established itself as a world leader in the understanding and simulation of statistical variability in nano CMOS devices. The group has developed a suite of high performance tools for statistical variability simulation and GRID computing solutions that already provide the semiconductor industry with fast and accurate prediction of statistical variability. Prof Asenov's research led to the formation of a new venture, Gold Standard Simulations Ltd, delivering services and developing stand-alone software to industry.

The "Statistical design and verification of analouge systems" (StatDes) project will draw on years of research by the Universities of Glasgow and Edinburgh in the development of tools for the simulation of nanoscale silicon chip devices and their circuit behaviour. In particular StatDes will translate world leading statistical compact model extraction and circuit simulation and verification technology, methodology and tools. These were developed in the framework of a £4.5M EPSRC eScience Pilot Project NanoCMOS, in which the Universities of Glasgow and Edinburgh were key partners. The capabilities of the tools and the knowledge generated will be exchanged with the major design and semiconductor houses and Small and Medium Enterprises (SMEs) in Scotland.

Why it is important

The StatDes project will deliver capabilities that will allow designers to develop products faster and more reliably with high yields and reliability. The tools will allow a reduction in the power consumption of future analogue, digital and mixed signal consumer products. The project will also produce case studies that will help encourage SMEs to start using the translated technology in product development. These will highlight how the toolset can be used and the likely benefits for product development from using the tools.



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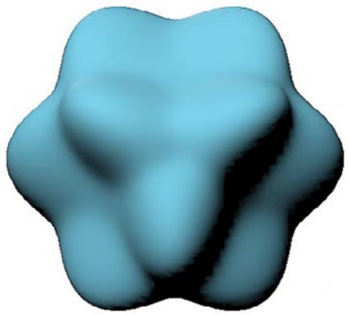
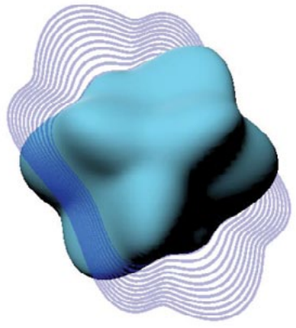
Carrier transport in p-channel MOSFETs: alternative materials and architectures

Dr C. Riddet and Prof A. Asenov





The challenge

As CMOS technology is scaled, high drive current is needed in order to increase circuit speed. As such, the investigation of alternate channel materials for CMOS applications has experienced a revived impetus, with Germanium proving especially promising for p-channel MOSFETs where higher carrier mobility and drive current compared to conventional Silicon devices has already been successfully demonstrated. The performance of Germanium based devices can be improved further by employing strain and exploiting different crystallographic orientations. The choice of device architecture is also of importance, with a suitable design required to properly take advantage of the benefits of the material. Predictive simulation of these systems is required to understand and quantify their potential

How it is solved

Accurate simulation of these devices is complicated by the nature of the materials themselves and the complexity of the architectures, which are now truly 3D. Therefore, 3D transport simulations using the Monte Carlo approach offers a solution that can capture the important physics while maintaining computational efficiency. The initialy basic model can be made more sophisticated by including a full array of carrier scattering mechanisms, the impact of quantum mechanics and a detailed approximation of the energy bandstructure, all of which allow for fast, reliable and predictive simulation studies of alternative materials and scaled structures to be conducted, giving a strong indication of their potential for use in future technology generations.

Why it is important

CMOS scaling has driven the growth and advancement of industrial and consumer electronics over the last four decades, allowing for modern communication and computing devices to be smaller and lighter but with increased power and functionality. Maintaining this trend requires development of future generations of smaller and faster CMOS devices allowing for denser integrated circuits. Simulation of these devices is vital in the design process, and must be accurate, predictive and efficient in order to be useful. Monte Carlo transport simulation offers a flexible approach that can be easily extended to include new physics and is applicable to aggressively scaled devices.

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Time-dependent variability

Dr L. Gerrer and Prof A. Asenov

The challenge

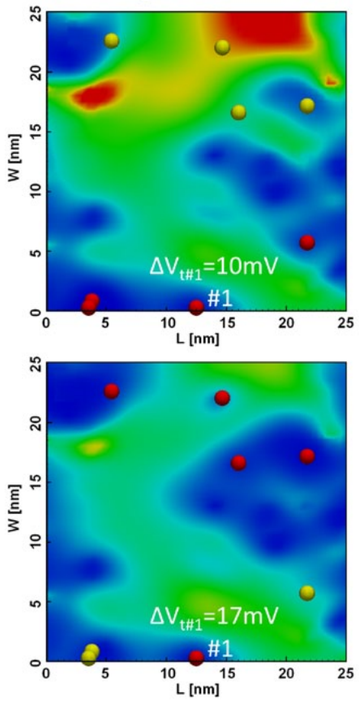
Dynamic charge trapping into the oxide represents a growing challenge for microelectronic leading to performances degradation with time (BTI, RTN). Interactions with statistical variability affect device parameters distribution. Moreover, the stochastic character of trapping leads to a strong dispersion of performances within the same device from one use to another, thus the device activity in a given circuit needs to be considered at atomistic level and transferred into circuit models.

How it is solved

We developed a reliability module following the most recent development in oxide degradation understanding and traps characterisation measures; we are able to predict time-dependent variability behaviour, including interactions with statistical variability and traps impact interactions (see picture). Each single trap activity is simulated and its impact dynamically evaluated to simulate both permanent and recoverable parts of degradations. Interfacing our simulator with first principle simulations on one hand and with compact models extraction strategies on the other, we are able to transfer the best available physic understanding of oxide degradation up to circuit level simulations and by turn to industrial reliability projections.

Why it is important

This simulator is the most complete and most efficient multi-scale simulator of time-dependent simulation, pushing forward microelectronic simulations capabilities. Not only it will provide valuable reliability projections, but it will also strongly help circuit designers to reach their targets. In turn, circuit performances will increase and design time will be reduced. Multi-scale simulators are absolutely necessary to address growing concerns of future microelectronics such as 3D device architectures or molecular devices.



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CASE STUDY: Gold Standard Simulations Ltd

Prof A. Asenov

http://www.goldstandardsimulations.com/

A spin-out company from the University of Glasgow is developing world-leading technology that could save the semiconductor industry billions of pounds from silicon chip failure by predicting how performance will be affected in future generations of miniature transistors.

Intel founder Gordon Moore correctly predicted in the mid-1960's that increasing miniaturisation would make it possible to double the number of transistors on a microchip every two years, leading to a phenomenal increase in computing power.

A typical silicon chip contains one billion transistors – electrical switches at the heart of microchip complementary metal oxide semiconductor (CMOS) circuits - that have led to an explosion in the capability of devices such as iPods, mobile phones, computers and games.

However, as the demands of the global semiconductor industry have pushed the continual scaling of transistors to truly nano-scale dimensions, their performance started to vary due to atomic imperfections in their structure – a phenomenon known as 'statistical variability'. This has led to decreasing yield, increasing manufacturing cost and increasing rates of chip failure for the $300 billion a year semiconductor industry. It currently takes companies 18 months, on average, to bring a new product to market and delays caused by chip failures close to product release can lead to businesses losing millions of dollars and significant market share. Gold Standard Simulations Ltd (GSS), a spin out company from University of Glasgow's School of Engineering, is leading the world in predicting the impact of 'statistical variability' on microchip performance.

GSS was formed to commercialise the advanced simulation tools developed in the University's Device Modelling Group and now produces and sells software and services for 3D 'atomistic' TCAD simulation of devices, advanced variability compact modelling and statistical circuit simulation. GSS uses these tools to predict variations in the performance of next generation transistors up to two years before they come to market, allowing the semiconductor manufacturers who produce them to optimise their designs in order to improve performance and yield.

Prof Asenov (head of the Device Modelling Group and CEO of GSS) believes that these techniques could save the semiconductor industry up to $2 billion a year, rising to $4 billion in the next five years, and Gold Standard Simulations is aiming to be the first to market with these tools.

GSS was formed three years ago and now supplies simulation software and services to some of the largest semiconductor companies in the world.

