Abstracts of Poster Presentations

Microbial communities forming green-coloured spots in tombs of the Necropolis of Carmona (Seville, Spain)

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Abstract:

The microbial colonization of masonry and historic wall painting by fungi, algae and bacteria is a known phenomenon. In many cases, this colonization induces deterioration processes that lead to structural or aesthetic damage. The Roman Necropolis of Carmona (Seville, Spain) represents one of the most significant burying sites in Southern Spain used during the 1st and 2nd centuries A.D. Some of these tombs show colonization by microbial communities.

Both molecular and culturing techniques were used in this study to analyse the microbial biodiversity with an approach to the functionality of the microorganisms. Molecular methods aimed to the detection of microorganisms from DNA and RNA directly extracted from samples collected at the tombs and did not require the culture of microorganisms. The experimental protocol included PCR amplification of genes encoding the small subunit of rRNA of bacteria (16S rDNA), genetic fingerprinting by denaturing gradient gel electrophoresis (DGGE), construction of 16S rDNA clone libraries, and comparative phylogenetic sequence analyses.

The bacterial communities of two green-pigmented biofilms sampled from tombs of the Necropolis of Carmona were studied. One of these biofilms contained bacteria phylogenetically related to the Proteobacteria (41%), Actinobacteria (25%), Cyanobacteria (18%) and Firmicutes (16%). The nearest phylogenetic relatives of bacteria from the second green-pigmented biofilm were members of the Proteobacteria (41%), Cyanobacteria (35%), Actinobacteria (6%), Fibrobacteres/ Acidobacterias (6%), Nitrospirae (6%) and Bacteroidetes (6%). The majority of sequences obtained from the bacterial communities of the investigated green biofilms presented homology to so far uncultured microorganisms.

The present study represents a significant step forward to understand the biodeterioration at the Necropolis of Carmona tombs by providing information on the microorganisms thriving at this historical and cultural site.

Keywords: Cultural heritage, Microbial diversity, Biodeterioration

Auto-ignition of n-heptane/toluene mixtures at high pressures modelled with detailed chemical kinetics

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Abstract:

Homogeneous Charge Compression Ignition (HCCI) offers the potential of simultaneously increasing fuel efficiency in internal engines as well as reducing harmful emissions such as NOx and particulate matter. Many HCCI combustion strategies have been studied by various investigators and included in these studies are efforts to develop and improve detailed chemical mechanisms suitable for modelling HCCI combustion.

Gasoline is a particularly attractive fuel because of its well-established infrastructure. Compared to single components, however, a distillate fuel such as gasoline offers the additional complexities of having a near continuous spectrum of hydrocarbon constituents. In these cases it is beneficial to employ a surrogate fuel with a finite number of components and a standard composition to analyze detailed chemical models.

In this work a surrogate gasoline kinetic model has been developed for a fuel mixture consisting of n-heptane and toluene with starting net mechanisms for each fuel component retrieved from the literature. The kinetic model for the mixture has been validated against new high-pressure shock tube ignition delay time data with a fuel mixture consisting of n-heptane 35% and toluene 65% by liquid volume.

Also, a single zone engine model has been used to evaluate how well the mechanism captures auto-ignition behaviour for conditions corresponding to homogeneous charge compression ignition (HCCI) engine combustion and the model can qualitatively predict the actual point at which auto-ignition occurs. In addition, the model can predict the relative ignition crank angle decrease when the n-heptane content is increased to from 36 to 50% by liquid volume.

Keywords: HCCI; Toluene reference fuels; Auto-ignition; Fuel chemistry; Chemical kinetics

Branching ratios for the dissociative recombination of hydrocarbon ions

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Abstract:

In a recent series of measurements[1-3] at the ASTRID storage ring in Aarhus, Denmark, branching ratios for the dissociative recombination of hydrocarbon ions with the general formula C2H3+, C3Hm+ (m=1-8) and C4Hm+ (m=1-9) have been measured. A grid-detector technique was used to distinguish the final channels of the reactions. The detector used did not have sufficient energy resolution to distinguish hydrogen atoms either free or attached to carbon atoms so the measurements determined the relative distributions of carbon atoms among the dissociation products. For most of the ions that were in linear isomeric form, the fragmentation patterns were predictable from the structure of the parent ion. For cyclic isomers however, this was not so clear and indications are that ring opening occurs prior to dissociation. Results obtained for C2H3+ and C3H7+ are in excellent agreement with measurements performed at CRYRING[4, 5].

