Abstracts of Oral Presentations

Numerical methods in turbulent flow prediction: LES, DNS and 2-equation modelling

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Abstract:

In recent years there has become a greater demand for air travel. More communities are now affected by the noise of civil aircraft. In order to lessen the impact, it is a necessity to improve various aerodynamic aspects of aircraft. This study focuses on the acoustic-efficiency of the aircraft body, and in particular cavity flows such as landing gear well and fuel vent.

Results of 3 types of numerical study will be presented, and their individual context and basis explained.

i) A 2-eqn turbulence model adapted for intermittency, k-w-g, was used to profile the probability of flow transition to turbulence over a surface[1]. Hoping gain a more computationally efficient method, this work showed the viability of implementing such a procedure.

ii) DNS of shearless turbulence interaction allowed fundamental turbulent mechanisms to be highlighted in the absence of mean shear[2]. It has been shown that turbulence intermittency, scales linearly with the logarithm of the energy ratio, up to 1000, beyond this value an asymptote is reached.

iii) LES has been employed to study an aspect of turbulent flow control, reduction of turbulent stresses in channel flows through wall oscillation[3]. By altering the oscillation period and displacement, relative to the channel flow velocity, an optimum perturbation has been identified.

[1] Bailey, MEng Thesis,CFD Transition Modelling, University of Leicester (2005)

[2] Iovieno,Tordella, JFluidMech549 (2006)

[3] Tordella, Bailey, Iovieno, EFMC6, Stockholm (2006)

Keywords: Turbulence; LES; DNS; Transition; Cavity

Metabolomics, diabetes and oxidative stress - the role of capillary electrophoresis

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Abstract:

The classical animal model for type I diabetes investigations is the streptozotocin (STZ) rat. STZ causes oxidative damage and β cells of pancreatic islets death. Simultaneously, markers of oxidative stress increase and it is generally accepted that the majority of complications associated with diabetes, such as cardiovascular disease, nephropathy or cataracts, are related to these increases.

Recently we have been working to characterise the STZ rat model by developing suitable analytical methodology to profile the metabolites in biofluids and tissues. The ultimate aim of the project will be to make available an acute model of short term response for evaluation of in vivo activity of naturally derived antioxidant compounds. The antioxidant compounds we intend to interrogate will be components suitable for use as dietary components.

In order to accurately follow the 'therapy' for a chronic diseases such as diabetes type I, normalization of a targeted aspect of the metabolism (without disruption of other metabolic pathway regulation) must occur. Furthermore, it is increasingly recognized that assessment of limited biomarker compounds to monitor the efficacy of the therapy is fundamentally flawed and that more comprehensive snapshots of multiple metabolites must be taken. Such an approach is commonly refereed to as Metabolomics.

The analytical measurement techniques which are commonly employed in Metabolomics are required to provide efficient, reproducible and quantitative high resolution data, and ideally, with minimal sample preparation. In this presentation, the benefits of Capillary Electrophoresis for such analyses will be discussed along with the procedures necessary to visualise and interpret the resulting data.

Keywords: animal model; nutraceuticals; bioanalysis; biomarkers; metabolic fingerprinting

Development of flexible solar cells

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Abstract:

Use of alternative energy sources is getting more and more important to reduce exploitation of oil, gas and coal resources and to minimize greenhouse gas emission. In consequence, the photovoltaic market is growing at 30% a year. The Helianthos-Project at Akzo Nobel was started to reduce the kWh costs for photovoltaic devices.

A roll-to-roll process was developed to reduce production costs of solar cell modules. They will not only cover roofs and walls but also different kinds of surfaces and shapes like jackets, trousers or hand bags to recharge electronic devices.

The development of a solar cell can be split into several parts. One important part is the front electrode who should be transparent and electro conductive. The scattering of sunlight is a further property of the front electrode to increase the current flow in a solar cell.

The front electrode has a crystalline structure and can be classified as a kind of ceramic. Knowledge about the crystal grain growth, the chemical structure and the thermo dynamical stability is important to increase the optical, mechanical and electrical properties.

This presentation will show the part of a Marie Curie fellow with a mineralogical and crystallographical background in a solar cell project.

Encouraging output parameters of the final solar cell modules are observed.

Keywords: Flexible solar cells, TCO, SnO_2, roll-to-roll process

Innovative laser based Pick-and-Join tool for micro-assembly

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Abstract:

The increased complexity and rapid evolution of Microsystems require innovative micro-assembly concepts and methods. The aim of the current research is to develop, according to the Pick-and-Join technique, an advanced laser based tool with high robustness and flexibility in time and product. The new tool has to pick the components, precisely position them and realize the joining using laser radiation. Furthermore, for laser processes like Transient-Liquid-Phase bonding, silicon-glass bonding or transmission welding of thermoplastics a defined force has to be applied on the joining partners.

The concept of the Pick-and-Join tool is based on the integration of a fiber laser, a flexible beam delivery system, a device adapted gripper, a process monitoring system and a precise positioning system with force feed-back control, in order to apply the necessary force. This set-up avoids the use of additional clamping devices.

In order to realize this integration a solid state continuous wave fiber laser with its well-known advantages, e.g. high beam quality and efficiency, was selected as laser source. Then, for a high processing speed and increased flexibility, a compact galvanometric-scanner is used to deflect the laser beam on the working plane. A modular vacuum gripper, transparent for the laser radiation, was realized for picking and positioning the joining parts. The high accuracy of the assembly process can be achieved due to the integrated visual monitoring system. First test on transmission welding of thermoplastics are presented.

Keywords: Fiber laser; Novel Pick-and-Join tool; Close loop visual control; Transmission welding of thermoplastics

The spread of central European modernism to earthquake prone areas of the continent and challenges for the preservation of reinforced concrete heritage buildings

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Abstract:

The idea of intensive urban development in an area limited within the surrounding nature has gained acceptance, as the sustainable planning philosophy. In earthquake prone regions it means more than maintenance and upgrading of existing buildings to changed living standards: facing the challenge of safety requirements. The distribution reinforced concrete buildings of the Modern Movement, sharing a common housing typology in Romania, Greece, Portugal, Slovenia, Spain and Italy is analysed, with comparative studies of this early XXth century building type on the adopted architectural language; preservation requirements in urban areas of high/low seismicity, taking into account different ranges of cultural value; attempts and distribution determined need for seismic rehabilitation; the relationship of the time of construction to the earthquakes occurring and codes. Multidisciplinary research interferences are reached between sociology, architecture, construction technology, building economics, geophysics, urbanism, and structural engineering. Functional demands of the future are addressed seeking further for ways to enhance the acceptance for retrofit measures. Possibilities of dialogue with citizens are investigated in the research on participative aspects in multi-actor decision making, using the method of documentation of examples of best practice. The project is funded with a Marie Curie Intra-European Fellowship by the European Commission, contract nr. MEIF-CT-2005-009765.

Keywords: Reinforced concrete; Housing; Architectural heritage; Seismic retrofit; Decision making

The effect of socio-economic factors on sleep quality

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Abstract:

Sleep is essential for health and well-being, yet there has been relatively little research on how social factors influence the quality of sleep. The paper advocates building on the insights and methods from research on Inequalities in Health to analyse Inequalities in Sleep.

Sleep is profoundly gendered, since it is mainly undertaken as a shared activity, influenced by both partners and responsibilities for children.

The paper presents a conceptual model for analysing the determinants of poor quality (or disrupted) sleep, which includes socio-economic circumstances, marital status and living/sleeping arrangements, environmental factors (such as disruption by light, noise, neighbours), worries, health status, as well as a range of partner behaviours (such as snoring) and disruptive activities by both younger and teenage/adult children.

The paper illustrates the conceptual model by analysing a UK self-completion survey of 1445 women aged 40 and over collected in an European Union funded multi-method study (Sleep in Ageing Women, QLK6-CT2000-00499). Logistic regression is used to examine how a range of factors influence quality of sleep, and how different variables mediate these relationships. There are strong influences of socio-economic circumstances on women's sleep (with high education, home ownership, and being employed associated with good sleep), which interact with partner behaviours that have a disruptive effect on sleep, as well as disruption from older and younger children. There are also adverse impacts of worries and the woman's own physical and psychological health status on their sleep quality, in turn linked to socio-economic circumstances.

Keywords: Gender; Health; Sleep; Socioeconomic factors; Couples

Afro-European encounters: Migration narratives

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Abstract:

The presence of increasing numbers of migrants from developing countries in European conurbations has stirred a growing interest for allogenous communities. Together with various forms of documentary literature, new genres are proliferating which give voice to the individual experience of the expatrié and shed light on the dynamics of cultural interaction. Immigrant autobiographies as well as fictions centred on displacement are being published all over Europe. These texts constitute, in my view, a re-elaboration of the old picaresque genre adapted to the reality of contemporary multicultural Europe. This paper looks at migration narratives by sub-Saharan Africans in Southern and Western Europe focussing on two illustrative texts from Britain and Italy. The sense of alienation and the development of survival strategies typical of picaresque characters acquire here the specificities of intercultural and interracial (dis)encounters. The subjective experience becomes emblematic for a whole community and foregrounds a cultural confrontation between a minority and a dominant group, raising questions about the implications of being black in a white country, of being African in Europe. In this sense, these texts are the pioneers of a nascent Afro-European literature, characterized by linguistic and cultural plurality (with regard to the different languages, origins and locations of the authors) and yet finding common ground both in the narrative strategies and in the thematic focus on identity and cultural negotiation.