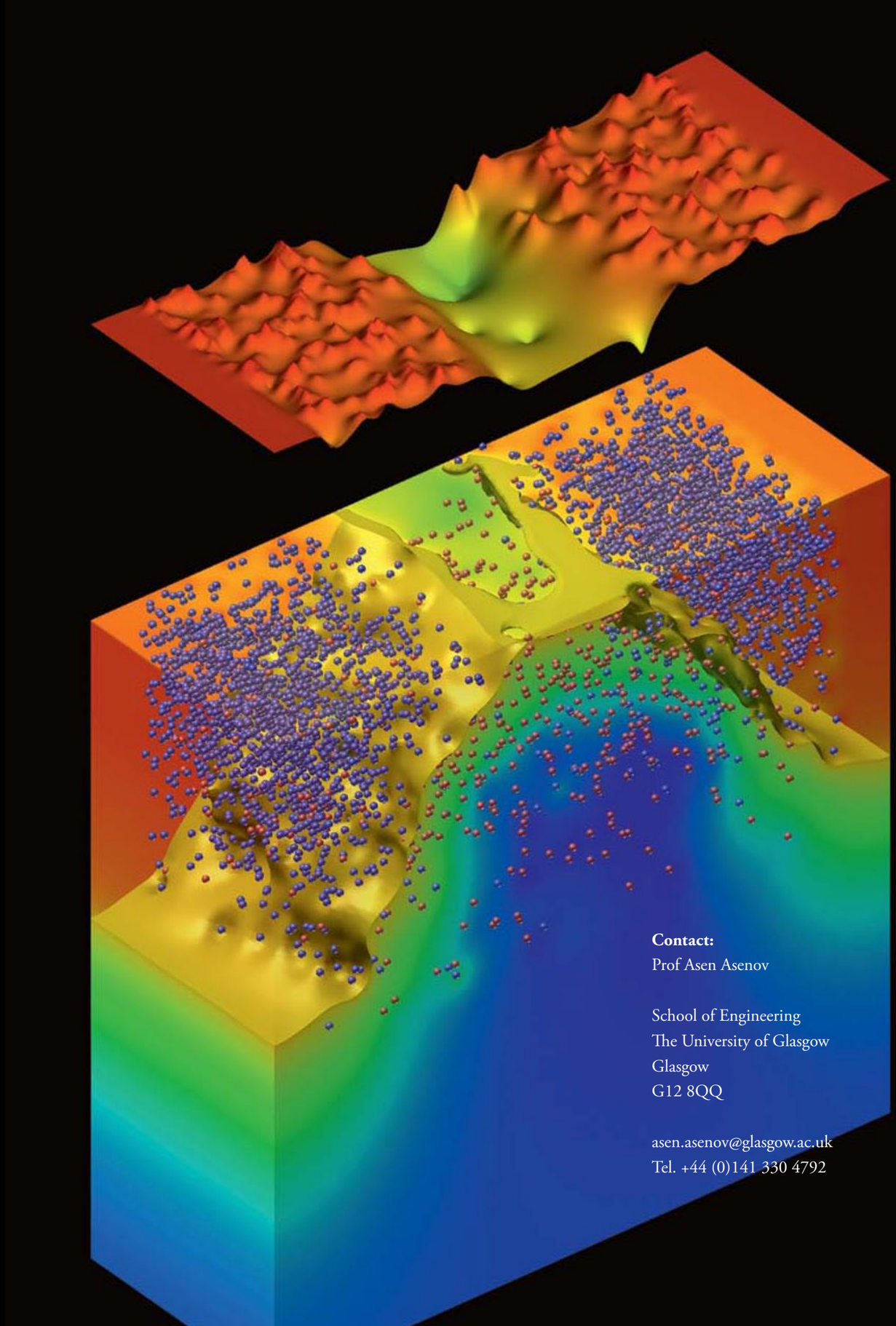
Prof Asenov's research group developed the tools in recent years with funding from EPSRC, the European Commission, and the European Nanoelectronics Initiative Advisory Council (ENIAC). Prof Asenov started the development of the simulation tools 15 years ago when he was approached by NASA, who believed there might be a problem with the randomness of dopants – that are introduced to silicon to make the transistors.

The problem arises because it is impossible to predict how the atomic dopants' atoms will be arranged within the transistors. In what has become known as the Christmas pudding effect, the dopants are like raisins in the pudding mix and no one knows how they will end up positioned in each pudding which exemplifies transistors in the silicon chip. This leads to variations in the current flow and disruptions.

"When we told companies about this 10 years back, they said the transistors are so big we can't see the dopants affecting their performance," said Prof Asenov. "They said it might happen in 15 or 20 years but we can't worry about it now."

"We were lucky to start to develop the tools well before this was recognised by industry. Now the industry has woken up to the fact that this is a big problem and we are the only company in the world that can do the predictive simulation that can help solve these problems."

On the right: Carrier concentration and potential in a modern nano-scale P-Channel MOSFET. The individual dopant atoms are shown and it is clear that they strongly influence the way that the current flows through the device.



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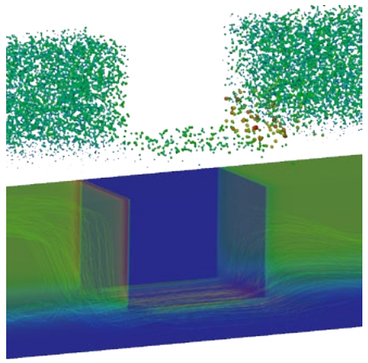
Numerical modelling of high-mobility channel transistors for future digital applications

Dr E. A. Towie and Prof A. Asenov



The challenge

The continued scaling of metal-oxide-semiconductor field-effect transistors (MOSFETs) for digital applications in microchips into the nanometre scale is incredibly challenging using traditional architectures and materials. The typical silicon bulk MOSFET structure is not expected to meet the requirements as set in the International Roadmap for Semiconductors (ITRS) at sub-20nm technologies. This has resulted in huge interest in different materials and designs of MOSFETs to improve performance and reduce power consumption including III-V materials that are predicted by the ITRS to enter production in the sub-15nm technologies.

How it is solved

We have developed a three dimensional numerical simulation toolset that allows future MOSFET device designs and materials to be evaluated and optimised. In particular, the use of high-mobility channel materials such as InGaAs and Germanium and advanced device architectures including quantum-well and multi-gate designs can be accurately simulated and their performance predicted. We use a 3D Monte Carlo simulator that captures non-equilibrium, quasi-ballistic carrier transport effects which has been extended to allow for simulation of high-mobility channel materials including degeneracy and multi-valley transport.

Why it is important

Completing numerical simulations with Monte Carlo of future high-mobility channel MOSFETs allows industry designers to understand the performance benefits before production begins, potentially saving costly development time. The MOSFET can be optimised using numerical simulations to achieve the best performance and the impact of reducing the supply voltage to reduce power consumption can be examined. Coupled with the ability to highlight potential pitfalls in a MOSFET design benefits the $300 billion a year semiconductor industry.

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Molecular electronics

Dr V. P. Georgiev and Prof A. Asenov

The challenge

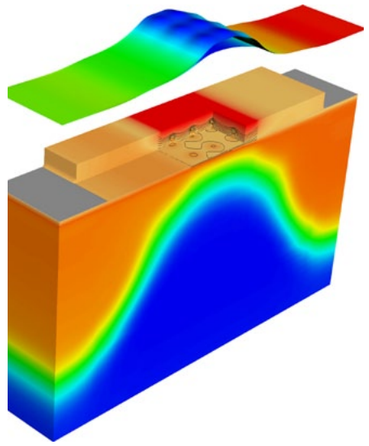
The main challenge is to demonstrate functional circuits using molecular metal-oxides (MMOs) with the ultimate aim of achieving the molecular limit in data storage and processing; i.e., realising inorganic, single molecule transistors. Additionally, the project aims to establish a link between the two traditionally distinct fields of molecular design and modelling, and device design and modelling, and to exemplify the synergy derived from the diverse expertise held at each side.

How it is solved

The challenge is solved by taking an interdisciplinary approach, involving chemical synthesis and experimental characterisation of the MMOs (X-Ray, ESI-MS, cyclic voltammetry, etc), DFT modelling of their electronic properties and device-level modelling and simulation of the Flash-Cell and circuits. This is achieved providing a stimulating environment for researchers from the School of Engineering and the School of Chemistry to liaise and share knowledge and ideas.

Why it is important

The programme is important from both fundamental and applied points of view because success will enable not only cheaper electronic circuits but also the development of a range of molecular based nanosystems. Moreover, a ‘real-time’ technology transfer will allow us to immediately seize any commercial development opportunities thereby building a better understanding of where we should focus our effort to benefit both UK society and economy.