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Keywords: Dissociative recombination; Hydrocarbons; Branching ratios; Storage ring

ESPResSo: Extensible simulation package for research on soft matter systems

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Abstract:

We present the Molecular dynamics simulation package ESPResSo. It has been designed to be a flexible and extensible simulation code which allows a broad range of applications in for example polymer science, biophysics, solid state physics or chemistry. ESPResSo is a parallel code which contains many state-of-the-art algorithms, especially for the calculation of long ranged interactions, and can be used for the simulation of systems with millions of particles, as well as for small scale simulations on a single workstation. The code is published under the terms of the GPL and is currently used in more than 30 international institutions. See also http://www.espresso.mpg.de for more information.

Keywords: Simulation; Molecular dynamics

Production of microbial protein using activated suspension technique (AST) in indoor tanks

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Abstract:

Microbial protein is generated in the ponds when organic matter is decomposed by microbial organisms such as bacteria and protozoa under aerobic conditions. Both aerobic and anaerobic conditions coexist in aquaculture ponds at the sediment-water interface. A large accumulation of organic matter in pond bottoms increases oxygen demand and favours the development of anaerobic decomposition which decreases the bacterial cell yields per unit substrates along with producing unwanted gases like methane and ammonia. Activated suspension technique (AST) is one of the practical solutions to avoid reducing conditions by which continual aeration is done to mix the organic matter throughout the water column and allow aerobic decomposition. However, the decomposition process is greatly influenced by the carbon to nitrogen ratio (C:N) of the substrates. The adjustment of the C:N ratio can be done by manipulation of the C:N ratio in feed and/or application of carbonaceous substrates to the system. Preliminary results indicate that application of low quality fish feed (higher C:N ratio) resulted in high quality microbial food in AST system.

The present research is designed to investigate the possibility of producing microbial protein in indoor tanks by manipulating C:N ratio. Different level of protein feed are applied to the tanks in tropical aquarium laboratory of the institute of Aquaculture. The daily feed application rates are similar to application rates used in intensive fish tanks. Carbohydrate is also applied to the tanks to keep total ammonia nitrogen (TAN) level below 1 mg l^{-1}. Continuous aeration and mixing is done to keep organic matter circulating in the water column and to maintain at least 5 mg l^{-1} dissolved oxygen (DO). Efforts will be made to answer the following research questions after the completion of the experiment.

1. How longer does it take to develop mature microbial flocs under different level of protein fed systems?

2. How much increased flocs can be developed and how much ammonia can be reduced by adding CHO in a low and high protein fed system?

3. Are there any effects of protein levels on water quality?

4. What is the nutritive value of microbial flocs?

Once the mature flocs develop, warm water fish tilapia will be stocked to study their growth and welfare in activated suspension systems.

Keywords: Microbial flocs; Activated suspension technique; Aquaculture; Tilapia

Polynuclear luminescent complexes for photonics applications

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Abstract:

Luminescent lanthanide complexes have fascinating optical properties which make them largely technologically used in lighting devices (luminescent lamps, emitting diodes), optical fibres and amplifiers, television and computer displays, lasers, in fluoroimmunoassay and fluorescence microscopy. Recently there has developed interest in the photophysical properties of lanthanide complexes which are luminescent in the near-IR region, such as ytterbium(III), neodymium(III), praseodymium(III) and erbium(III), in their potential for medical applications, in particular for cancer detection. Unfortunately, lanthanide ions themselves do not absorb light effectively because the relevant f-f transitions are theoretically forbidden. This often means that they require to be bound to a sensitising molecule (organic ligands or transition metal complexes) in order for them to be effectively used as luminescent probes.