Keywords: African migration; Immigrant literature

A novel approach to investigate the cell biology of the mitochondrial protein IF1, the ATP saver

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Abstract:

The maintenance of cellular activity requires energy. That energy is stored in the chemical bonds of a molecule, adenosine trisphosphate: ATP. ATP is primarily made in small structures within cells, the mitochondria. It has a turnover rate of ~ 60 Kg per day and is synthesised by an enzyme known as the F1-F0–ATP synthase, driven by the flux of hydrogen ions down a gradient (the mitochondrial potential) established by mitochondrial respiration. Under potentially lethal conditions, such as hypoxia or ischemia, the potential falls, and the enzyme reverts from ATP synthesis to ATP hydrolysis. Glycolysis becomes the only source of ATP and mitochondria act as ATP consumers. The mitochondrial protein IF_1 acts as an inhibitor of the ATPase activity. It binds to the ATPase and limits its hydrolytic activity, protecting the cell from mitochondrial driven ATP depletion, and therefore represents an important determinant for cell survival. We have measured its expression in various tissues in relation to the F1-F0–ATP synthase and imaged its intracellular localization. We have also genetically manipulated the expression levels of the protein to determine its role in the cellular response to hypoxia. To this end, we have devised and built an instrument to explore the relationships between ATP (measured with firefly luciferase luminescence) and other aspects of mitochondrial and cell (patho)physiology – mitochondrial potential, redox state, calcium and pH, measured using fluorescence indicators. This instrument, (Fluminometer or Fluoro-luminometer) combines measurements of fluorescence and luminescence signals aiming to extend our knowledge of the relationships between changes in cellular pathophysiology and ATP homeostasis in intact cells.

Keywords: ATP; Mitochondria; IF_1; Ischemia; Fluminometer

Diffractive grating structures for colour-separating backlights

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Abstract:

The light management in present liquid crystal displays (LCDs) is not very efficient. One of the factors limiting the light throughput is the absorption in the colour filters. It has been shown[1] that a promising way to reduce this absorption is the use of diffractive colour separation by a grating on top of a lightguide in the backlight.

Recently it has been shown[2] that it is possible to combine colour separation with polarised light emission by the use of a surface-relief grating with a birefringent coating. In that way also the absorption in the polarisers can be reduced.

The principle of this colour-separating polarised backlight is as follows. A surface-relief grating with a period of approximately 400 nm is applied onto a lightguide. The grooves of the grating are filled with a birefringent material having its optical axis along the grooves. Furthermore, the ordinary refractive index of the birefringent material is matched to the grating material, whereas its extraordinary refractive index is significantly higher. As a result, light with polarisation along the grooves (s-polarised light) can be diffracted, whereas light with polarisation perpendicular to the grooves (p-polarised light) will propagate unaffectedly in the lightguide due to total internal reflection. If this structure is used in a side-lit geometry, red, green and blue light with s-polarisation is coupled out in slightly overlapping angular regions between –30 degrees and +30 degrees.

The structures used up to now showed the feasibility of our concept but were not yet optimised. We performed calculations of the grating efficiency as a function of the material and structure parameters. For high efficiencies of the colour-separating polarised backlight, the extraordinary index of the birefringent material should be high. The modulation depth of the grating is preferentially between 300 and 500 nm. The grating efficiency is affected by the shape of the grating as well.

In order to obtain the desired grating structures the interference pattern produced by two laser beams coming from the same source has been used to induce an anisotropic polymerisation process in photosensitive materials. An etching procedure can be applied thereafter to realize the surface relief morphologies. We will show a first optical characterization of the obtained structures that evidences their novel features.

[1] Y. Taira et al., SID 02 Digest, 1313 (2002); F. Yamada et al., Eurodisplay 2002, 339 (2002).

[2] D.K.G. de Boer et al., Eurodisplay 2005.

Keywords: Displays; Backlights; Holography; Diffraction Gratings; Colour-separation

Development of a co-culture system for tissue engineered vascular grafts

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Abstract:

Surgical replacement or bypass surgery is the most common treatment for coronary and peripheral atherosclerotic diseases, with over 28,000 bypass cases performed each year in the UK. However, many patients do not have appropriate blood vessels for use as replacements and the development of tissue engineered vascular grafts (TEVG) offers a possible solution to this problem. Smooth muscle cells (SMC) and endothelial cells (EC) exist within close proximity to each other within the blood vessel interacting in a variety of ways which can regulate the normal function of both cell types. As such establishing a stable co-culture system is vital for the development of a TEVG. For a TEVG to be fully functional it must be able to withstand the variety of mechanical stresses present in the dynamic vascular environment. These physical cues also provide signals to both the SMC and EC, regulating the development of the vessel. The mechanical stresses in vivo are extremely complex, but can be approximated by use of a bioreactor system.

The main aim of this research is to develop a tubular co-culture system of SMC and EC that can be used within a coronary artery bioreactor system. In order to achieve this goal, a well-established 2D porous membrane system was initially developed, which established that co-culture with our cell types was possible. Growth curves have been carried out to determine a media suitable for both cell types, and SMC and EC markers are being assessed by RNA analysis and immunocytochemistry. Based on this work a system of direct co-culture is being developed and assessed for its suitability for use within the bioreactor system.

Keywords: Vascular; Co-culture; Tissue engineering; Smooth muscle cell; Endothelial cell

Simulation in cardiovascular dynamics: Lumped parameter models as a complement for 3D refined modelling

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Abstract:

Studies of the cardiovascular system require a multidisciplinary approach, bringing together expertise from a number of branches of experimental and theoretical science. Interdisciplinary teams provide the key to answering questions concerning the diverse forms of biological interaction amongst individual organs, between these organs and their environment and their reactions under physiological conditions or specific inputs. Modelling of biological systems represents a challenge and the use of complex 3D physiological models remains at the frontier of what can be currently achieved with specialized software.

The use of finite elements (FE) models to represent the whole system is computationally prohibitive and a multiscale approach is an attractive alternative. Detailed FE models can be used where accuracy is needed. These can then be coupled to more global lumped models of the rest of the system.

Significant resource has been directed to the use of FE modelling but less to advanced lumped modelling. Quite simple approaches for the lumped parts (e.g. block diagrams) are often used. This may limit the usefulness of these models. In this work, a simple model of the left ventricle will be presented. The energetically coherent approach used aids understanding of the dynamics of the left ventricle. Whilst the model is too simple to be used in clinical diagnosis, it can provide adequate boundary conditions for FE models of the arterial system.

The natural extension of this work is the core of the Marie-Curie funded project C-CAReS, in which a coupling of a simple ventricular Bond Graph model with a 3D model of the aortic valve is being developed. The ultimate goal is to determine the closure force of an aortic valve as a function of patient physiology.

Keywords: Cardiovascular modelling and simulation; 3D models; Lumped parameter models; Boundary conditions

Eastern Europe: Post-industrial welfare state for industrial economies

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Abstract:

This paper surveys a certain paradox of the Eastern European welfare state. On the one hand, post-communist countries are mostly adopting a very 'liberal' welfare state model. Four of the eight post-communist countries that have recently became EU members have flat-rate income taxation. Five of them have partly 'privatised' their pension systems and now have mandatory funded pension schemes. Attempts at privatising healthcare are widespread. With weak unions and infrequent industrial actions and not many institutional labour market rigidities (such as occupational pensions), few Western European structural problems trouble policy-makers in the East.

On the other hand, the post-communist economies rely dominantly on the growth based on traditional industrial operations, plants based on economies of scale and massified workforce. This is driven by foreign direct investment (FDI). R & D spending is low. Not much of a middle class is being created with existing income patterns and some policy changes (flat rate personal income tax) even seem to be aiding a retardation. The policies that many call for in Western Europe in order to break the power of the 'median voter' (Esping-Andersen) are applied easily in the East - where no median voter capturing an oversized welfare state exists. The post-communist states seem to be depriving themselves of the means (welfare state and taxation mechanisms) to invest in the knowledge economy and create a vibrant middle class!

Keywords: Post communist; EU; Welfare state; Post-industrial; Middle class

Relating personality with song preference

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Abstract:

With more music content available through digital means (e.g., Internet, MP3 players, etc.), there is an increasing need to personalize this content to individuals' specific content preferences. To accomplish this, a better understanding of individual differences in music preferences is necessary. This study investigates the relation between the music preferences of 36 participants and their personality traits, as measured by the NEO-PI-R (Costa & McCrae, 1992). Participants listened to 18 different 10-second song clips of music, which varied by tempo (fast/slow) and 9 genre categories. Participants gave several responses after each clip, including a measure of liking/disliking. Participants also completed the NEO-PI-R after all clips were played. Significant correlations found between participants' song preference and their measured traits are discussed.

Keywords: Personality; Traits; Music; Personal preferences; Personalization technologies

An adaptive virtual structured network topology for P2P systems

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Abstract:

P2P and Grid computing are two technologies used to respond to users needs and distributed application requirements. The former focus is on resource sharing, such as Gnutella, etc. One of the features of these systems is that the resources are gathered dynamically due to their availability and services they can provide.

The later attention is in computing resources and system performance. Usually the system resources are booked in advance. The challenge here is to design and implement techniques for efficient management and utilisation of all system resources.

In this project we propose "DGET: Data-Grid Environment and Tools", a system which benefit of these two technologies.

In this paper, we will focus on how to design efficient search and discovery techniques to optimise the system response time? We use techniques based on structured network topology. Therefore, we propose a new self-reconfigurable network topology, called TreeP. TreeP is based B+tree model. We conducted both theoretical and experimental studies of TreeP. TreeP topology is of diameter O(log_d(N)), is O(d) connected and is built using O(Nlog_d(N)) messages; Where N is the number of peers in the system and d the order of the tree. The TreeP system is then stressed in real-world heterogeneous computing environment and proved to be very efficient. TreeP is a component of DGET.

Keywords: P2P; Grid computing; Virtual network topology; B+tree; Heterogeneous systems

Excess in the sky

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Abstract:

Some small excesses of galaxies in some areas of the sky tell to astronomers what the Universe is made of. How?