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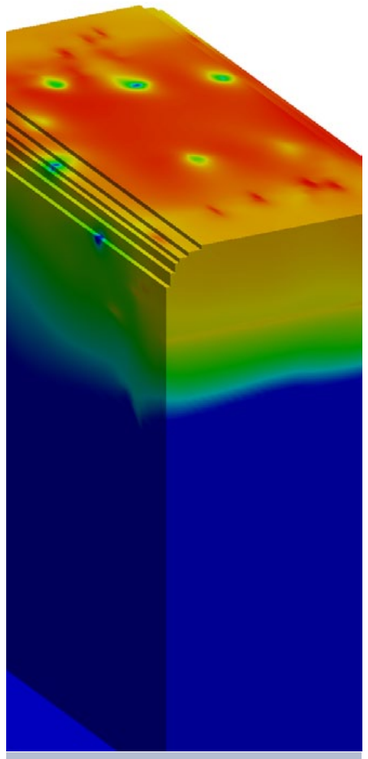
Advanced simulation of variability and reliability of nanoscale MOSFETs and flash memories

Dr S. M. Amoroso and Prof A. Asenov



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The challenge

One of the biggest challenges that CMOS Reliability-Aware Design methodology faces today is the statistical variability associated with the discreteness of charge and granularity of matter in nanoscale transistors. Recent publications clearly demonstrate the interplay between the statistical variability and the degradation phenomena in transistors, implying that their performance and reliability-related parameters must be evaluated as stochastic variables. It was experimentally established that the capture/emission dynamics of oxide traps underlie both random telegraph noise (RTN) and bias-temperature-instability (BTI) phenomena, thus motivating the inclusion of these effects in statistical simulations of contemporary devices and circuits.

How it is solved

The aim of this project is to address the simulation of reliability of nanoscale transistors through a multi-scale approach. The main physics underling the reliability phenomena of nano-CMOS devices can be, indeed, captured already with semi-classical approaches like a 3D Drift-Diffusion system of equations. Such a first-order approach allows to efficiently run thousands of statistical simulations and, in turn, to study the stochastic distributions of the device figures of merit. A full 3D Monte Carlo approach is, instead, employed when the aim is to evaluate in detail variability effects related to the charge transport. This approach is, however, extremely time consuming and allows the simulation of only few hundreds of devices. When also the quantum aspects have to be addressed, then a 3D Non Equilibrium Green Function (NEGF) approach is necessary. This approach is the most time consuming and allows only the simulation of a few small devices.

Why it is important

The main objective is to develop new paradigms in integrated circuit design which will enable the manufacturing of reliable, low cost, high-yield complex products using unreliable and variable devices. The project will provide device engineers and designers in the nano CMOS industry with simulation tools, reference databases and examples of how to produce future devices that are economical, efficient, and meet high performance, reliability and degradation standards.

Process simulation of electron devices including emerging non-planar architectures

Dr L. Wang and Prof A. Asenov

The challenge

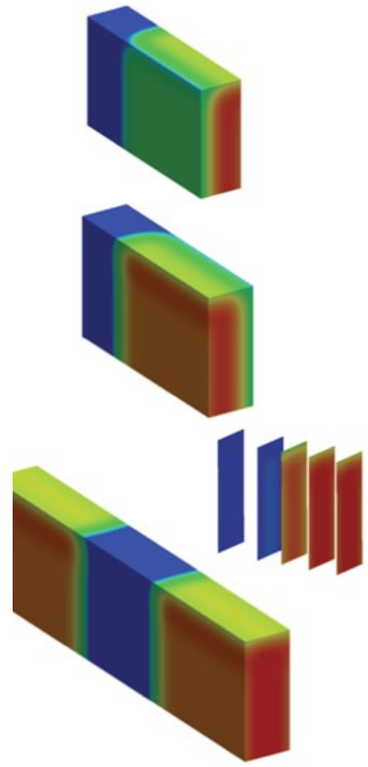
With the continuous scaling down of semiconductor devices into nanometer regime, the planar MOSFET is approaching the end of useful life, and novel architectures such as FinFETs and fully depleted (FD) SOI transistors have been introduced in the contemporary CMOS offerings to combat the leakage, performance and variability problems. For emerging device architecture such as FinFETs, conventional 1D or 2D TCAD simulations are not applicable. For reliable process simulation of FinFETs, state-of-the-art 3D simulation techniques are needed for critical process steps including ion implantation, diffusion, strain engineering etc.

How it is solved

Traditionally the commonly used methods in TCAD tools for the simulation of ion implantations include Monte Carlo method and the distribution moments method. The Monte Carlo method is a physically based “atomistic” method, offering flexibility and accuracy, but it is time consuming, especially for 3D structure. The “moments” method calculates the dopant distribution by applying an analytical distribution function in the domain. It involves convolution of the point response functions that can be constructed from “moments”. It becomes more complicated for the 3D structure of non-planar devices. We have developed a set of analytical models based on either Pearson or Gaussian distributions, specially formulated considering ion implantations in the 3D structure of FinFETs. A C^{++} simulation module has been developed as part of the 3D “atomistic” simulator GARAND. This will be further enhanced by future work on non-ideal 3D geometries, emerging doping technology such as Plasma Immersion Ion Implantation, process variations etc.

Why it is important

TCAD (process and device simulation) provides deep insight into the device performance and information of how certain production processes influence the device behaviour, which is very important for IC production. The design of the doping profile in the source/drain and extension regions is crucial when optimising the performance of the non-planar devices such as FinFETs. The software we are developing will provide efficient, reliable, accurate and concise process simulation tools, forming the bases for accurate prediction of device performance and structure and process optimisation.



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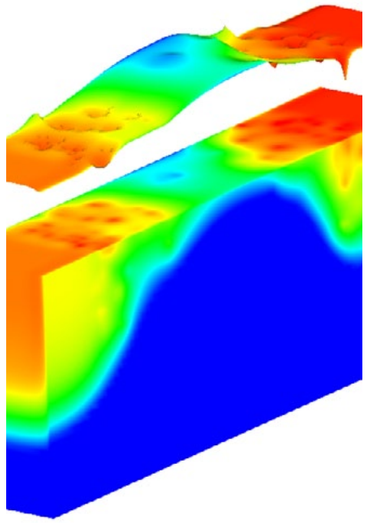
Automatic calibration of Glasgow “atomistic” drift-diffusion simulator

Dr D. Balaz and Prof A. Asenov



The challenge

In order to study the challenges posed by the statistical variability in transistors, it is necessary to perform large numbers of simulations. We need to be able to obtain accurate results yet use methods that are computationally efficient. The challenge is to bridge from precise but computationally demanding methods, e.g. Monte Carlo, to computationally efficient methods, such as the drift-diffusion model.

How it is solved

An automatic optimisation software is being developed that allows for calibration of the drift-diffusion models to the results obtained by more accurate methods like Monte Carlo. Various optimisation methods, such as Levenberg - Marquardt algorithm, COBYLA or BFGS are used to perform the task. The goal is to find values of parameters that will reproduce the simulated MC I-V characteristics with the Glasgow “atomistic” simulator for a device with a uniform doping. Then, those parameters are used to perform the statistical variability simulations.

Why it is important

The automatic calibration of the Glasgow “atomistic” simulator is an important step in assessing the impact of statistical variability of electronic devices, such as transistors. The development of the automatic calibration process will allow for fast and efficient transfer of data from computationally accurate to computationally efficient calculations and hence help investigate the statistical variability.

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Simulation of novel 3D finFET: reducing variability and leakage power

Dr X. Wang and Prof A. Asenov

The challenge

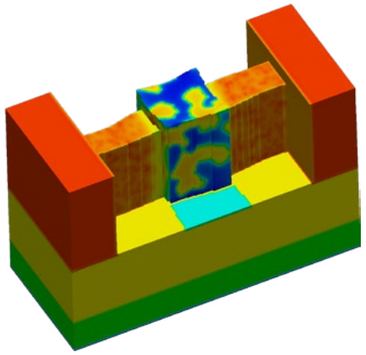
Metal-oxide-semiconductor field-effect transistor (MOSFET) is the main tiny build block of digital integrated circuits. When MOSFET is progressively scaled in nanometer regime, even two closely paired transistors demonstrate a large difference in the device parameter such as threshold voltage. This is caused by the purely random effect. The random discrete charges and granular matter in nanometer scale MOSFETs causes the statistical variability and reliability. The statistical variability and reliability will bring problems in such as mismatch, leakage power, and circuit yield. It has become the critical concern since 32/28nm node technology and finally is driving the MOSFET architecture change towards FinFETs.