In the proposed study using the different synthetic approaches we are preparing new dinuclear (and larger) molecular complexes and solid-state coordination polymers which combine a strongly-absorbing d-block unit (e.g. cyanometallates, or complexes with peripheral carboxylate units) with a near-infrared luminescent lanthanide unit. We will thoroughly investigate their physico-chemical properties (structural, optical and others). The results will provide an in-depth understanding of the detailed interactions in these new species and will be a major step forward in the rational design of new near-infrared luminescent molecules and solid-state materials, for use in applications as diverse a biological sensing and opto-electronic devices.

Keywords: Lanthanide; Luminescence; Energy-transfer; Polynuclear complexes; Crystallography

Development of new target prototypes for the production of radioactive ion beams at CERN

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Abstract:

CERN (European Organization for Nuclear Research) is the world's largest particle physics laboratory. Cancer therapy, medical and industrial imaging, radiation processing, electronics, measuring instruments, new manufacturing processes and materials, the World Wide Web, these are just some of the many subject areas to which CERN has made major contributions as a spin-off of research in particle physics.

ISOLDE (Isotope Separator On Line), is a long-standing experiment at CERN illustrating the use of a variety of technologies. It consists in producing radioactive nuclides for nuclear physics, astrophysics and medical applications. Radio isotopes are produced by the interaction of particles accelerated in the CERN particle accelerator complex onto serious solid refractory materials so called "targets". They are extracted under vacuum and at high temperatures, purified, ionized and delivered as intense beams for various experiments. The target and ion source units are therefore a central part for the production of these beams.

The Marie Curie fellowship undertaken at CERN consists in being a part of the R&D team designing targets/ion source prototypes at ISOLDE.

This is a multidisciplinary experimental activity which involves nuclear physics, radiochemistry, material science, surface physics. A few examples of prototypes developed and successfully tested will be presented.

Keywords: Particle Physics; Ion sources; Radioactive beams; Isotopes

Data acquisition for the CMS experiment

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Abstract:

The CMS experiment will study proton-proton collisions at CERN's new collider facility, the Large Hadron Collider (LHC). The LHC will allow the exploitation of physics in a unprecedented energy range, giving access to the production of new heavy particles (e.g. the Higgs particle) and new phenomena (e.g. Supersymmetry).

The experiment is carried out by a large international collaboration.

At present about 2000 scientists from 164 institutes and research laboratories from 36 countries are involved in the CMS collaboration.

At the LHC, the proton beams cross each other 40,000,000 times each second. At the highest LHC beam intensities, there will be roughly 25 proton-proton collisions for each crossing. Recording all the information from these collisions in the CMS experiment, requires, for every second of operation, the equivalent of 10,000 Encyclopaedia Britannica.

The task of the Trigger and Data Acquisition System is to select, out of these millions of events, the most interesting 100 or so per second, and then store them for further analysis.

The central DAQ team is responsible for delivering the hardware and software to acquire data from sub-detectors, DAQ system and assemble, monitor and record the event data. This involves custom hardware and commercial computer and networking equipment. The software is mainly written is C++ and Java and requires expertise in system programming, networking, web applications, databases and GUI technologies.

Keywords: Data acquisition; CMS; LHC

Semi-automatic home video editing

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Abstract:

In recent years the use of camcorders for recording personal experiences increased strongly. More and more users shoot videos of their experiences, but this raw material is rarely watched again; most of the times the captured video documents appear boring and have low aesthetic quality.

Video editing could help, but current tools are too complicated for the average user. Fully automatic solutions have been presented in recent years and are appearing on the market. These automatic video editing tools, however, do not allow users to tailor the final result to their own style and wishes.

This project aims at developing new solutions for home video editing to overcome these problems. While editing home videos, users should not be aware of complicated technical details like shot cuts, transitions or video effects. At the same time users should be able to efficiently interact with the system in order to get the desired final result.

Our goal is to develop a video editing system that automates a wide set of professional movie-making rules (or film grammar rules) and low level video editing operations. Additionally the interaction with the system should be based on high-level concepts, such as mood, style, characters, locations, and scene semantics.

Multimedia content analysis algorithms are researched to achieve automatic understanding of structural and semantic concepts of the video documents.