At the beginning of time, Universe was filled with some very hot gas crossed by waves of matter like wrinkles in water. These waves propagated while the Universe was cooling. Then, like water freezing at zero degrees, waves of matter froze when the Universe became cold enough: they formed some matter concentrations. Matter attracting matter because of gravitation, more galaxy clusters were formed near matter concentrations than in the other parts of Universe. They are these excesses of galaxies that some astronomers discovered in the sky in 2005, revealing that the waves of matter froze when their size reached 500 million of light-years.

This last distance is an important clue to know what the Universe is made of. Why? The Universe expands like a balloon and distances are related to this expansion: the faster the Universe expands, the more the distances between two distant points increase with time. But expansion is also related to the Universe content: for instance the matter slows down expansion. Astronomers have thus concluded that to explain the figure of 500 million light-years, the Universe should be filled by 30% of matter and 70% of an unknown component called dark energy. Whereas the first one slows down expansion, the second one accelerates it, the whole explaining how expansion allowed the wave of matter to reach the size of 500 million of light-years.

Keywords: Cosmology; Astronomy; Observation; Galaxy; Dark energy

Alternative anode materials for solid oxide fuel cells

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Abstract:

A fuel cell is a highly-efficient and environmentally-friendly energy conversion device. Using solid oxides as electrolytes and operating at relatively high temperatures (600-1000 ^{o}C), a solid oxide fuel cell (SOFC) can use hydrocarbons (e.g. natural gas) directly as fuel without external reforming, which makes them, amongst the other fuel cell systems, potentially more competitive within the present technologies for energy production. To realize this advantage, an efficient anode is particularly important. The current Ni-based cermet anode material has a number of disadvantages including nickel coarsening, sulphur poisoning, carbon deposition and volume instability upon cyclic reduction-oxidation (redox). Therefore, alternative anode materials are desired. In this project, ceramic-based materials are explored as such an alternative. These materials are either single phase perovskite oxides with mixed ionic/electronic conduction (e.g. $La_{1-x}Sr_xAl_{1-y}Mn_yO_{3-\delta}$ and $La_{1-x}Sr_xTi_{1-y}Mn_yO_{3-\delta}$), or multi-phase composites containing a good electronic conductor (e.g. donor-substituted $SrTiO_3$), a good ionic conductor (e.g. YSZ) and a very small amount of catalyst (e.g. Ni). Promising results have been obtained with these new materials and will be presented on the conference.

Keywords: Solid oxide fuel cells; Anode materials; Ceramic

Dispersion of single-walled carbon nanotubes

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Abstract:

The ability to miniaturise devices has completely changed our society, and modern technology is constantly pushing towards smaller and lighter devices with enhanced and more diverse functionalities. Single-walled carbon nanotubes (SWNTs) display unique structures and remarkable physical properties and are promising candidates for the realization of smart nanomaterials. They have nanoscale dimensions, and can be modified through covalent bonding of functional organic molecules, opening the way to structural materials of high technological importance. One of the major bottlenecks to applications is their aggregation into bundles. Many methods have been suggested to de-bundle the SWNTs, including both covalent functionalisation and non-covalent funtionalisation with surfactants, polymers and macromolecules. These methods have their advantages but the ideal situation must be to dissolve and de-bundle the SWNTs in an appropriate solvent at concentrations that are useful for their implementation in applications. In this work I will show our simple methodology to disperse and de-bundle SWNT using organic solvents as dispersants. Using Atomic Force Microscopy we observe the bundle diameter distribution to decrease dramatically with concentration. Near-infrared Absorption and Emission Spectroscopy were carried out on all solutions confirming an increase in the population of individual nanotubes with decreasing concentration.

Keywords: Nanotube; Nanotechnology; Dispersion; Bundles; Spectroscopy; Microscopy

Nano-scale accuracy analysis of diamond films for advanced technologies using uleSIMS and other techniques

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Abstract:

Diamond is well known for its extreme properties, e.g: the hardest substance known, high thermal conductivity combined with high electrical resistance, high electrical breakdown strength, and excellent chemical resistance. Although artificial diamond has been used in industry for applications such as abrasion and cutting for many years, it is only recently that diamond production techniques have improved sufficiently that it is possible to grow high quality single crystals several millimetres in size[1]. It is also possible, by adding impurities in an appropriate way, to tailor the material's electrical conductivity to produce a semimetal, a high mobility type p semiconductor or an extremely good insulator[2]. Consequently, a whole new range of applications has become feasible, including high power, high voltage electronic devices, and devices for use in extreme environments.

In this context, our work deals with the accurate characterization of the layer structures essential to electronic device design and fabrication, with emphasis on the subtle details that distinguish between ultimate and poor performances. For this task, we use ultra low energy secondary ion mass spectrometry (uleSIMS), an analytical technique developed in this group[3] which plays a fundamental role in the semiconductor area. In this presentation, we will show analysis performed in unique diamond samples containing very thin boron doped layers (deltas), and explore the limitations of the analytical technique for this sort of material.

[1] J Isberg, J Hammersberg, E Johansson, T Wikstrom, DJ Twitchen, AJ Whitehead, AE Coe, GA Scarsbrook, Science 297 (2002) 1670.

[2] CE Nebel, M Stutzmann in "Properties, Growth and Applications of Diamond" Ed. MH Nazare, AJ Neves (2001) INSPEC, London. p45.

[3] M. G. Dowsett, N. S. Smith, R. Bridgeland, D. Richards, A. C. Lovejoy, and P. Pedrick, Secondary Ion Mass. Spectrometry SIMS X, edited by A. Benninghoven, B. Hagenhoff, and H. W. Werner (J. Wiley & Sons, New York (1997), p. 367.

Keywords: Synthetic diamond; uleSIMS; Delta layers; Single crystal diamond; Near-surface analysis

Illuminating the black box: Computational investigations of numerical cognition

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Abstract:

The current work illustrates the application of two very different modelling techniques, applied to clarify a debate within the cognitive neuroscience of numeracy concerning the way in which quantity is represented in neural systems. Though different in detail, most contemporary theories of numerical cognition refer to some sort of intermediate, analogical representation scheme for numbers – a scheme that complements the more evident verbal / symbolic codes (such as the number words, "one, two…"). There remains great debate as to the precise format of this putative representation scheme.

Here, we focus on "quantity comparison", a key component of the "number sense". The first technique compares the representational theories in terms of the way in which each interacts with biologically plausible learning. Better representational theories should permit closer agreement between model behaviour and empirical data. The second technique involves the "evolution" of numerically sensitive behaviour in an artificial ecosystem, with the goal of recovering those quantity representations that emerge spontaneously.

Taken together, these techniques offer a practical way to explore the traditionally elusive question of the balance between Nature and Nurture in cognitive development. Yet they also embody a fundamental distinction between two apparently inconsistent frameworks for understanding cognitive systems; attempts to resolve this inconsistency are a critical element of our current work.

Keywords: Cognition; Number processing; Neural networks; Learning; Evolution

Manipulation of molecular properties by coherent light fields

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Abstract:

Recent efforts of the physics scientific community have led to the development of fields such as ultracold physics, quantum information processing, Rydberg physics, and control of chemical processes. The success of many of these endeavours depends on the ability to precisely manipulate quantum level systems by laser fields. Practically all schemes of laser manipulation of quantum states rely heavily on the use of strong field effects in light-matter interactions, which can be interpreted in terms of the Autler-Townes (AT) effect. The AT effect is usually observed as splitting of the excitation spectrum measured by a weak probe laser field due to "dressing" of the molecular energy levels by a strong laser field. The AT effect itself has a potential for development of novel applications, like the recently demonstrated technique for lifetime and branching ratio measurements using cw laser fields.

Keywords: Laser manipulation; Quantum states; Light-matter interaction; Autler-Townes effect

Digital-handwriting: Automation of manual work in a handwrite-computer system interaction

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Abstract:

Scope:
In ages of digital writing the handwriting on paper seems to be inefficient and obsolete. Nowadays many walk of live digital writing is invented or even forced at several work places, even though most of people write by hand significantly faster and more correctly. Our aim is to present a solution that provides paper forms for handwriting as input, produces digitalised data for companies' electronic systems requiring no or very little further human work.

Objectives:
To apply OCR (Optical Character Recognition) in enterprise environments proving maturity of such technology in business environment (SME).

Methods:
We evaluate digital pattern technologies according to usability, flexibility, ease of integration, and security. In evaluation process we select the ones which promise feasibility. We identify technical boundaries with prototype implementations.

Results:
During the project the chosen part solutions of technology providers (SRS, Hallbach) were integrated into our selected enterprise system (genesisWorld). Prototype implementations were successful. Continuity is granted by the first enterprise customer.

Conclusions:
Integration of pen based OCR technologies into enterprise environment is feasible. An adopted digital pen interface in my company's main product (CRM) proves it. As a consequence it turned out that manual work of digitalisation is significantly reduced. As a side effect the solution speeds up businesses process in some cases

Keywords: Digital pattern; Digital pen; Small and medium enterprise; genesisWorld

The role of interstellar turbulence on the formation of stars and planetary systems

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Abstract:

Stars and their planetary systems form in dense (molecular) gas clouds within the interstellar medium. The latter is far from being quiescent. Turbulent motions manifest themselves in all scales from the large scales of molecular (hydrogen) clouds to the smallest scales of protoplanetary discs. A complete theory for the formation of stars and planetary systems must take into account the dissipation of turbulent energy from the large to the small scales (turbulent cascade) self-consistently, i.e. one cannot just study star and planet formation at the smallest scales and in isolation. The physical complexity of the systems studied as well as the many orders of magnitude over which their density and radius evolve in the process of star and planet formation make it necessary that theoretical work is based on numerical hydrodynamic simulations. In this work we conduct large scale numerical simulations of dense parts of the interstellar medium in the presence of turbulence where we ensure that the numerical resolution is sufficient to follow the formation of young stellar objects and low-mass (and possibly planetary) companions around them. In this paper, we give an overview of the observational constraints of the star formation process, present our model and numerical approach as well as some preliminary results on the evolution of gaseous discs around young stars and the possible role of such discs on the formation of planets around stars.