How it is solved

When statistical variability and reliability derives from intrinsic sources, it is impossible to completely remove their random effects in nanoscale MOSFETs, but we do have some countermeasures to manage or even reduce fluctuation magnitude. The first possible solution is to optimise the traditional bulk planar MOSFET process to reduce statistical variability in processes such as gate-last. The second is to change the circuit design paradigm from the worst-case design to statistical modelling and circuit design. However, these two methods do not remove the “bug” from the root. The third method is to adopt the novel MOSFET architecture such as three-dimensional FinFETs. For the first time the integrated transistors are no longer on “Flatland”. Due to its multi-gate action, it allows low channel doping, which eliminates the traditional dominant contributor of statistical variability source: random dopants. FinFETs have the steep switch from on to off, significantly reducing the standby power rendering it a green energy consumption technology. FinFET is the future.

Why it is important

Dramatic statistical variability and reliability is one of the main causes for the yield loss and leakage power dissipation. Novel 3D FinFETs drive the continuous scaling of nanoscale devices and the success of the Moore’s law, and most important it reduces the variation among transistors, enables ultimate integration of large systems and reduces the chip leakage energy computations. Therefore it is important to have the early predictive information about FinFET technology and its statistical variability for future nano integration through accurate physical simulations.



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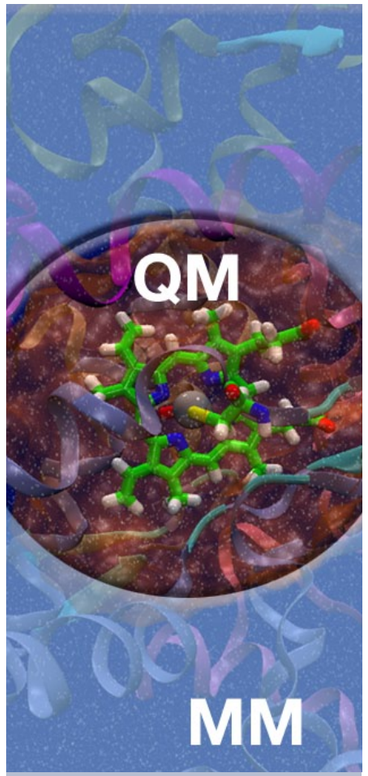
Atomistic modelling of chemical reactivity and molecular simulations

Dr H. M. Senn



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The challenge

The overarching aim is to elucidate the mechanisms of chemical reactions; that is, to understand in atomistic detail how chemical bonds are formed and broken during a reaction. This includes identifying and characterising the structures and spectroscopic properties of reaction intermediates and transition states; calculating the energetics (reaction and activation energies); and studying the dynamics of the reaction event.

Of particular interest are reactions catalysed by enzymes and transition-metal complexes (homogeneous catalysis).

How it is solved

To describe accurately the making and breaking of chemical bonds, we use quantum-chemical (QM) methods, which provide approximate solutions to the electronic Schrödinger equation. We mainly apply density-functional theory (DFT) methods, but also use semi-empirical and correlated *ab initio* methods. To model large biomolecular systems, we use molecular mechanics (MM) and molecular dynamics (MD) based on classical force fields.

Combined QM/MM methods allow us to incorporate the effects of the protein environment on the chemical processes in the active sites of enzymes.

Why it is important

Detailed insight into chemical reactions, including knowledge about reaction intermediates and the energetics of each step, provides the basis for rationally improving and designing chemical transformations. Understanding homogeneous catalytic processes and enzyme catalysis are of particular relevance because they yield the desired products with exquisite selectivity and efficiency of energy and materials.

Reaction mechanisms in homogeneous catalysis

Dr G. Hill

The challenge

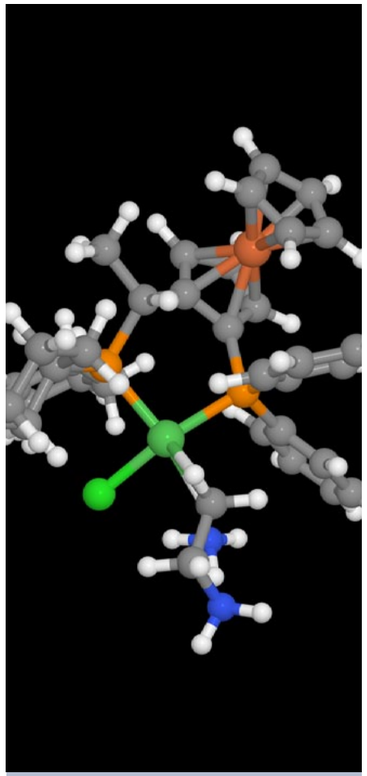
Homogeneous transition metal catalysis is vitally important in the synthesis of fine chemicals, which are often used as precursors in the production of pharmaceuticals. The chemical reaction cycles that occur during a catalytic process are typically complex and difficult to describe experimentally, preventing detailed mechanistic understanding and rational design of improved catalysts.

How it is solved

A number of recent advances in fundamental theoretical chemistry are being combined into a powerful, standardised computational technique able to effectively model catalyst behaviour. Unlike competing methods, the high-accuracy of this approach will produce quantitative predictions of reaction barriers and elucidate reaction mechanisms. To achieve this for catalytic processes of an industrially relevant size, only the most important atoms are treated at the highest level, with more computational efficient techniques employed for the ligands.

Why it is important

Application of this computational protocol to existing catalytic reactions will provide enhanced understanding of the mechanisms involved. This knowledge will then enable the *in-silico* design of new catalysts and processes, and the potential of industrial and university-based experimental research groups to employ these advances holds the promise of benefits to the economy and the environment.



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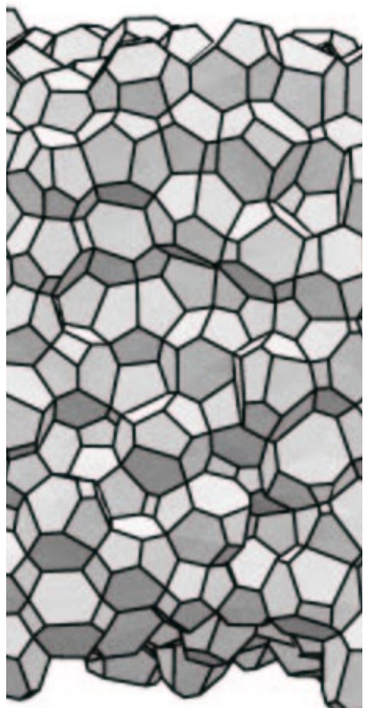
Porous materials: from the inside out

Dr P. Harrison



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The challenge

Computer Aided Engineering (CAE) is increasingly powerful and ever more useful from an industrial perspective.

The computational capability afforded by current technology, made readily available by high performance supercomputing, can be harnessed to provide cost effective solutions to a range of materials-based engineering problems. We focus on porous materials.

How it is solved

Various methods of numerically generating porous microstructures are available; open and closed cell polymer and metal foams have a distinct topology which can be generated using computational methods such as energy-minimised Voronoi tessellation in both two and three dimensions.

Other porous materials such as aerogels are better modelled using mathematical based methods such as Diffusion Limited Cluster Aggregation or more physically-based Molecular Dynamical modelling. By informing these algorithms with data from powerful 3-D imaging techniques, such as microCT, Dualbeam SEM technology or 3-D TEM, we aim to drive the creation of digital topologies towards realistic statistically representative microstructures and use these models for accurate modelling of porous materials.

Why it is important

Porous materials are important due to unique characteristics such as high specific mechanical properties, high compressibility, permeable microstructures that permit intracellular flow of fluids and high internal surface area.

The goal of this research is thus to develop CAE software to create representative porous microstructures of a broad range of porous engineering materials for multi-scale computational analysis.

Synthetic (metallic and polymer foams, aerogels) and natural porous materials (wood, bone) can be found in a wide range of applications in both industry and nature (e.g. lightweight and self-healing structures, impact energy absorbers and attenuators, supercapacitors, acoustic insulation & filters).

Understanding and predicting the relationship between microstructure and macrostructure is a key requirement in optimising properties and modelling mechanical and physical behaviour.

Virtual forming of technical textiles

Dr P. Harrison

The challenge

Advanced textile composites lie at the centre of the cost-performance spectrum of structural materials and are attracting growing interest from both academia and industry.