We are following a user-centred design in which ease-of-use is a key requirement. Our video editing solution should be effective and at the same time as simple to use as a TV remote control. For this purpose novel interaction concepts are tested with user experiments.

Keywords: Video editing; Home video; User-centred design

DMLX Software, the languages of Spain and the linguistic normalisation programs

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Abstract:

Our goals are to assess quantitatively to what extent programs of "linguistic normalisation" of Catalan, Basque and Galician in six Autonomous Communities in Spain have succeeded in restoring both competence and usage in these languages, and to project future trends using new demolinguistic software. The near-simultaneous introduction of normalisation programs in the 1980s in six parallel but distinct contexts provides us with a natural laboratory in which many of the historical and social variables that might affect success are controlled, and where comparable data are collected by the same instruments - the census and other official surveys.

We draw on the language questions in the 1991 and 2001 censuses to analyse the dynamics of linguistic competence and on comparable sample surveys in the six communities to study context-dependent usage. The demographic projections of our web-based program DMLX incorporate formal models of L1 transmission, school acquisition and linguistic integration of immigrants. On the usage side, we model the specific connection of these processes with a range of private and public interactions.

Our analysis discerns distinctive change tendencies in competence and patterns of usage in each community. The differences between projections based on the 1991 census and figures from the 2001 census particularly revealing. We interpret the differences among communities in terms of sociolinguistic, demographic and political factors.

Keywords: Demolinguistic projections; Minority languages; Linguistic revival processes; Knowledge and language use; Catalan, Basque and Galician

Akt improves Ca^{2+} handling and contractility in cardiomyocytes by phosphorylating key Ca^{2+}-handling molecules at CaMKIIδ-specific sites

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Abstract:

The proposed studies aim to address a relevant problem of cardiac biology, that is, how to modulate cardiac function by targeting pathways alternative to the b-adrenergic receptor pathway in the normal and disease states. In recent years, it has been demonstrated that by modulating Ca^{2+} handling at the cellular sarcoplasmic reticulum level, it is possible to significantly improve cardiac function in normal and heart failure settings. Cardiomyocytes (CMCs) adapt to physical stress by increasing cell size while maintaining cell function ("physiological" hypertrophy). This is in contrast to maladaptation, in which the increase in cell size is not accompanied by maintenance of cardiac function. The biochemical pathways involved in "physiological" hypertrophy are beginning to be unraveled, and the protein kinase Akt seems to be among the key molecules of this process. We found that Akt has a profound effect on cardiac function and it does so by phosphorylating critical regulators of intracellular Ca^{2+}. The insulin-like IGF-1 pathway, in which Akt is involved, appears to be critical in determining the type of cardiac hypertrophy that occurs in athletes during physical training. We believe that our data have already contributed to understanding some of the molecular aspects of this "physiologic hypertrophy", characterized by increased left ventricular wall thickness, increased LV cavity diameter and increased cardiac function. In previous studies, we and others showed that Akt overexpression increases CMC size and improves cardiac function in transgenic (Tg) mice. Moreover, we showed that Akt overexpression increases myocardial inotropism and lusitropism at the cellular level and demonstrated indirectly that Akt improves sarcoplasmic reticulum Ca^{2+} uptake compartimentalization. In addition, forced expression of active Akt in the heart has been associated with improved angiogenesis through the activation of S6 kinase. Thus, Akt overexpression may be a promising therapeutic tool for heart failure.

In the present study, we further investigate the molecular mechanisms of Akt's action on Ca^{2+} handling. We show that Akt overexpression causes phosphorylation of two key Ca^{2+} handling proteins, phospholamban (PLB) and the ryanodine receptor 2a (RyR), at their Ca^{2+}-calmodulin dependent kinase IId (CAMKIId) site, but not at the protein kinase A (PKA) site. Moreover, direct phosphorylation of PLB by Akt at the CAMKIId site is shown to increase SR-Ca^{2+} uptake using biochemical assays *in vitro*. This result is further proved by the effects of an active Akt mutant directed specifically to the SR, which induces PLB phosphorylation and increases SR Ca^{2+} uptake, without causing hypertrophy in cultured CMCs. Thus, we demonstrate a new mechanism through which Akt overexpression improves Ca^{2+} handling and myocardial contractility by direct phosphorylation of PLB and RyR2.