Keywords: Star formation; Planet formation; Protostellar discs; Interstellar turbulence; Numerical hydrodynamics

The crystal structure of the RET receptor tyrosine kinase

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Abstract:

The receptor tyrosine kinase RET is proto-oncogene, whose aberrant activation cause a variety of cancers, primarily affecting cells derived from the neural crest, such a thyroid C-cells and the adrenal gland.

In order to determine the molecular nature of mutations causing RET activation, we have solved the three-dimensional structure of the receptor tyrosine kinase alone or in complex with a kinase inhibitor, which is currently being tested as an anti-cancer drug.

Keywords: RET; Cancer; Drug; Receptor tyrosine kinase, crystallization

ADMIRE: A new framework for distributed data mining on grid computing environments

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Abstract:

Distributed data mining (DDM) deals with the problem of finding patterns or models in an environment with distributed data and computations. The main aim of the DDM techniques is to exploit fully the benefit of distributed data analysis while minimising the communication. Usually, DDM techniques perform local data analysis followed by the generation of a global model by aggregating the local results. These two steps are not independent since naive approaches to local analysis may produce an incorrect global data model. This is even more critical when the datasets located on different sites record different sets of features (heterogeneity). Furthermore, today we have a deluge of data from not only science fields but also industry, commerce fields. Massive amounts of data that are being collected are often heterogeneous, geographically distributed and owned by different organization. To face with these problems, Grid Computing can be used as infrastructures to provide an effective computational support for distributed data mining applications.

In this paper, we will present the architecture of ADMIRE, a new framework for developing novel and innovative DDM techniques to deal with very large and distributed heterogeneous datasets in both commercial and academic applications. The main ADMIRE components will be detailed as well as interfaces allowing the user to efficiently develop and implement their DDM techniques on a Grid platform such as DGET, a Data-Grid middleware developed in University College Dublin.

Keywords: Distributed data mining; Grid computing; Data-Grid; Distributed systems; Heterogeneous datasets

Ion source development for high intensity radioactive ion beam production

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Abstract:

Radioactive ions provide an analytical tool which can be used to probe the structures of atomic nuclei and materials as well as having applications in nuclear astrophysics, bio-medicine and the environment.

Radioactive ions are produced by nuclear reactions induced by the bombardment of a target (from various materials) with a primary beam of protons, neutrons or stable ions.

In order to accelerate, transport and separate the different isotopes produced in a same reaction, the atoms have to be ionized, using an ion source.

In an ion source, the atoms are positively or negatively ionized, generally by collisions with photons or energetical electrons, or by exchanging electrons with the walls of the source when hitting them.

For the ionization of radioactive isotopes, an ion source has to be efficient, fast and selective, so that the desired isotope can be ionized and extracted before decaying.

ISOLDE is a top facility for the production of radioactive ion beams by the ISOL (Isotope Separation On-Line) method. The objective of the Marie Curie fellow at ISOLDE is to improve the actual ion sources, so that they can provide beams with higher intensities, needed for the future European facilities.

The phenomena inside the ion sources used at ISOLDE are presented, as well as the limitations which have to be surpassed for their improvement.

Keywords: Nuclear physics; Ion sources; Radioactive isotopes

Atmospheric pressure plasma chemical etching for continuous c-Si solar wafer processing

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Abstract:

Plasma enhanced chemical etching of silicon wafers has been carried out at atmospheric pressure. A linear extended DC arc with a width of 150 mm for plasma activation was used to develop the etching process. The technology operates in a remote (downstream) mode. The experimental set-up allows continuous processing which is advantageous in terms of in-line capability and consequently reduced effort for substrate handling. The technology comprises the potential to be inserted in different silicon wafer processing steps such as reduction of reflection losses by surface texturing, removal of n-doped silicon, phosphor silicate-glass removal, etc.

Etch gases like CF_4, CHF_3, NF_3, SF_6 and SF_6/O_2 were injected into the afterglow plasma of a linear extended DC arc. In-situ Fourier Transform Infrared (FTIR) gas phase spectroscopy inside the plasma etching area have been used for characterising the intermediates and products of the plasma chemical process. A range of species has been identified giving evidence to the key products of the etching reaction as well as onto competing side reactions.

The plasma generated fluorine containing intermediates have been successfully utilized to etch (100)-mono-Silicon wafers. Static etch rates of over 11 µm/min and dynamic etch rates of 1.5 µmAm/min have been achieved so far. The process conditions have been optimized to obtain different surface textures such as micron-sized pyramids or nano textured surfaces, reducing noticeable the reflectivity of the smooth silicon surface. UV/VIS/NIR reflection spectra (300 nm to 1000 nm) showed that by means of surface texturing the reflection of bare-polished (100)-monosilicon wafers was reduced from 40% to less than 2%.

Removal of the emitter (n-doped silicon) from the rear side surface of solar cells has significant potential for future solar cell concepts. In this contribution fluorine radicals generated in the atmospheric pressure plasma reactor were used to completely remove the rear side emitter without etching front side structure. Cell efficiency data comparable to established wet chemical etch processing were achieved.

Feasibility of phosphor silicate-glass removal has been demonstrated. FTIR spectra exhibit decrease in the Si-O phonon band after plasma chemical etching at atmospheric pressure, similar to that after wet chemical etching (reference process). Wafer characterisation is underway to evaluate and optimize SiO2/Si-selectivity by atmospheric pressure plasma etching.

Keywords: Plasma etching; Silicon wafer; Atmospheric pressure; Photovoltaics; Fluorine

Consumer expenditures and home production: New evidence from Germany

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Abstract:

The europeanwide increase in the fraction of people above age 60 in the population raises the interest in the living conditions of this large population group. I investigate the differences in consumer expenditures –often used as a measure of well-being– of German households before and after they enter retirement. A distinct drop in spending upon retirement entry has been documented already for the US and the UK. It poses an empirical puzzle since standard economic theory predicts that forward-looking agents maximize their utility by smoothing consumption over the life cycle. Out of the various explanations being put forward to explain this puzzle, I explore the role of home production in substituting some part of consumer expenses.

Taking a combined look at consumer expenditures and time use pre and post-retirement, I find a significant drop of about 17% of pre-retirement expenses at retirement which coincides with an increase in time spent on home production of an additional 30% per day.

Keywords: Economics; Consumer demand; Time use; Life-cycle model; Retirement

A novel bionanotechnology tool provides innovative strategies to culture cells for clinical use

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Abstract:

Animal cells, whose dimensions are in the range of several tens of micrometers, perceive and react to chemical, structural and mechanical signals that are spatially distributed on the nanometer and the micrometer scales. Therefore, a man-made substrate whose chemical composition, structural features and mechanical properties are perfectly controlled down to the nanometer range is an ideal tool to regulate cell behaviour. And this is where nanotechnology advances can give a helping hand.

A novel nanolithography technique which allows the creation of periodical nanopatterns of biochemical signals that are perceptible by cells was recently developed at the University of Heidelberg (Germany). By appropriately choosing the identity of the chemical signals and the way in which they are spatially distributed, surfaces produced using this technique can be used to switch on and off targeted cell functions. As well as forming the basis for advances in fundamental research, this new technology provides ways to design materials that are intended to interface with cells. More particularly, in the present project we want to develop substrates nanopatterned with chemical signals that will sustain cells in culture in the absence of animal serum. Serum is routinely added to cell cultures as a source of nutrients, but its use has significant disadvantages, including contamination risks which compromise the use of in vitro-cultured cells for clinical purposes. Thus, removing the need to use serum will greatly benefit fields such as stem cell research and tissue engineering.

Keywords: Biomaterial; Nanotechnology; In vitro-cultured cells; Animal serum

GloLab for transfer of knowledge

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Abstract:

The world-wide web has become humankind's most powerful tool for the transmission of knowledge. We suggest to start the creation of the Global Laboratory Network (**GloLab**) for scientific and teaching on-line experiment, and discuss the main principles of the GloLab building[1]. We show a practical example of remote experiment for teaching of magnetism (http://labfiz.uwb.edu.pl/exp/domeny/). Such experiment could be used for different levels of education: pupils, high school, university and PhD students. It would be great to realize the idea in larger, the European scale. Thus, there are excellent reasons - and it is within reason - to create a GloLab sharing effort among different institutions, each contributing unique building blocks: access to singular experimental set-ups corresponding with their accumulated scientific and teaching potential, their unique equipment and samples. Both view-type and fully remote experiments performed according to the highest standards can have importance for the wider society - while giving quick access to every interested physicist world-wide. Besides developing the common scientific base, the GloLab will disseminate knowledge and research results to a non-expert audience, inspiring and attracting young talents to Science.

[1] A. Maziewski, W. Dobrogowski, V. Zablotskii. Physics World, February (2006) 17.