Our research is driven by the anticipated need to design, process and model with these materials.

How it is solved

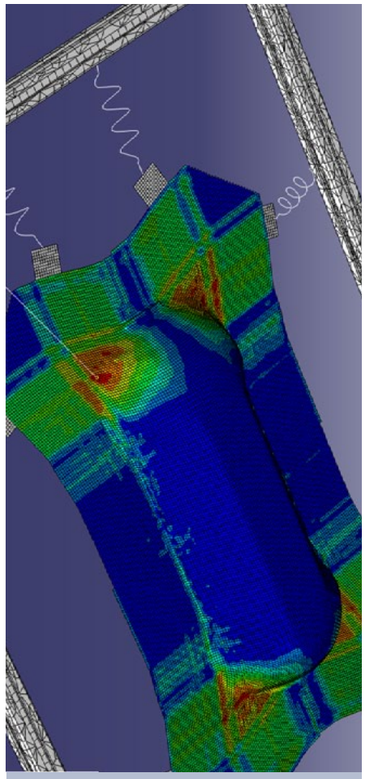
In our group, constitutive models based on multi-scale analysis are being developed and implemented in finite element software (e.g. AbaqusTM) to create a virtual manufacturing environment for the composite forming process.

In particular, novel constitutive models based on multi-scale analysis have been developed and implemented in finite element software (e.g. Abaqus) to create a virtual manufacturing environment for the composite forming process (Fig 1). The aim here is to predict the forming behaviour of these materials from information such as fibre volume fraction, textile weave style and matrix rheology. In addition, novel algorithms to incorporate off-the-roll fibre direction variability, as measured from several commercially available textiles, have been developed in order to predict error bars in the final mechanical properties.

Further challenges include: modelling multi-layer forming and characterisation of inter-ply and tool/ply friction. Models are validated through an experimental programme employing specialised equipment including novel shear-characterisation apparatus and a custom designed thermoforming station.

Why it is important

The drive to improve efficiency in industry has created a desire to 'get it right first time' when implementing new processes in the factory or when changing existing ones. This research is driven by the anticipated need to manufacture complex parts using advanced composite materials without having to spend large amounts of time and effort in designing tooling by a trial and error approach.



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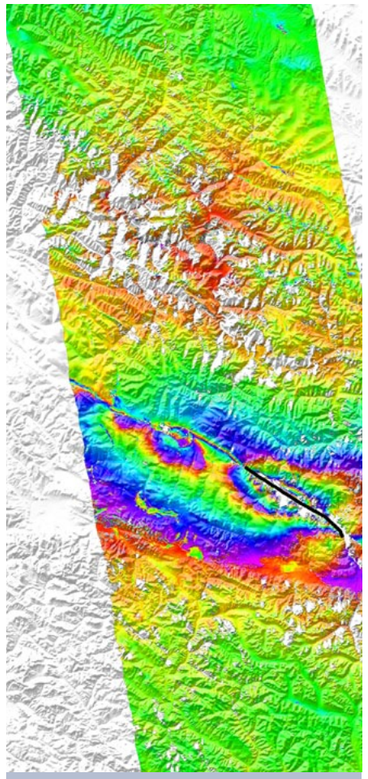
Geodetic modelling for earthquake and landslide hazards

Dr Z. Li, Mr W. Feng and Mr A. Singleton



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The challenge

Determining the real physical mechanism(s) behind geophysical phenomena such as earthquakes and landslides with space geodetic observations is a big challenge. Having calculated the Earth's surface displacements using satellite radar imagery, we are interested in modelling the earthquake cycle including interseismic strain accumulation, the earthquake itself, and postseismic adjustments. Knowledge of the location and mechanisms of faults is critical in estimating the effects of earthquakes on nearby habitation. The rate and distribution of strain accumulation across earthquake fault zones is a key piece of information in the estimation of future seismic hazard.

With regard to landslides, following the detection and accurate measurement of unstable slopes, we aim to model the sliding mechanism and the relationships between the landslide movement and various external triggering factors.

How it is solved

A first major step is to use geodesy techniques to process satellite data to obtain precise surface displacements, which often involves several models/techniques developed in-house to reduce as many measurement errors as possible.

For earthquake hazards, we have developed numerical simulations (including highly effective linear and non-linear algorithms) which can be used to determine fault geometry and slip distribution from geodetic observations.

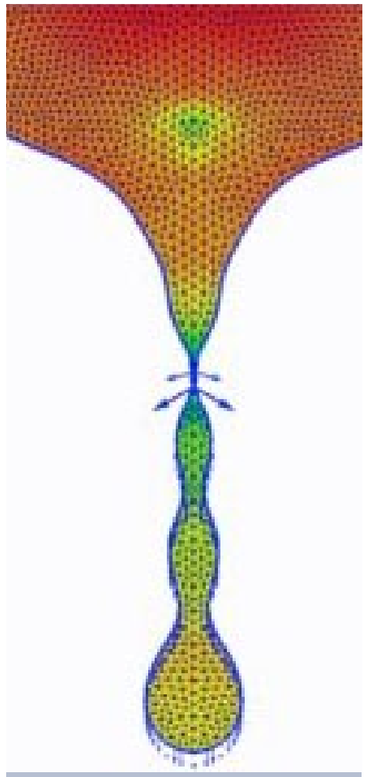
For landslide studies, we use time-dependent deformation data to infer the mechanism of movement. Without additional information, simple limit equilibrium models can infer the slope's response to external factors such as rainfall, reservoir level changes and/or earthquakes as well as the depth of the sliding surface. The availability of geological data could allow more comprehensive landslide models to be run (e.g. FEM).

Why it is important

Focusing on the use of remotely acquired satellite data, we can effectively model earthquake and landslide hazards without the requirement for fieldwork and ground instrumentation. This obviously has some important cost savings and also means we can study numerous, large areas with relative ease. Our work then allows a far better understanding of the Earth's most destructive natural hazards and consequently promotes a reduction in future vulnerability to similar events by developing appropriate remedial measures.

Modelling of micro-fluids

Dr L. Kaczmarczyk and Prof C. Pearce



The challenge

Fluid flows, particularly those at the microscale, underpin a range of technologies, including drug delivery, advanced diagnostics, paint formulation and food production. Understanding the interactions between liquids and air, between liquids and liquids or between liquids and solids is hugely important in healthcare, industry and food production. However, the computational modelling of fluids at this scale is a significant challenge.

How it is solved

The phenomenon of surface tension is extremely important for fluids at micro-scales; it is responsible for the size, shape and behaviour of liquid droplets. Our work focuses on the development of a computational model for fluids that includes surface tension, enabling us to more effectively and accurately predict the response of micro-fluid droplets subject to external excitation. We adopt an Arbitrary Eulerian Lagrangian (ALE) approach that enables surface tracking and large distortions to be modelled efficiently and accurately

Why it is important

This framework will enable us to contribute to the improved design of SAW (surface acoustic wave) devices for microfluidic applications within the medical and food industries. We are working with colleagues in Biomedical Engineering (Prof. Jon Cooper & Dr. Julien Reboud) to create a virtual modelling environment that will allow them to explore a range of design parameters for SAW devices without the need for multiple physical prototypes, thereby rapidly shortening the development process.

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Simulation and predictive modelling of materials and structures

Prof C. Pearce and Dr L. Kaczmarczyk

The challenge

Predictive modelling of materials and structures requires simulation tools that are physically accurate, numerically robust and computationally efficient. Complex materials, from composites to biological materials, often require novel multi-scale solution techniques. Extreme events, such as fire, and long-term considerations, such as durability, involve strong coupling of the solid, liquid and gas phases that are not easily resolved in the same computational setting. Moreover, these computationally intensive simulations demand bespoke solution strategies.

How it is solved

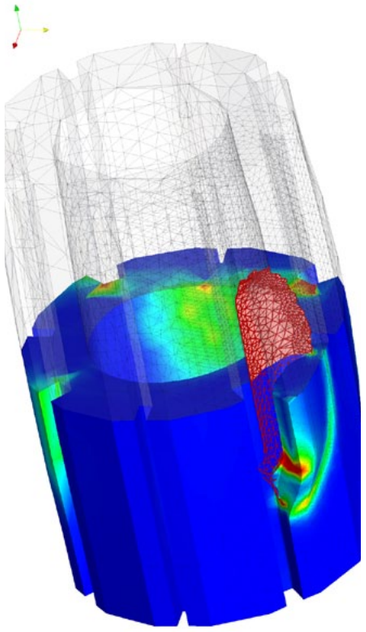
We are developing finite element based computational tools and methodologies that enable us to simulate and predict the behaviour of complex materials and structures. This virtual laboratory allows us to explore extremes of size and condition that cannot be undertaken efficiently or practically with physical experiments.