Acknowledgment: This research was in part supported by a *Marie Curie International Fellowship* within the 6th European Framework Program, by grants from the Italian Ministry of Research and Education, the Italian Ministry of Health and from the National Institutes of Health.

Keywords: cardiomyocytes, hypertrophy, calcium handling, akt, phospholamban

Low grade brain edema is not involved in the motor alterations observed during the early stages of encephalopathy in the hepatic devascularized rat

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Abstract:

Hepatic encephalopathy (HE) associated with liver failure includes neurological symptoms ranging from alterations of the motor function to coma. It has been demonstrated that cirrhotic patients present increased conduction time and decreased amplitude of the motor evoked potentials. These alterations were proposed to be the consequence of a low grade cellular edema along the cortico-spinal tract. In order to assess this hypothesis, we evaluated the motor function of rats with acute liver failure (ALF) induced by hepatic devascularization at different grades of HE and after mannitol injections at early stages of the encephalopathy.

Both latency and amplitude of the motor evoked potentials were respectively significantly increased and decreased ($p<0.05$) at early stages of the encephalopathy (after 6 hours of liver ischemia) when no neurological symptoms or brain edema were detectable. Mannitol injections performed 6 hours after liver ischemia significantly reduced brain water content but had no significant effect on the alterations of the motor function.

In conclusion, early stages of encephalopathy induced by ALF reproduced the motor alterations observed in cirrhotic patients. The absence of effect of decreasing brain water content after mannitol injections on motor evoked potentials suggest that low grade brain edema is not involved in the apparition of these motor alterations in hepatic devascularized rats. These results do not support the hypothesis that neuronal dysfunction in HE is secondary to astrocytic edema.

Keywords: Hepatic encephalopathy; Motor evoked potentials; Low grade cerebral edema; Acute liver failure; Mannitol

Experiment control system for LHCb

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Abstract:

LHCb is one of the four detectors being built for large hadron collider (LHC) at CERN. It aims to study rare decays in b-meson systems and precise measurements of CP violation. LHC experiments make use of wide range of hardware with millions of electronic channels for readout, and huge data processing farms. LHCb alone has over 2000 computing nodes running complex software's for data processing. To handle this unprecedented complexity would require a robust experiment control system (ECS) running in distributed environment of over 100 computers.

Slow control system is "sine qua non" to supervise and control changing technical parameters. Control infrastructure should ensure safety for both equipments and personnel.

Sub detector components are categorized into control domains based on their behaviour and functionality. PVSS - a commercial SCADA system tool is widely used by LHC experiments for its cynosure ability to control and monitor both hardware and software. The tools have diverse functionalities for integration with custom software, user interfaces (run control) and data management system. Lack of abstract behaviour modelling, automation mechanisms and error recovery in PVSS is compensated through use of custom developed finite state machine software (FSM). FSM containing state management interface toolkit provides means for allocating states, actions and their transitions for components based on their control domain. FSM and other common software components comes with a framework (JCOP) which provides comprehensive set of tools and guidelines for a homogenous control system, critical to operational and maintenance issues. This integrated ECS will ensure the detector to meet the experimental requirements of LHCb.

Keywords: Automation; Control; Hardware; Monitoring; Software

The York Institute for Tropical Ecosystem Dynamics

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Abstract:

The York Institute for Tropical Ecosystem Dynamics (KITE), a Marie Curie Excellence Centre, has been established in the Environment Department, the University of York UK, following a £1 million award from the European Union. The research cluster will combine new environmental data sets on past environmental change with modelling initiatives to explore past, present and future ecosystem dynamics at a number of sites along the Eastern Arc Mountains of Kenya and Tanzania, an area regarded as one of the world's hotspots of plant biodiversity. At the heart of KITE is the need to link palaeoecology, bioclimatic modelling and research on past human impacts to gain a holistic understanding of vegetation dynamics and biodiversity in the Eastern Arc Mountains. KITE will combine expertise from a number of disciplines to understand how ecosystems respond to climate change. For example, do high levels of biodiversity result from buffering of global climatic changes due to the close proximity of the Indian Ocean monsoon system, or is this a response to high climatic and environmental variability? The research will improve forecasting climate variability impacts on ecosystem functioning, and will lead to an increased scientific understanding for environmental conservation under a changing climate and societal impacts. KITE will develop an international profile for environmental change research at the University of York, and foster new international relationships by encouraging knowledge transfer between Europe and East Africa. Such closer links will be increasingly important as policies on managing the consequences of global climate change move from the national to the international political arena.