Keywords: Transfer of knowledge; Remote experiment; Science popularization; Magnetism

The production of astatine negative ion beams

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Abstract:

Astatine is radioactive and essentially unavailable in nature. Its name, derived from a Greek word meaning "unstable", emphasizes the instability of all its known isotopes with respect to the radioactive decay. The longest-lived isotope of astatine has a half-life of about 8 hours, thus the only way to work with the element is in a laboratory having the facilities to produce it. In addition, chemical operations with milligram amounts are impossible (even if such quantities were available), given the enormous release of heat and radiation. The radiochemistry of astatine has been only investigated from trace concentrations in aqueous solutions, typically 10-11 to 10-15 M since greater concentrations lead to radiolysis of the water with consenquent formation of hydrogen peroxide and oxygen either masking or influencing the behaviour of astatine. This makes the astatine concentration comparable to that of the least of the impurities in the experimental system and leads to irreproducible and uninterpretable results. For all of these reasons, there is a great request from the scientific community for astatine ion beams. At ISOLDE some of the astatine isotopes can be produced with good yields but the relevant positive ion beams are contaminated with isobars from francium and radon. Here we report our results on the development of astatine negative ion beams free of contaminants

Keywords: Astatine; Negative RIBs; Halogens; Target; Ion source

Extreme value statistics in strongly correlated systems

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Abstract:

Much of our information about the physical world is of a statistical nature: average rainfall, infant mortality rate, stock market volatility, etc. When average quantities are reported it is often assumed that the fluctuations around the average are negligible. In some processes, however, extreme statistics have the greatest physical impact. For example, earthquake magnitudes follow a decaying probability distribution in which small earthquakes are very frequent, while large earthquakes are very rare. Yet such rare events are of primary relevance. Extreme value theory concerns itself with the statistics of rare events. Many 'classical' results are known for uncorrelated processes, i.e. when the assumption of identically and independently distributed random variables holds. As a statistical physicist, I am interested in investigating processes where this assumption breaks down, particularly within critical (scale-invariant) phenomena, where fluctuations cannot be neglected. The problem, therefore, is to extend extreme value theory to include correlations.

The aim of my talk is to give an overview of extreme value theory, to explain why such a theory is desirable and useful, and to report on some of the progress within physics to understand how extreme value statistics work in correlated systems.

Keywords: Extreme value statistics; Rare events; Critical phenomena; Statistical physics

Improving the properties of a biodegradable polymer: The case of nanofilms of PHB

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Abstract:

Poly(3-hydroxybutyrate) (PHB) is a natural and biodegradable thermoplastic polyester produced in small amorphous granules by some bacteria to store energy inside the cell. As soon as the polymer is isolated from the cell it crystallizes and thus embrittles in short times if stored at room temperature. The polymer, even if relatively cheap, free of industrial solvents, highly biodegradable and thus environment friendly, has not reached a large success.

However, it was recently shown that, probably due to interaction with the substrate, films of this and other semicrystalline polymers thick a few nanometers [1-3] can be obtained in the amorphous state and been stable for months. Such a general trend opens the possibility to prepare samples stable in time and suitable for nanotechnological applications of PHB and other polymers Taking advantages of the polar character of PHB, dielectric spectroscopy was used in order to monitor the degradation induced by crystallization. Isothermal cold crystallization of amorphous bulk and ultrathin films of PHB was monitored at different thickness and different temperatures in real time. The different crystallization kinetics are followed and analyzed in terms of reduction of mobility and volume fraction of the amorphous phase. Moreover the use of a powerful derivative technique, based on the logarithmic variation of the permittivity constant within crystallization time, permits a faster and more sensitive analysis of the acquired data.

It was observed that decreasing the thickness of the polymer layer leads to an increase of the crystallization time, from less than 2 hours for a 50m bulk sample up to more than 27 hours for a 26nm ultrathin film, and a reduction of the Avrami parameters, and thus the dimensionality of the process, as estimated from the here proposed derivative technique. In addition no effect on glass transition temperature and thermal evolution of the structural relaxation is observed down to 26nm, indicating that the slowing-down of the crystallization kinetics is probably due to interface effects.

[1] M. Despotopoulou et al., Macromolecules, 29, 5797 (1996)

[2] H. Schönherr et al., Macromolecules, 36, 1199 (2003)

[3] M. J. Capitán et al., Macromolecules, 37, 5653 (2004)

Keywords: PHB; Ultrathin polymer films; Crystallization in confinement; Biodegradable polymers; Nanoscience

The use of vegetative cover and mycorrhizal colonisation in the remediation of soils contaminated with metals

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Abstract:

The aim of our research was to investigate the coupling of vesicular-arbuscular mycorrhizal fungi (VAM) with plants in the remediation of soils contaminated with metals.

The research design included lab pot-trials, ex-situ lysimeters experiments, and field experiments. Five types of treatments coupled with phytoremediation have been investigated: inoculation with VAM, spraying with 2-Aminoethanol (2-AE) on leaves, amendment with green manure, top soil, and with compost. We estimated phenological and physiological parameters of plants, concentrations of metal in water, soil and plants, control parameters of metals behaviour in water and soil.

The enhancement of metals contamination in soil increased the oxidative stress and decreased the biomass. Even under the application of acid water, the mycorrhization attenuated the stress. The most common beneficial effect of VAM was increased uptake of immobile nutrients, especially phosphorous. Supplementary application of 2-AE further reduced the stress and increased the biomass. The effect of the green manure application was contamination dependent (beneficial at high soil contamination). Amendment with compost strongly reduced the oxidative stress and increased the plants biomass. The contaminants in the upper part of the soil were transported by rainfall and added to the pollutants in the deeper part.

Keywords: Phytoremediation; Heavy Metals; Lupinus angustifolius; Secale cereale; WAM

Perceptual and algorithmic representation of music similarity

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Abstract:

The aim of the project is to model perceptual similarity of popular music and to apply these models to algorithmic assessment of similarity. The project combines two scientific approaches: 1) perceptual experiments to analyze subjects' evaluation of similarity between songs and to understand how people perceive similarity in music, and 2) the development of algorithms able to predict the results found in the perceptual experiments. The algorithms will be evaluated in their ability to predict the data collected in the first phase of the project. The focus here will be on Western popular music.

This work addresses several basic questions in cognitive and musicological sciences and also has some potential applications. For example, automatic evaluation of similarity between songs can lead to the implementation of automatic playlist generators, music browsers and music structure analysis tools.

One perceptual experiment has already been performed in December '05 and the results will be shown in the presentation.

This project is part of Marie Curie Early Stage Training project (CONTACT) granted to Philips Research.

Keywords: Perception; Music; Music similarity

Probing nanoparticle growth with light: Real-time non-destructive measurements

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Abstract:

A prominent issue in nanotechnology is the inability to accurately determine nanostructural dimensions using non-destructive and real time methods. Traditional nanostructural methods such as electron microscopy and X-ray diffraction are difficult to incorporate into experimental arrangements due to costs and accessibility. Optical techniques such as laser interferometry are usually limited to dimensions about one quarter the wavelength of the light source, or of the order of 100 nm. Ellipsometry is advantageous in that it measures both the intensity and the phase shift of light reflected from a surface, whereby changes of the order of 0.1 nm in the thickness of a surface layer can be easily observed. Recent advances in ellipsometric hardware and software now allow real time ellipsometric measurements to be performed, with information being now limited primarily by theoretical models used to fit the data. Examples of the growth of plasma deposited and also chemically reduced silver nanoparticles, measured in real time and in situ, will be presented. A model to determine the size of the particles based on plasmon resonances will be briefly presented and the results will be compared with electron micrographs of the nanoparticles.

Keywords: Nanoparticles; Plasmons; Ellipsometry; Nanocomposites

From Pliny to Virgil: Menopause and diabolical perspectives in the art of Hans Baldung Grien

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Abstract:

Hans Baldung Grien (d.1545) utilized the classical Italian humanist perspectives of his mentor, Albrecht Durer, but with significant differences of artistic purpose. For Baldung, Aristotelian hierarchies were overturned in a 'topsy-turvy' world of witches and diabolical disorder. He conscientiously subverted classical perspectives in order to show the Satanic underpinnings of the fallen, corporeal world. Inversions of meaning, and deliberate visual ambiguity in rendering familiar objects 'unheimlich' or uncanny, served to demonstrate satanic machinations at work through the feminine insurrection of witchcraft. Representations of wild and unruly night time revels, amid demoniacally animate landscapes, were deployed to fool the eye and emotional response of the viewer as to precisely who or what was being depicted. Liminality, deceptive ambiguity and the confounding of visual expectations served to destabilize a clear reception, reading and interpretation of the image. In seeking to confound the eye and bewilder the viewer with demoniacal uncertainty and 'melancholic' doubt through the 'lustful' or unruly display of classically rendered female bodies, Baldung inverted the usual aim of the classical Italianate Renaissance perspectives used by his teacher. Far from clarifying, or objectifying visual elements and representations, Baldung conscientiously inverted rational 'harmonies' and 'orders' in order to achieve moral confusion and uncertainty in the consumer of the image - a porous mentality that was, itself, then interpreted as a diabolical condition. Operating within the 'humanist' hermeneutics of the early Reform, the image's perspectival dynamics and control of presentation determine viewing and perception, morally operating as 'pious' interrogation, evidence of sin, and chastisement in one and the same moment of reception.

Keywords: History; Art history; Gender studies; Cultural studies; European studies

The influence of present and prior alternatives on risk aversion

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Abstract:

The idea that preferences may be elicited by the context is receiving increased attention (e.g. Usher & McClelland, 2004). Although frame and anchor effects have been initially considered independent, both may be seen as instances of a broader family of accessibility effects, a conception compatible with more recent theoretical treatments of judgment and decision making (Kahneman & Frederick, 2005). This conception is worth exploring because it is consistent with so much psychological evidence, and to our knowledge, it has not been applied before to analyze how individuals make sequential and non-sequential choices, two situations by which decision-makers may assess options at any particular point.

We created an experimental setting with hypothetical choices presenting mixed gambles with asymmetric payoffs in two financial domains: lottery and portfolio. A total of 1175 respondents participated in the studies.

Our main results can be summarized as follows. No reduction of risk aversion was found when an option with higher expected value was included in a high probability of loosing set. Nevertheless, it was found such reduction when the probability of winning was high mediated by frame. In the lottery treatment, the higher the probability the higher the anchor effect of the added option. In the between-trial condition, when subjects focused on gains (losses) they were less risk averse after a high risk background with high probability of winning (loosing). In the portfolio treatment, neither within-trial nor between-trial effects were found, showing that a small frame manipulation was successful in making individuals context-independent. The results are consistent with our predictions.