Multi-scale and multi-physics analyses enable us to capture the influence of the evolving microstructure and the effect of coupled processes (mechanical, thermal, hygral) on the overall response. New modelling techniques for evolving geometries are employed for capturing processes from fracturing to growth.

To solve large-scale problems, we increase numerical efficiency by employing advanced numerical tools that are tailored for high performance computing.

Why it is important

Our work is funded by both industry and research councils. The transformative potential of composites for infrastructure, driven by their extraordinary mechanical properties, is key to a resilient, adaptable, low-carbon infrastructure. Our modelling tools will bring confidence to their long-term performance, investigating and quantifying the degradation processes and their influence on the microstructure. Our modelling framework for crack propagation in brittle materials is being developed as part of project to rationally assess the integrity of safety critical structures.



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A prototype detector for the cosmic-ray muon tomography of legacy nuclear waste containers

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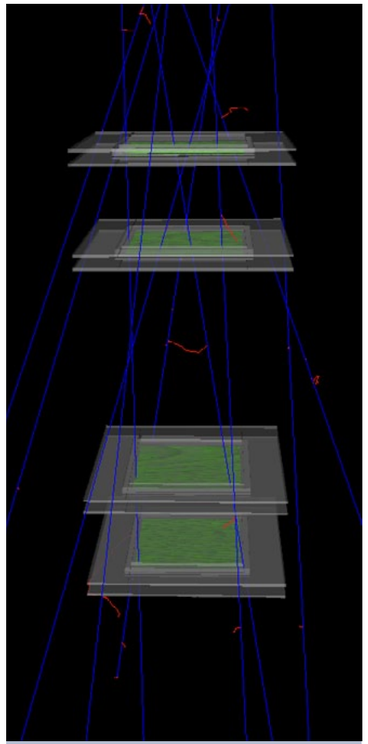

The challenge

The storage of 'legacy' nuclear waste is a challenging issue for the UK Nuclear Industry. In recent years, Sellafield Ltd. has funded multi-million pound research which has been carried out by the National Nuclear Laboratory and the Nuclear Physics group at the University of Glasgow to develop a particle detector system with the potential to make a significant impact upon future storage policy and contribute to the continuous improvement of safety at the Cumbria site.

How it is solved

This system detects muons, produced when cosmic rays impact on the Earth's atmosphere. These interact with matter primarily through Coulomb scattering from atomic nuclei. The extent of this scattering is dependent on the atomic number of the material. This relationship can be exploited in muon tomography to image objects within industrial waste containers, which would otherwise block conventional forms of imaging radiation, such as X-rays. To test this concept, a prototype detector has been developed using AutoCAD modeling and Geant4 simulations. By reconstructing the incoming and scattered muon trajectories, the scattering location and magnitude are determined. The contents of the container can then be imaged and any potential nuclear waste material can be identified.

Why it is important

The feasibility of this detector technology in identifying high-density waste material within containers has been confirmed through accurate Geant4 simulations and dedicated image reconstruction software. Preliminary results from a constructed prototype detector have verified these initial findings. It is foreseen that with further development, a muon tomography system will be deployed at Sellafield in the future, and will play an important role in ensuring the safety of the UK's nuclear waste storage.

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Nanoscale pattern formation in materials science

Dr D. P. Bourne, Prof M. A. Peletier^ and Dr F. Theil*

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The challenge

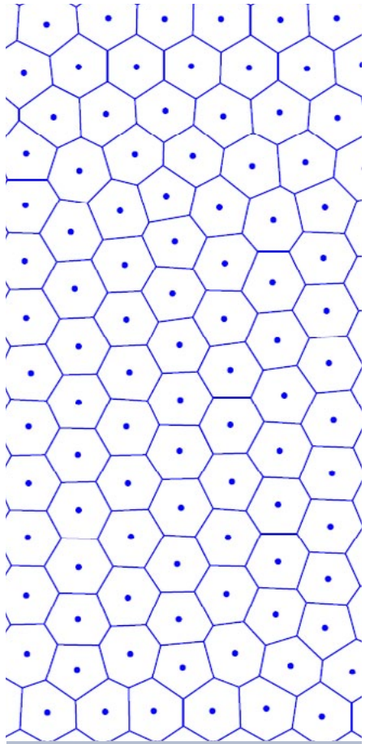
A block copolymer is a type of polymer that is built from blocks of monomers. If you zoom into the nanoscale of these materials you observe periodic structures such as spheres, hexagonally packed cylinders and lamellae. The type of nanostructure determines the properties of the material at the macroscale. The challenge of this project was to derive models of block copolymer melts and to perform simulations to predict and control the nanostructures.

How it is solved

Starting from a statistical mechanics model of a diblock copolymer melt, rigorous asymptotic methods were applied to derive simpler models that are computationally tractable. In order to solve these equations, we developed a novel algorithm that is built on a deep connection between optimal transportation problems and computational geometry (Voronoi tessellations and power diagrams). The nanostructures we predicted theoretically match those observed in experiments.

Why it is important

Block copolymers are used in the manufacture of rubbers (e.g., shoe soles), plastics and adhesives. Due to their property of spontaneous self-assembly at the nanoscale, they are being employed by researchers as nanostructuring agents to design new rubbers and plastics with tailored properties. In addition to experiments, advances in modelling and simulation are essential to unlock the full potential of these materials.



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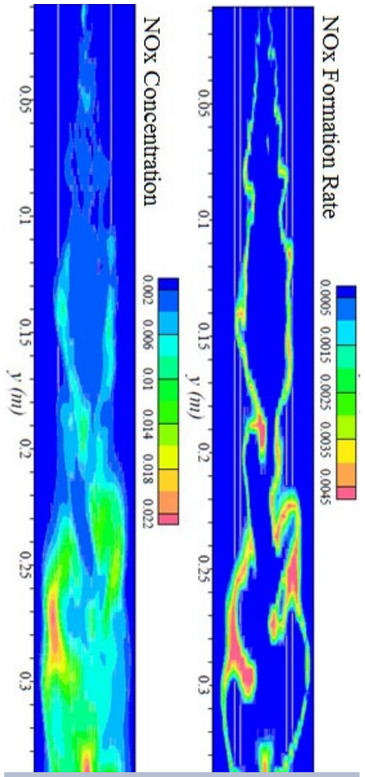
Combustion and gasification modelling

Dr M. C. Paul



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The challenge

The world's power production is heavily dependent on fossil fuels and their consequences on the environment and humankind are drastic. In the UK, coal, gas and biomass power stations are producing much of the country's energy demand, and this is equally true for Scotland. The Scottish Government is committed to reduce its emissions level by 42% and internationally the UN's target on the Kyoto Protocol is 18% by 2020. These altogether give extreme pressure to the power production industries, globally, to work on the refinement and optimisation of their combustion systems

How it is solved

We develop advanced computational fluid dynamics (CFD) based modelling methods and apply these to optimise combustion and gasification of various fuel sources, e.g. pulverised coal, gas, biomass, algae, waste, underground coal and syngas. We have a unique expertise in large eddy simulation (LES) and direct numerical simulation (DNS) for turbulent combustion, and our methods successfully applied to several industrial burners including Rolls-Royce's Gas Turbine Engine. We systematically optimise the combustion performance by implementing new chemical kinetics capable of correctly predicting emissions, temperature, and other gaseous and solid (nano-scale soots) species. Thermodynamics and chemical controls to the reduction of emissions (e.g. toxic NOx) are also examined.

Why it is important

Our CFD work has major environmental, technological as well as economical impacts and will potentially benefit a number of industries operating in power production including coal, oil, gas, biomass, algae, waste, underground coal etc. Modelling is a cost-effective solution method for them and would also help to improve the designs of their combustion systems.