Keywords: Africa; Biodiversity; Climate change; Modelling; Palaeoecology; Tanzania

A combined CFD-Experimental approach for the analysis of the agglomeration mechanism in the bayer process

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Abstract:

Aughinish Alumina produces over 1.8 million tonnes per annum of alumina (Al2O3) by treating bauxite ore, using the Bayer process. The Bayer process mainly consists in crushing the beauxite ores and mixing it with a high caustic concentration solution to dissolve the aluminium as sodium aluminates. Both quality and production of alumina are dependent of the precipitation process step of the gibbsite agglomerates. Thus parameters that allow agglomeration during the seeded crystallization of gibbsite (supersaturation, seed charge density, process temperatures and hydrodynamic conditions) have to be well known in order to obtain a robust process that can lead to a constant end quality product. A campaign of experiments and numerical simulations have been undertaken in a crystallizer designed to have, hypothetically, a perfect mixing, where all the particles are in suspension and for which the main hydrodynamic parameter (i.e. power per unit volume) can be defined for scale up. Through a series of numerical simulations of the vessel former described, it has been shown that considering an angular velocity derived from the scale up criteria, it is not possible to achieve a good mixing, and part of the solid phase accumulates at the bottom of the vessel. With the aim of improving the mixing of the solution, without altering the angular velocity, the effect of a draft tube, introduced into the vessel, has been analyzed, both numerically and experimentally.

Keywords: Alumina; Crystallization; Hydrodinamic

Synthesis of charge containing comb-like copolymers and surface-tethered polymeric brushes by controlled radical photopolymerization

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Abstract:

The controlled/living radical polymerization, such as Iniferter[1] and Nitroxide-Mediated Radical Polymerization (NMP)[2] are used for the preparation of polymers possessing well-defined compositions, architectures (linear, branched, comb, stars) and functionalities. These techniques have also potential to be employed for surface modification of solid substrates (silica, gold, glass, iron oxide) by growing polymer chains from a suitable surface immobilized initiators[3].

In the current work, we have used a combination of NMP with dithiocarbamate photoiniferter chemistry for the synthesis of charge containing amphiphilic copolymers with comb-like structure. The photoirradiation of various protected monomers of (meth)acrylic acid (e.g. 2-tetrahydropyranyl methacrylate THPMA, *tert*-butyl acrylate *t*BuA) was started from dithiocarbamylated polystyrene (PS-DC). A purified graft copolymer of PS-*g*-PTHPMA-DC with reactive end group (DC) was subsequently used for chain extension with cationic type monomer, 2-(dimethylamino)ethyl methacrylate (DMAEMA). Selective deprotection of the acid functionality should yield a new type of water soluble zwitterionic polymers with interesting pH - responsive behaviour.

In the second part of this work, we attempted to use iniferter approach for the modification of silica nanoparticles by initiation of controlled polymerization of above mentioned functional monomers from surface anchored DC photoiniferter. Eventual applications of surface-attachted functional polymers include surfactants, adhesion and separation technology, biosurfaces (e.g. artificial implants, cell culture dishes, biosensors, drug delivery vehicles), nonfouling biosurfaces, miroelectronics and many others.

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Keywords: controlled radical polymerization; photoiniferter; comb copolymers; silica nanoparticles; polymer brushes

The use of sonoelectrochemical technology for the preparation of bioactive calcium phosphate coatings on carbon materials

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Abstract:

Bone replacement is often required in patients suffering from bone degeneration, diseases such as cancer, or catastrophic destruction caused trauma.