Keywords: Behavioural finance; Decision making; Risk aversion; Frame; Anchoring

Bioreactors and tissue engineered coronary arteries

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Abstract:

Atherosclerosis, characterised by the thickening of artery walls and vessel occlusion, remains one of the leading causes of death in Western society. Current clinical treatments for this disease include the use of allografts, autografts, and polymeric vascular grafts. However, the long-term patency for small diameter vascular grafts (<6mm) still remains low. Therefore, tissue engineering offers huge potential for this application. To achieve this goal of tissue engineered vascular grafts (TEVG), a bioreactor and model artery system was developed in this study.

In vivo, the endothelial cells located on the inner wall of the artery are subjected to a range of mechanical forces including a pressure of 80/120mmHg and a shear stress of 10-40dynes/cm2. To this end, a monolayer of primary endothelial cells (ECs) was seeded in a tubular construct and subjected to these biomechanical forces for up to 24 hours. The biological response of the ECs was evaluated using H&E, phalloidin and Hoechst staining methods.

Preliminary results show that for up to 24h in the bioreactor, the ECs remain attached in a monolayer and do not show any signs of cell death. A notable reorientation of cells was observed perpendicular to the direction of the flow. This is in contrast to the case in vivo, where ECs are oriented parallel to the direction of flow. This difference may be due to the fact that the cells were only subjected to biomechanical forces for 24h. The novelty of this work lies in the fact that both, shear stress and pressure were investigated on a monolayer of ECs in a tubular construct.

Keywords: Atherosclerosis; Tissue engineering; Vascular grafts; Biomechanical forces; Bioreactors

Design and bioproduction of recombinant elastin-like polymers showing tailored bioactivity and self-assembling properties

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Abstract:

Nature provides us an incredible amount of protein materials that exhibit an ample range of functional applications. These proteins must have properties that fulfil the most diverse functions and purposes that the living organisms need to live. Materials science is learning from the nature obtaining polymers that mimic the incredible properties of the natural macromolecules. Protein-based polymers (PBPs) are polymers that include sequences of the natural proteins and other sequences designed de novo using the knowledge obtaining from the observation of the natural proteins. Elastin-like polymers (ELPs) are a really interesting kind of protein-based polymers. These polymers show the mechanical properties of the natural elastin, are highly biocompatible, show self assembly properties and they can be tailored using DNA recombinant technologies. One of the more interesting properties of the ELPs is the smart behaviour. They show an inverse temperature transition (ITT) that make them smart polymers responsive to changes in the temperature. Furthermore, this ITT can be modified in some ELPs as a respond to external stimuli obtaining smart-protein polymers with a wide range of sensitiveness.

Another interesting property of the ELPs is the self assembly. This is one fervent field of the actual materials science due to is potential in nanotechnological and nanobiotechnological applications. The Elastin-like polymers (ELPs) are based on the recurrence of certain short monomers that are considered as building blocks in the natural elastin. The most representative polymer of this family is poly (VPGVG), and the vast majority of the ELPs described in the literature are made from selected modifications of this pentamer or its permutation[1].

The adaptation of genetic engineering techniques to material field has opened the possibility of obtaining these polymers with absolute control and absence of randomness in the primary structure. This has allowed the production of multifunctional polymers that can combine physical, chemical and biological functions[1]. All this at a very competitive cost of production and under very favourable environmental considerations1. Aiming to obtain expression of elastic protein-based polymers we use established E. Coli strains[2]. In this work we present two ELPs specially designed for tissue engineering purposes. The produced polymers comprise different building blocks, each showing a different functionality.

First, the final matrix has been designed to show a mechanical response comparable to the natural extracellular matrix, so they are produced over a base of an elastin-like polymer of the type (VPGIG)n. Along with the desired mechanical behaviour, this base has shown an outstanding biocompatibility[3]. The second building block is a variation of the first. It has lysine substituting isoleucine so the lysine-amino group can be used for cross-linking purposes while retaining the properties of elastin-like

polymers[2]. The third group contains cell attachment sequences found in the human fibronectin. In polymer A, this sequence is the RGD loop, while in polymer B is the CS5 domain, which contains the endothelial REDV cell attachment sequence. In addition, polymer B also contains the elastase target sequence VGVAPG to favour its bioprocesability by natural routes The polymers and their crosslinked matrices have been subjected to mechanical tests, physical-chemical, biochemical and "in vitro" analysis (HUVEC, IOBA-NHC cell line[4] and fibroblasts). The results clearly confirm the excellent behaviour of the matrices for the pursued purpose, as expected from the combination of functionalities and properties of the building blocks used in its molecular design.

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Keywords: Biomaterials; Bio nanotechnology; Tissue engineering; Recombinant elastin-like polymers; Smart behaviour

Overview of wave energy converter modelling

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Abstract:

Many of the offshore Wave Energy Converters (WECs) designed and tested to date are formed by an oscillating floating body linked to a Power Take-Off (PTO) system that could be either a hydraulic system or a direct driven linear electric generator. A general approach to the modelling methodology is proposed here. A preliminary hydrodynamic comparison of different oscillating bodies by frequency domain analysis allows the estimation of the absorbed power and therefore, a criterion to identify an optimal geometry. In this initial design phase a linear system is assumed. A time-domain analysis is also illustrated here for some simple PTO mechanisms and applied to different wave climates. A linear generator scheme is then introduced and some possible solutions for the grid connection are sketched. Finally, the problem of developing safe, cost-effective and reliable mooring arrangements that minimise the impact on the power output performance of the overall WEC system is addressed. Although some choices may seem specific, this approach is intended to be a general study and to give a global overview of the design methodology of offshore wave energy converters. It is intended to be a platform for further collaboration on modelling and the integration of modelling techniques that are often applied in isolation. It is seen how the expansion of such collaborative efforts leads to a more standardised approach for the holistic system modelling of offshore wave energy converters.

Keywords: Renewable energy; Ocean engineering; Moorings; Energy conversion; Hydrodynamics

Tracking in the ZEUS experiment

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Abstract:

The HERA collider and ZEUS detector taken together may be thought of as analogous to an enormous electron microscope with a resolution fine enough to see features on scale one thousandth of the size of the atomic nucleus.

ZEUS, which has dimensions of 12m x 10m x 19m and weighs 3600 tons, is indeed dedicated to identify the nature and properties of particles produced by the high energy electron-proton collisions.

The momentum and the charge of the particles can be calculated by measuring and fitting their trajectories in a magnetic field. This is the goal of the Central Tracking Detector. At its centre, this component of the ZEUS detector is completed by a Micro Vertex Detector. Situated close to the beam line, this subdetector is designed to measure precisely the tracks near the interaction point (the vertex).

These two essential tracking components will be described briefly and the various techniques used to determine the track parameters and the vertex positions will be shown.

Keywords: Track; ZEUS; Particle; Vertex; High energy

A new automatic artery lumen identification algorithm for carotid ultrasound images

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Abstract:

Many properties of the common carotid artery (CCA), e.g. (the change in) lumen diameter and wall thickness, can be measured non-invasively with ultrasound techniques. Usually this requires manual identification of the region of interest within the ultrasound image. To eliminate such a user interaction we developed a novel CCA automatic lumen identification algorithm, acting on the envelopes of the received radio frequency echo signals, eventually composing the ultrasound image. To reduce computational load the available data undergo decimation, according to the 2-dimensional resolution characteristics of the echo system, followed by dynamic range reduction. Subsequently, parametrical template matching, based upon the expected diameter range and *a priori* knowledge of the typical pattern of the echo envelope covering an artery, is performed, resulting in the estimation of the lumen centre position along each signal considered. Finally, in order to reject wrong estimates, a spatial and temporal clustering method is applied. The proposed algorithm was tested off-line on 128 realistic echo data recordings over a few seconds. In more than 98% of the images considered the artery was properly identified. Further developments involve: a) real-time implementation, in order to have full automation and better quality feedback for measurements of wall properties, and b) extension to other anatomical structures.

Keywords: Ultrasound; Artery; Pattern recognition; Automatic identification

Dendrimers as detoxication agents

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Abstract:

Dendrimers are a new class of nanotechnological polymers with a well-defined molecular structure. They are monodisperse polymers with high molecular weight and it results in a multitude of physical properties. They possess many functional end groups and empty internal cavities which are responsible for high solubility and reactivity. These specific properties make dendrimers suitable for targeting of DNA and RNA, catalysis, microarray and drug delivery systems. Based on dendrimers the new contrast agents for magnetic resonance therapy are developed. The main idea of our project is studying the possibility to use dendrimers as new detoxication agents. It was found that dendrimers are able to complex both with hydrophobic fluorescent probes (as model toxins) and hydrophobic endogenous toxin bilirubin. As a result of binding the solubility and photostability of bilirubin sharply increased. Based on these results we proposed that dendrimers can be used in haemodialysis systems for effective removal of bilirubin. Also, the effect of dendrimers on transport and enzyme proteins was studied. It was found that dendrimers can change protein conformation, intramolecular dynamics, binding properties and enzyme activity. Based on these results the conclusion was made that in studies on application of dendrimers for targeting, catalysis, drug delivery and detoxification the impact of dendrimers on proteins should be taken into account.

Dr Dzmitry Shcharbin is a beneficiary of a Marie Curie International Incoming Fellowship within the 6th EU Framework Programme (grant 510018).

Keywords: Dendrimer; Detoxication; Endogenous toxin; Bilirubin; Serum albumin

LHCb data management on the grid

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Abstract:

The LHCb detector is one of four being built for the Large Hadron Collider (LHC) at CERN, Geneva. The LHCb Computing Model outlines how the experiment wishes to utilise computing resources that are distributed across many collaborative institutions. This distributed computing model is required as the volume of data produced by the new detector would overwhelm individual institutions or even countries. LHCb's DIRAC system was designed to perform physics related computing operations using dedicated LHCb resources and as an interface to the LHC Computing Grid (LCG), currently the world's largest Computing Grid. DIRAC is made up of many components one of which is the Data Management System (DMS). The DMS allows the manipulation, movement and deletion of files on remote storage resources and the interaction with Grid File Catalogs to maintain a consistent picture on their locations. New functionality has recently been incorporated into the DMS to integrate use of gLite's File Transfer Service (FTS) and new LCG File Catalog bulk operation functionality. In this paper the DMS will be detailed as well as measurements of its performance in recent LCG Service Challenges.