Cell motility analysis

Dr J. Kim

The challenge

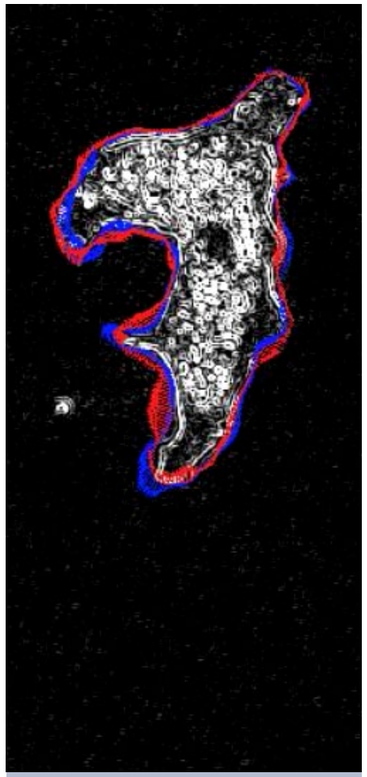
There are two distinct ways of cell migration: pseudopods and blebs. These can be observed even in the same cell at the same time in different parts of the cell. The pseudopods are expanded by mainly actin polymerisation with a relatively gradual increase of velocity. On the other hand, blebs expand rapidly and they have rounded morphologies. Full identification these mechanisms are yet to be realised.

How it is solved

The algorithm for unravelling the pseudopod and bleb mechanisms has the following parts: i) a finite number of image pixels on the cell boundary are extracted; ii) the kinetics of each pixel is established as a set of stochastic differential equations; iii) using the distance measured in i) and the model in ii), the velocity and acceleration are estimated by solving an estimation problem; v) acceleration and morphological characteristics of identified cell boundary are used to classify pseudopods and blebs.

Why it is important

Cell movement is essential in many important physiological phenomena including wound healing process, immune response, and metastasis. Metastasis is of particular interest from medical science as it is the way that cancer or disease cells spread over other parts of human body. It is triggered when cancer cells migrate out from a tumour into blood, lymph or other tissues. Therefore, understanding factors initiating the metastasis is of vital importance to develop optimal strategy for fighting cancer and disease.



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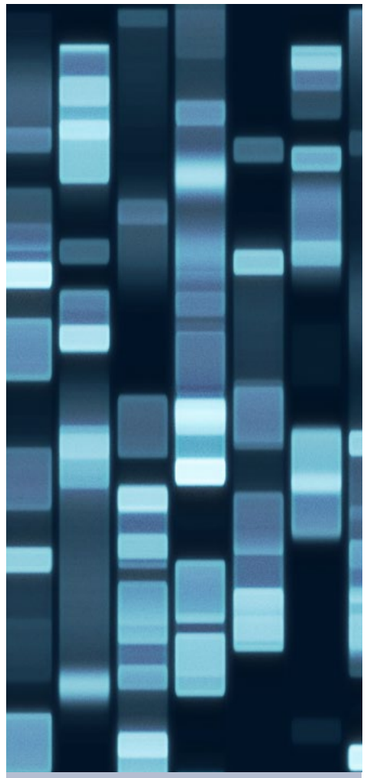
Parameter estimation in systems biology

Prof D. Husmeier



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The challenge

Modern approaches to molecular biology aim to mathematically describe the processes of gene expression, transcriptional regulation and post-translational modification as the result of complex interactions in signalling pathways and regulatory networks. The models are typically based on Michaelis-Menten and mass action kinetics, and depend on a range of parameters describing the chemical kinetics and thermodynamic equilibria. While the numerical solution of these equations has allowed us to understand the essence of some regulatory processes at the qualitative level, the real challenge is to infer the unknown kinetic parameters driving these processes from noisy postgenomic data, and to identify the correct pathway structure by means of statistical model selection and hypothesis testing. While the availability of high-performance computers has rendered the mathematical modelling feasible, statistical inference remains a challenging task, as every parameter modification in an iterative optimization routine has to be followed up by a numerical solution of the differential equations describing the system, which is not viable unless the system is restricted to only a few interacting components.

How it is solved

Our work focuses on approximate computational inference that bypasses the need for an explicit solution of the differential equations. The basic idea is to perform smooth regression of the data, then match the slope of a tangent to the interpolant against the predicted derivatives from the differential equations. The problem of this approach is that the parameter estimation hinges critically on the nature of the chosen regression model, which is aggravated by the presence of noise and the limitation of measurements in affordable time course experiments. The approach we take is based on the insight that the differential equations can be used for regularisation, by feeding them back into the regression scheme so as to influence the shape of the interpolant. Extensive comparative evaluations reveal that this leads to more accurate and robust parameter estimation.

Why it is important

The prospects of reliable, robust, and computationally feasible inference in mechanistic models of biological networks and signalling pathways promises to lead to a deeper insight into the nature of molecular regulatory processes. This has a wide spectrum of applications, from shedding light on the interaction between circadian regulation and metabolism in plants, which influences biomass production in crops (relevant to biofuel production and food security), to unravelling the molecular signatures of various diseases, most notably cancer.

Radiation dose evaluation using Monte-Carlo methods

Dr B. Seitz

The challenge

The evaluation of the precise dose delivered to a patient is of prime importance in cancer treatment using ionising radiation. It will ensure a proper treatment of malign tissue while keeping the effect on healthy tissue to a minimum. The interaction of radiation with matter is complex and difficult to predict. Treatment planning systems rely on statistical computer models, hence the prediction of the delivered dose will depend on the quality of these models.

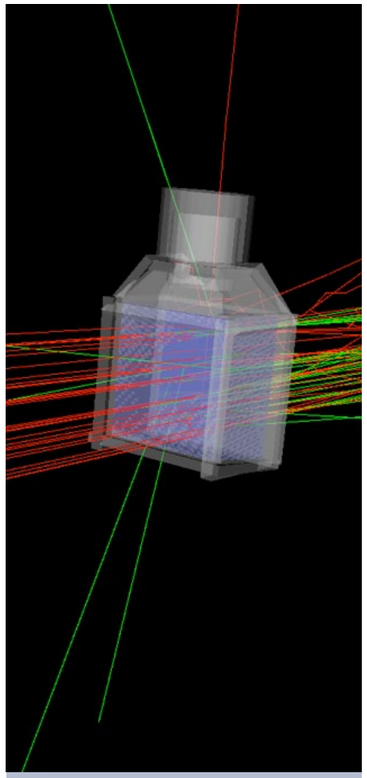
How it is solved

The interaction of ionising radiation with matter is relevant to a large number of applications, from fundamental research in nuclear and particle physics to the prediction of radiation doses delivered in radiotherapy and the design of radiation protection. These interactions are stochastic and hence are mostly modelled by Monte-Carlo simulations. The results will depend on the Monte-Carlo model applied.

Based on the expertise acquired in large scale nuclear physics experiments, we study a large variety of different models in close comparison to experimental data. This allows us to develop the model most closely matching reality for any given application, ranging from X-ray energies in CT scans to very high energy particles from modern accelerators.

Why it is important

Amongst many different causes, cancer is a disease related to age. Current estimates show that about one third of the population will develop cancer in their lifetime, necessitating a detailed understanding of all treatment modalities. This will allow precise prediction of therapy doses, optimising the kill rate for malign tissue while spearing healthy tissue as much as possible.



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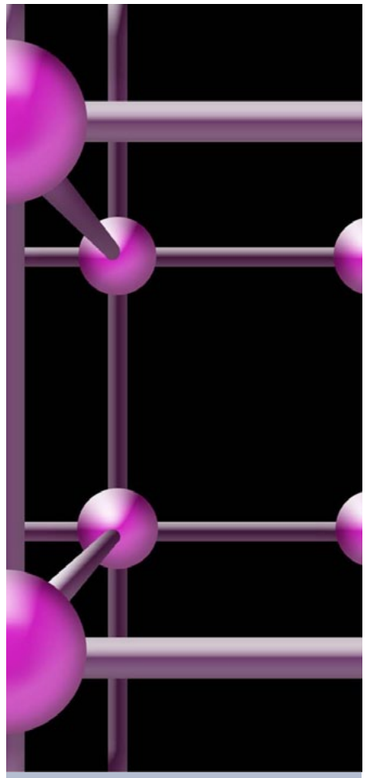
The quandary of the quark