Carbon is an attractive material in the biomedical field owing to its excellent biocompatibility, good endurance in physiological environments, and a modulus similar to that of bone. However, the bioinert carbon materials cannot directly produce or induce the regeneration of bone tissue when used for bone repair or replacement. The introduction of bioactive coatings, such as calcium phosphate (CaP), is an effective and convenient way to provide carbon material with bioactivation potential. Calcium phosphate ceramics have been demonstrated to have good biocompatibility and osteoconductivity. When implants are used with calcium phosphate coatings, they can combine the mechanical properties of the substrates with the bioactive character of the coating. In the present study, we combined sonochemical technology with electrodeposition, named sonoelectrochemical method, to directly produce uniform bioactive calcium phosphate coatings, with preferable bonding force, on carbon fabric surfaces under mild conditions. Preliminary results show the technique, can generate nano-CaP coatings with an appropriate morphology and structure. Furthermore this method is also feasible for coating other conductive substrates including titanium and its alloys.

Keywords: Biomaterials; Calcium phosphate; Coatings

Study of Spanish baroque paintings by analytical non-destructive techniques

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Abstract:

Baroque paintings (XVI-XVII c) found in artworks like altarpieces, organs and wall paintings, were studied by different characterizations techniques, (more than 100 specimens) to solve technical historical problems to deduce the original appearance and to establish the chemical and physical conditions of restoration and conservation.

The paints as heterogeneous mixtures of organic and inorganic compounds formed complex multi-layers. All the samples were identified by standard SEM technique. Separate layers, pigment particles and organic constituents were visualised well in paint cross sections. The backscattered electrons (BSE) enable a good compositional contrast within the paint layer, because heavy elements with high atomic numbers result in higher electron back scattering than lighter elements. X-ray energy dispersive detector (EDX) supplied a spectrum of the elements in the paint cross-section. Mineral phase composition of the pigment was determined by X-ray diffraction (XRD). FTIR gave information on the distribution of compounds with specific chemical functional groups. For example, carbonates (from pigments or supports) and carbon-hydrogen bonds (derived from binders, oils, or varnishes) can be characterised and localised in paint cross-sections.

All the samples consisted of a multilayered mixture of pigments, binding media and showed a range of colors: white, red, brown, gold. Lead carbonate, green earth, gold, cinnabar and bass were identified by XRD and corroborate the presence of these compounds for EDX. The organic compounds e.g. egg yolk, egg white and animal glue were identified using FT-IR. The information on this painting by FTIR is related to both the inorganic compounds present and to the nature of inorganic binding medium it was identified to be a mixture of protein related to animal glue.

Keywords: Painting; Pigments; XRD; FTIR; SEM/EDX

Schistosome mitochondrial genomes: phylogeny and diagnostics

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Abstract:

Schistosomiasis (also known as Bilharzia) is one of the most important 'neglected diseases' according to the World Health Organization, affecting over 200 million people worldwide. Symptoms include hepatosplenomegaly, colonic polyposis with bloody diarrhea, cystitis, portal hypertension with hematemesis, etc. Several species of schistosomes, the causative agents of the disease, are therefore of considerable medical and veterinary importance. Complete or nearly complete mitochondrial genomes are obtained for *Schistosoma mansoni*, *S. haematobium*, *S. spindale*, *S. guineensis*, *S. incognitum*, *S. japonicum*, *S. mekongi*, *S. malayensis*, *Orientobilharzia turkestanicum* and *Trichobilharzia regentii*.

An independently derived phylogeny of the schistosomatids reveals the patterns of evolutionary change within the mt genomes. Non-Asian *Schistosoma* species are characterized by a unique gene order revealing a split within the *Schistosoma*. Our data show that this gene rearrangement evolved with the speciation of *S. incognitum*, enabling us to clarify different theories for the origin and subsequent radiation and dispersal of the schistosomes providing a better understanding of the evolution, distribution and possible future spread of schistosomes.

Complete mitochondrial genomes allow assessment of the phylogenetic utility and information content of mitochondrial genes, individually and combined, over a broad evolutionary time-scale. Additionally, comparison between genomes indicates regions of high and low sequence variability, thus suggesting genes and gene regions best suited as molecular markers for a variety of purposes such as diagnostics (species, strain and life cycle stage identification) and population genetic analysis (evolution and spread of drug resistance and detection of selection).