Keywords: Data management; Grid computing; LHCb

Application of the large eddy simulation technique to study the flow over an incompressible cavity and evolution of a planar turbulent jet

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Abstract:

The main goal of the present research is to apply a rapidly developing numerical approach to understand the physics behind the using of active control methods to various fluid mechanics problems. In particular, we are interested in the problem of changing direction of a free turbulent jet using its interaction with small scale unsteady jets.

To gain an experience in using the Large Eddy Simulation technique and an in-house code Lithium a flow over a 2D cavity was simulated and possibility of reducing self-sustained cavity oscillations has been examined.

Our results showed that incompressible flow over a 2D cavity enters the state of the self-sustained oscillations if no control has been applied. Simultaneous injection and suction near the upper corners of the front and rear cavity walls were applied to reduce the oscillations. It was shown that when the injection/suction level was above a certain threshold value, the oscillations were ultimately completely attenuated, whereas when the injection/suction was below the threshold the oscillation process was hardly affected by the control.

The next step of the research project was to simulate isolated primary planar jet. The main emphasis was put on the effect of the shape of the inflow velocity profile on the jet evolution. The results demonstrated that the jet evolution depended on the degree to which the flow in the nozzle had developed. In the case of well-developed profiles, the symmetrical mode dominated the flow close to the nozzle exit, but the antisymmetrical mode developed and dominated further downstream leading to a clearly observed sinuous distortion of the potential core. A symmetrical mode, resulting in a jet 'puffing' prevailed in the case of undeveloped profiles.

Keywords: fluid shear flow, numerical simulation, flow control and instability, transition to turbulence

Dynamical behaviours and bifurcations in noninvertible maps of the plane and of the space

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Abstract:

Going directly to the subject of our presentation, it deals with the dynamic behaviour occurring in one- and two-dimensional discrete dynamical systems, smooth, piecewise smooth and piecewise linear, coming from several applications. We study different kinds of attractors and related bifurcations, both in the phase space and in the parameter space.

Our presentation starts with an introduction of some basic notions of dynamical systems theory, namely, we explain what is dynamical system, attractor, bifurcation and some other terms.

With some more details, two directions of our research can be distinguished:

(1) The first one is related to so-called border-collision bifurcation occurring in piecewise smooth dynamical systems (the systems which in several regions of the phase space are defined by different functions). Border-collision bifurcation may occur when an attractor collides with a border line separating the regions of different definition of the function. This subject is of top interest now, due to numerous applications of piecewise smooth systems, recently reported, in various fields of science, such as engineering, electronics, medicine, economics and others.

(2) The second direction of the research is related to the investigation of dynamics of applied models coming from economics, which are so-called business cycle models. This class of models is represented by two-dimensional noninvertible piecewise linear, or smooth, maps. It is already well known that the main bifurcation scenario which can be realized considering a business cycle model in a dynamic context is related to a fixed point losing stability with a pair of complex-conjugate eigenvalues. In the case in which such a model is discrete and defined by some smooth nonlinear functions, the Neimark-Sacker bifurcation theorem can be used. While for piecewise linear, or piecewise smooth, functions which are also quite often used for business cycle modelling, the bifurcation theory is much less developed. We describe a so-called centre bifurcation occurring in a family of two-dimensional piecewise linear maps whose dynamic properties are, to our knowledge, not well known.

Keywords: Nonlinear dynamical systems; Noninvertible maps; Business cycle model; Attractor; Bifurcation

Hypogean atmosphere as a natural reservoir of CO_2 during one complete annual cycle of continuous monitoring

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Abstract:

On the bases of the results of the automatic continuous monitoring system with eight environmental sensors (rainfall, inner air temperature and humidity, exterior temperature and humidity, atmospheric pressure, CO_2) it was found that:

1) Castanar de Ibor cave (Cáceres, Spain) is a natural reservoir all year around of CO_2. The annual average concentration of both gases are 3 226 ppm and 31 891 Bq/m^3 respectively. These are much higher values than the one found in the majority of the other caves, which indicates a very low interchange between atmospheres. This agrees with the high thermal-hygrometric stability. The thermal oscillation during the year is only 0.09ºC while the air is saturated in water with relative humidity of 100%. The exterior atmosphere has an annual thermal oscillation of 40ºC.

2) The dripping water can cause inner air temperature oscillations 0.06ºC (more than one half of the annual variation of the temperature).

3) The CO_2 and ^{222}Rn gases have higher concentrations during the winter and slightly lower in the summer. This pattern can be explained based on the role of water that isolates the cavity by filling the rock porous system (fractures and connected porosity). During the summer, the dryness of soil and rock layer causes the partial opening of the porous system and consequently the outgasing of the CO_2 and ^{222}Rn from the cavity. During the winter, the infiltration water, charged with CO_2 from the soil, favours the recharge of the cave atmosphere and its downward movement the water seals the host rock. Thus there is not outgasing with the increase of ^{222}Rn and CO_2 as a result.

4) In contrast to what is generally accepted, the gradient of temperature between the two atmospheres and atmospheric pressure variations is not enough to model this hypogean atmosphere.

Besides the importance of the results presented here for the environmental conservation of hypogean monuments, they can also give some insight concerning the actual subject of global budget of atmospheric CO_2.

Keywords: hypogean atmosphere, cave, radon, carbon dioxide

Improving media recommendation algorithms by exploiting relationships in usage and domain data

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Abstract:

With the steadily increasing amount of media items available through content distributors as well as directly stored on consumer electronics devices, personalized recommendation functionalities are increasingly being used to guide consumers in their selection and help them make their choices.

However, current recommendation algorithms perform sub-optimally as far as the accuracy of given recommendations and the portion of a given media collection they can produce recommendations for are concerned. We show the underlying causes for these problems in current recommendation approaches, and we outline our approach to reducing the problems by exploiting relationships in usage and domain data. We furthermore show why the performance of recommendation systems cannot be assessed purely based on comparative evaluations using test datasets. Realistic user tests are necessary in order to identify the real-world characteristics of recommendation algorithms, and measure their performance as perceived by the user.

Keywords: Digital media; Recommendation systems; Machine learning; User modelling

Substantive fairness and comparative evaluation in plea bargain decision making

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Abstract:

Defendant's willingness to accept plea bargain offer is significantly affected by the substantive fairness and comparative evaluation of the bargain, even when these variables are irrelevant to the expected outcome of trial. In Study 1, participants' willingness to accept offers increased with culpability, while Study 2 participants showed self-serving assessments of plea offer fairness. Study 3 revealed substantively fair outcomes serve as reference points that generate gain and loss frames and shape risk attitudes in plea choice. Study 4 showed how the comparative evaluation of offers impacts their rate of acceptance. Finally, study 5 found that, when both are present, substantive fairness and comparative evaluation generate independent main effects on plea acceptance but do not interact. The implications of these findings for the legal plea bargaining debate are discussed.

Keywords: Decision making; Law; Fairness; Egocentric bias; Prospect theory

How to strengthen the European Research Area: Lessons from a Marie Curie fellowship exploiting the use of molecular tools to study natural pest control

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Abstract:

This Marie-Curie Fellowship brought together a young researcher from the University of Innsbruck, Austria, and a leading scientist based at Cardiff University, UK, to assess the role of natural enemy biodiversity in sustainable pest control. Both scientists have specialised in the development of novel molecular approaches to the study of trophic relationships, allowing unique insights to be acquired into predator-prey interactions. This research will help to maximise the benefit arising from the exploitation of natural regulatory mechanisms and to create new approaches to sustainable land use.

The development of scientific skills in an outstanding academic environment, getting an inside view of how research is organised in one of Great Britain's leading Universities, and networking with scientists for future collaborations, are seen as highly rewarding aspects of this fellowship. Furthermore, the current project highlights that complex scientific questions can be tackled most successfully when expertise from various European researchers is brought together. Thus, besides providing the opportunity to participate in mobility programs, ample funding opportunities should be provided on a European level for high-quality research projects to establish long-term scientific collaboration between European researchers. Only when these issues are taken into account and brought into action will European researchers be released form their countries' boundaries and a European research area be created, pushing Europe's science to the forefront internationally.

Keywords: Sustainable land use; Molecular ecology; Researcher mobility; Research careers; European Research Area

Computer-based Learning and Research Support Environments

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Abstract:

The relationship between research and learning is strong: Research is in part learning in an uncharted domain.

There is as yet no widely-applicable computer-based virtual environment that comprehensively supports learning and research by individuals and groups. However, various computer-based virtual environments exist, and they support some of the activities involved in learning and research. It is inevitable that comprehensive support environments will start to be constructed.

As an outgrowth of the presenter's research into personal learning environments, this presentation is concerned with the nature of research as an individual activity, as a collaborative activity, and as a learning activity. A multidimensional space within which virtual support environments may be categorized will be described, and a few web-based tools and examples will be demonstrated.

Attendees will be encouraged to make the presenter think 'on his feet' as to how their research needs might be supported by future computational systems.

Keywords: Learning support systems, research support systems, virtual environments, ICT

The hormonal effects of cumulative partial sleep deprivation in healthy young men

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Abstract:

Cumulative partial sleep deprivation has been shown to impair many physiological functions. The current study shows the effects of sleep restricted to 4 hours per night on stress hormones (NPY, cortisol, and testosterone) and on CRP and Homocystein (two cardiovascular risk factors) in healthy young men.