Prof C. Davies



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The challenge

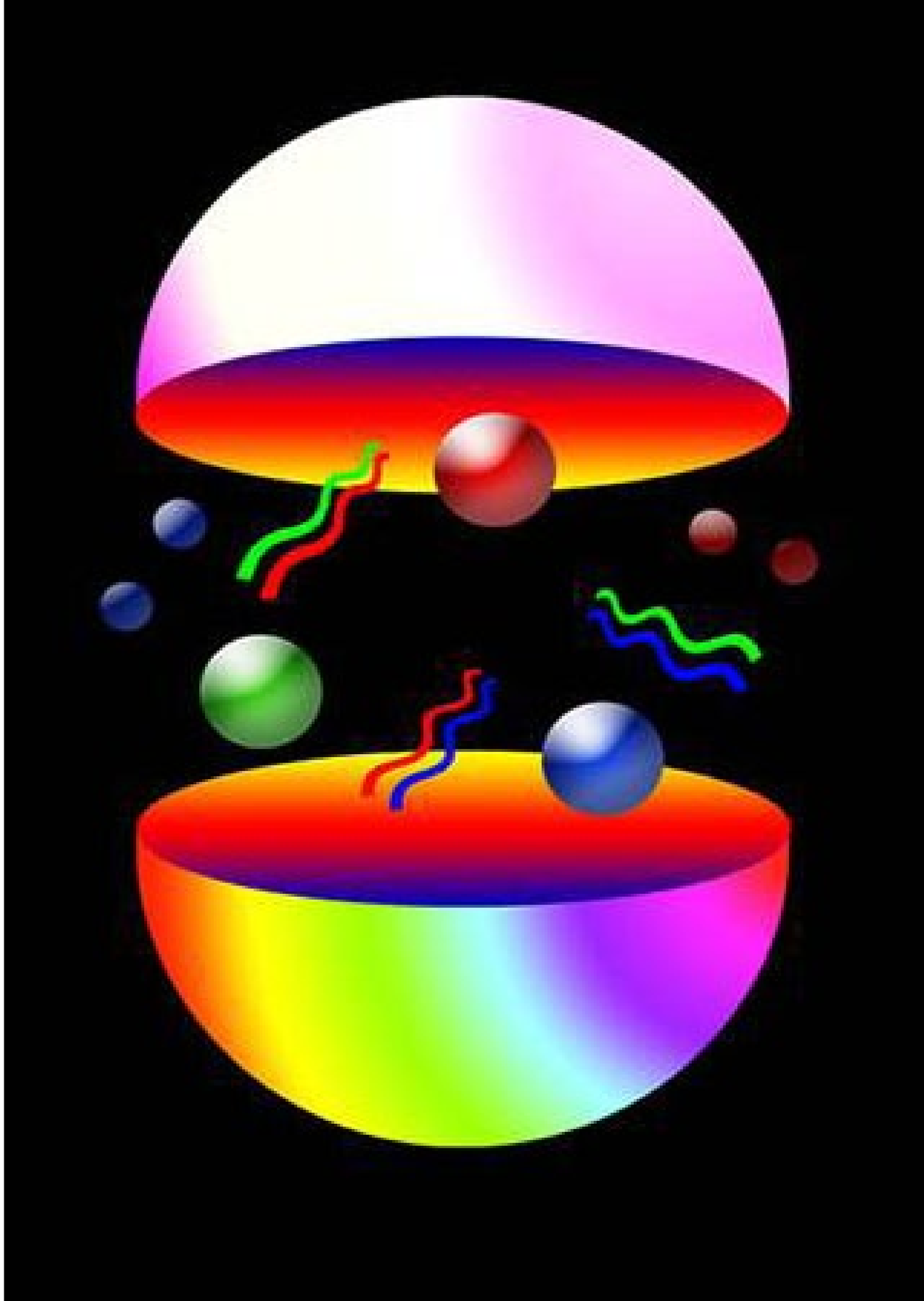
All matter is held together by the strong force, which binds quarks together into protons and neutrons and in turn provides the attraction between protons and neutrons to form nuclei. Indeed most of the mass of the atom (and therefore ourselves) results from the binding energy of the strong force. The theory for this, Quantum Chromodynamics (QCD), is simple to write down but can only be solved numerically. The calculations are very challenging but promise stringent tests of our understanding of the subatomic world.

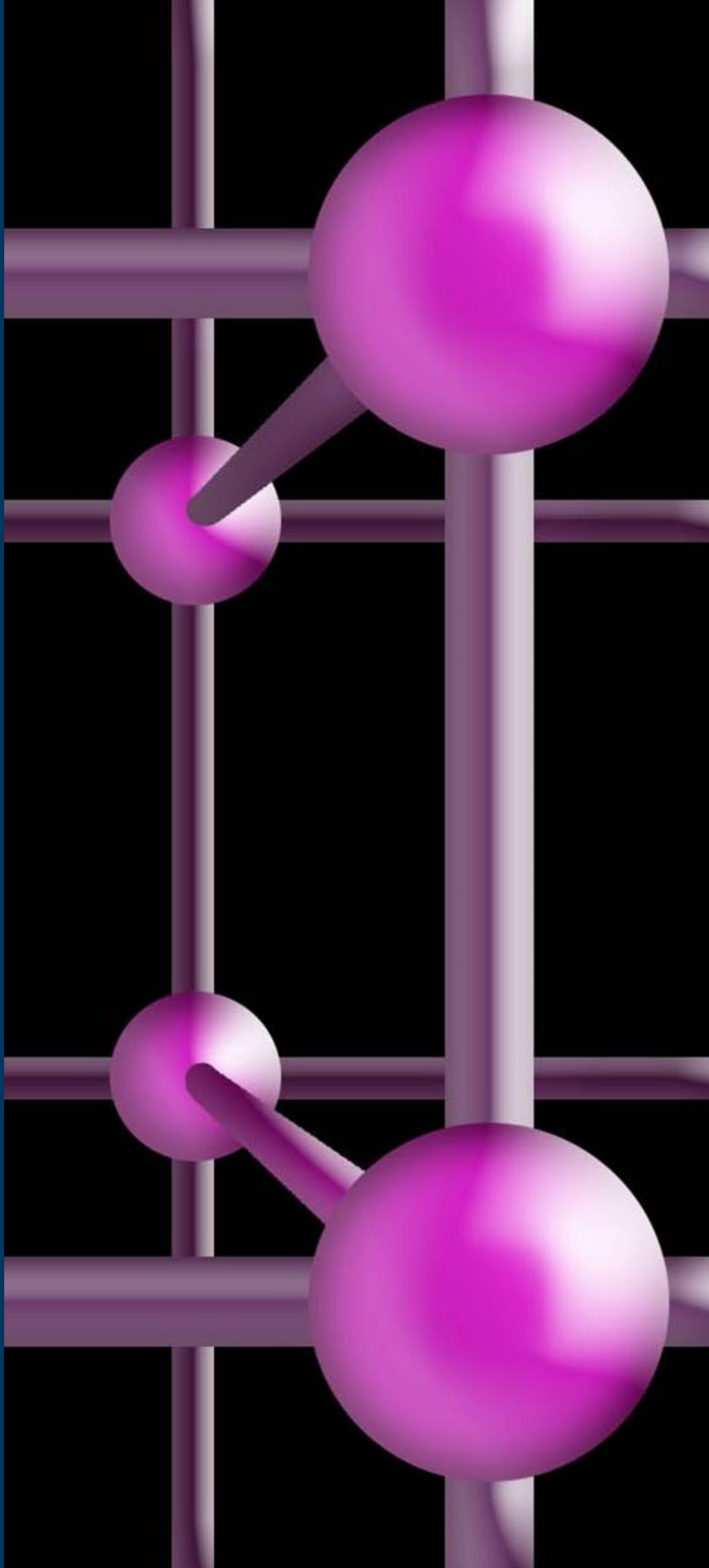
How it is solved

Tackling QCD numerically is a "grand challenge" that requires the world's most powerful supercomputers. Multi-million dimensional integrals over quark and gluon quantum fields living in a discretised space-time box are handled using Monte Carlo importance sampling techniques. Numerically most costly is the calculation of rows of the enormous sparse (and ill-conditioned) matrix that gives the solution of the Dirac equation.

Why it is important

These techniques are allowing us to calculate accurately the masses of a host of particles like the proton produced in high energy experiments at CERN in Geneva. Comparison to experimental results allows us then to work out, for example, what the masses of the different quarks have to be. Quarks are not accessible to direct measurements because QCD does not allow them ever to appear as free particles, so this is the only way to determine their properties. In addition the calculation of decay rates of various particles seen at CERN is allowing us, using experiment, to pin down other parameters of quarks. These will constrain the Standard Model of particle physics to the level where we hope new physics will be uncovered.





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