After 2 nights of normal 8 hour sleep, sleep of 15 young and healthy male subjects (mean age 22.9 yrs) was restricted to 4 hours during 5 nights. Hereafter, 2 nights of 8 hour recovery sleep were allowed. Blood samples were obtained at 08.00 AM after the first 2 nights of normal sleep (baseline), after 5 nights of restricted sleep (sleep deprived), and after 2 nights of recovery sleep (recovery). Blood samples were analysed for CRP, testosterone, and homocystein. Salivary samples for cortisol analysis were taken 10 times, and for NPY analysis 8 times on each of the 3 profile days (baseline, sleep deprived, and recovery).

Cortisol levels were not affected by sleep deprivation or subsequent recovery sleep. NPY and testosterone levels tended to decrease after sleep deprivation, but the effect was not significant. CRP levels started to increase modestly during the sleep deprivation and increased even further after recovery sleep ($p < 0.05$). Homocystein levels tended to increase as well after sleep deprivation, with a partial decrease again towards baseline levels after recovery sleep.

The serum concentrations of CRP and homocystein, 2 well established cardiovascular risk factors, were increased after 5 days of partial, cumulative sleep loss. Moreover, the CRP level continued to increase during the recovery period, indicating that a recovery period of 2 nights is not sufficient for full restoration from the effects of 5 days sleep restriction. The results also suggest that sleep deprived subjects may be at a higher cardiovascular risk.

Keywords: Sleep; Sleep deprivation; Stress hormones; Partial sleep deprivation; Cardiovascular risk

What to do with the soft heart of strong elementary particle collisions?

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Abstract:

The strong interaction, which binds the building blocks of atomic nuclei, is the most predominant interaction type in the Universe. It acts in the core of stars driving their energy production, and transforms nuclei to build up our present world. Few microseconds after the "Big Bang" the strong interaction dominated the evolution of the then very hot and dense Universe.

For half a century up to today, understanding the nature of the strong interaction has been one of the key issues of fundamental physics research, identifying the substructure of all strongly interacting elementary particles (hadrons) in form of confined quarks and gluons. The underlying theory, Quantum Chromodynamics (QCD), explains why the true nature of these constituents can only be revealed when they receive a high momentum transfer in a minute fraction of all the interactions.

In the dominant "soft" processes hadrons seem to act with all their components coherently - with a dynamics uncalculable from QCD. It is therefore an experimental challenge to constrain the large number of proposed approximations to QCD.

This presentation concerns the NA49 experiment at the CERN which covers the complete range of hadronic collisions, from the most elementary hadron+hadron via hadron+nucleus to nucleus+nucleus interactions. It will be demonstrated how model-independent information can be built up using these possibilities, allowing a detailed phenomenological understanding even in the absence of reliable theoretical predictivity.

Keywords: Particle physics; Nuclear physics; Strong interaction; Hadrons

Experimental and numerical investigation of fracture mechanisms and fracture properties of wood at varying moisture contents

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Abstract:

Changes in the fracture characteristics and fracture patterns of wood are experimentally and numerically evaluated and discussed. Four different wood species were chosen for the experimental programme to reveal the mechanisms of moisture transfer in softwoods and hardwoods when subjected to opening mode I fracture. Moisture contents chosen were 6, 12, 18 and 30 percent, to represent the full humidity range. Fracture mechanisms were investigated throughout the *in-situ* ESEM experiments, while fracture toughness and fracture energy were evaluated in *ex-situ* wedge-splitting tests.

The findings of the experimental programme confirmed that there exist distinct changes in the fracture behaviour, with moisture content being one of the most important parameters for fracture mechanisms. In green conditions, wood can be regarded as a poroelastic fluid-saturated media. It has been evidenced that the crack tip remains free of water in the lumens. At the next level of moisture content of 18 percent, only bound water is present in the wood cell walls, with diffusion as a main moisture transport mechanism. As wood dries to the in-service level of 12 percent and down to 6 percent, shrinkage is the main process that can affect the fracture pattern and fracture mechanism.

Differences in the fracture mechanisms were captured numerically using the lattice fracture model. It takes into account wood inherent heterogeneities through Monte-Carlo simulation of elastic and strength properties, assigned to finite element mesh. Lattice fracture model enables mimicking of fracture patterns in wedge-splitting samples, as well as simulation of load-deformation responses. The analysis showed good agreement between the experimental and numerical results.

Keywords: Wood; Moisture; Fracture; Damage; Mechanisms

Evaporative cooling of a magnetically guided atomic beam

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Abstract:

We report on the experimental implementation of the evaporative cooling of a magnetically guided atomic beam. A non-degenerate, but already slow and cold beam of particles, is injected into a magnetic guide where transverse evaporation takes place. In our experiment, $7x10^9$ atoms per second propagate in a magnetic guide with a temperature around 550 μK, at an initial velocity of 90 cm/s. The magnetic guide provides a transverse gradient of 800G/cm. The relatively high collision rate 5 s^{-1} has allowed us to start forced evaporative cooling of the beam to demonstrate a ten-fold increase of the on-axis phase space density. This ten-fold increase brings the phase-space density of the beam at about $2x10^{-7}$. In addition, we have recently implemented evaporative cooling by the adsorption of the most energetic atoms on a ceramic surface. We use a transverse magnetic field to shift locally the beam towards the surface, where atoms are selectively evaporated. With a 5 mm long ceramic piece, we gain a factor 1.5±0.2 on the phase space density. Our results are consistent with a 100% efficiency of this evaporation process. The flexible implementation that we have demonstrated, combined with the very local action of the evaporation zone, makes this method particularly suited for the evaporative cooling of a beam.

Keywords: Evaporative cooling; Magnetically guided beam; Phase space density

MRI-based visualisation and quantification of moisture migration in multicomponent food systems

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Abstract:

Moisture migration between components with different water activity is an important issue in the preservation of food quality during storage and/or preparation. Magnetic Resonance Imaging (MRI) is ideally suited for non-invasive imaging of water, and has found a broad range of applications in different areas. Appropriate choice of the MRI measurement method allows the visualisation of water migration in real time and the recognition of different transport mechanisms.

The aim of this work was to use MRI for monitoring redistribution of water in food systems comprising of phases with contrasting water activity (Aw). SPI and RARE measurement methods were used to monitor water redistribution in cracker shells with moist filling and soup inclusions in water. In the first case, slow migration was monitored for 2 months with time resolution in the order of days. In the second case, a fast hydration time resolution (in minutes) was achieved. 3D images with sub-millimetre resolution allowed visualisation of the time dependence of spatial redistribution of moisture during migration, the quantification of its speed and the extent of matrix swelling.

In order to understand the role of different transport mechanisms, a model system comprising of a hydrated gel phase in contact with an initially dry cereal-based solid matrix, was monitored for 3 days. In this case, SPI was used to visualise low and high hydration regimes. Swelling of the carbohydrate matrix as well as progress of migration through the gas phase were assessed.

The obtained results can be used for validating models for prediction of water redistribution in multiple phase systems in a quantitative manner.

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Keywords: MRI; Moisture migration; Multicomponent food

Purification of α-olefins from Fischer-Tropsch process using reactive extractive distillation

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Abstract:

The Fischer-Tropsch process poses an interesting possibility for the production of α-olefins. Many different chain lengths can be produced from a relative cheap feedstock. However, their purification is not so straightforward because many olefin isomers are co-produced which have very similar physical properties (boiling point etc.). Industrially it would be strongly favoured to apply distillation, but this fails because of a low selectivity. However, Reactive Extractive Distillation, which uses reactive solvents based on transition metal-ligand complexes, can purify the α-olefin from the other olefin isomers. The metal-ions reversibly react with olefins and the selectivity depends on the olefin structure. The ligands, organic molecules capable of reacting with metal ions, are derived from ligands developed and commercially applied in hydrometallurgy.

The feasibility of the proposed concept is evaluated by analysis of the hexene complexation behaviour in vapour-liquid systems with the developed solvents. The reaction stoichiometry and the effects of pressure, solvent and olefin concentration and temperature were all evaluated. The effect of ligand structure is determined by testing different functional groups and sizes of the organic tail. A simple equilibrium model is used to interpret the results and make a conceptual design for the Reactive Extractive Distillation process.

Various commercial metal extractants were tested and it was observed that their interaction with silver was either insufficient to stabilise silver or too strong such that the silver was not able to complex the olefin any longer. However, some ligands were identified that bond silver with an intermediate strength like D2EHPA (a phosphoric acid) and DNNSA (a sulphonic acid). Decreasing the size of hydrocarbon tail of D2EHPA and DNNSA showed that it is possible to increase the selectivity for 1-hexene over its isomers from around 1.0 without solvent to > 1.3 in the presence of a reactive solvent. It is estimated that the number of equilibrium stages inside a distillation column can be decreased from over 500 to 80 and produce 1-hexene at a commercial purity.

Keywords: 1-hexene; olefin isomers; Reactive extractive distillation; Purification; Separation; Extraction

Design and optimisation of process utility systems

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Abstract:

In process industry, the costs of utilities, such as heating, cooling and power, hold an important proportion of the total cost. Utility systems design is one of the most interesting topics in process engineering. Due to the complexity of equipment networks and operating conditions, it is still a challenging task to develop and optimise utility systems under the real industrial conditions, although many researches have been done in this field.

Under variable conditions, such as different electric power prices between peak and peak off time, changing load in batch processes and variable ambient temperature, several operating scenarios must be proposed. There exists a short period in which utility system transform from one scenario to another.

In this report, transient behaviour of utility systems is studied. Firstly, operating scenarios of an existing utility system are obtained from steady state models. Secondly, dynamic models are investigated for transient period simulation. Finally, transient behaviour of the utility system is examined based on dynamic modelling and simulation.

Transient research will be applied to check the feasibility of utility system design and optimisation. A successful design must satisfy the steam and power constraints in transient period. Transient period length analysis can help to identify the flexibility and stability of utility systems.

Keywords: Site utility systems; Transient behaviours