Keywords: Bilharzia; *Schistosoma*; Mitochondria; Phylogenetics; Diagnostics

Vibrational study of flavonoids with interest in the cultural heritage

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Abstract:

Paintings and textiles represent an essential part of Cultural Heritage having an important artistic and historical significance. The analysis of organic molecules employed as pigments or dyes is crucial to carry out studies on their conservation. Artworks are in general very complex objects and the organic pigments are often present only in very small quantities thus their study is difficult and a large effort has been devoted to find analytical non-destructive method to allow the *in situ* study of art objects without their destruction.

Vibrational spectroscopy (Raman and infrared [IR] spectroscopy) is a very useful tool for specific identification of molecules with very good spatial resolution. In particular the Surface-enhanced Raman spectroscopy (SERS) technique represented a remarkable improvement in the detection. These pigments are in many cases highly fluorescent, display a relative small Raman cross-section and are practically insoluble in water. All these facts make more difficult their study by normal Raman. SERS technique implies the use of nanostructured Ag or Au surfaces to enhance both the incident and scattered light resulting from the studied molecules.

In this work we present preliminary results derived from the application of SERS and Surface-enhanced Infrared spectroscopy to the flavonoids quercetin, luteolin, apigenin and kaempferol. Flavonoids are organic colouring materials known since the antiquity which have been used traditionally to prepare artist's pigments and textiles dyes. These compounds also have important biological activity. A previous assignation of Raman and IR vibrational spectra of flavonoids was made on the basis of the different position of the –OH groups existing in these molecules. SERS spectra of flavonoids display many differences when compared to normal Raman of solid and solution suggesting that these molecules undergo a clear chemical change upon adsorption on the metal surface. We have found that the chemical degradation depends on the flavonoid structure and it can also be modulated by changing the pH. The laser irradiation line employed as excitation also seems to have an influence in the pigment degradation on the metal surface.

Keywords: Vibrational spectroscopy; Surface-enhanced Raman spectroscopy; Surface-enhanced infrared spectroscopy; Organic pigments; Flavonoids; Cultural heritage

Origin and character of soil organic matter and its usefulness for elucidating anthropogenic and climate-induced landscape alterations in Galicia, NW Spain

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Abstract:

We investigate the soils around the archaeological study site Campolameiro in Galicia, NW Spain, famous for its prehistoric rock art. Early inhabitants have burned the original forests of Galicia multiple times, causing intense erosion episodes. The soils, classified as "cryptopodzolic rankers" contain a vast amount of plant-derived organic matter (OM), and formed upon 6 to 10 ka of erosion and sedimentation. We use the molecular fingerprint of the OM (as measured by pyrolysis-GC/MS) to identify and differentiate between human- and climate-induced landscape alterations. Before doing so, we had to stress that the OM had not been transported in aluminium-OM complexes, a process known as podzolisation.

From a pedological point of view, knowledge on these soils is urgent because (1) their abundance in Europe and beyond is persistently being underestimated, (2) these soils have a large carbon sequestration capacity (global warming), and (3) the process governing its formation is highly enigmatical. We showed that Al-OM complexes prevail, but that these do not migrate within the soil, which contradicts podzolisation. Thus, the pedogenesis of the soils of Campolameiro is in discordance with current hypotheses on similar soils. As a result, we can use the OM composition to reconstruct human-induced vegetation changes (agriculture, forest clearance), taking into account that the rate of OM decomposition and its selectivity is climate-dependant.

We observed a striking and unambiguous relation between charcoal lines (i.e. evidence of vegetation fire), and accelerated erosion and acidification. Forest clearance by use of fire is recognised in the Roman Era but also as early as 6,000 years BP. Currently, Py-GC/MS data are being processed, and preliminary results showed that the polyaromatic hydrocarbons phenanthrene, anthracene and naphthalene are resistant against microbial decomposition, allowing us to use these compounds to further specify the chronology of the burning events.

Ultimately, we expect the OM composition to reveal important information on the environmental circumstances at the moment of production of the rock art.

Keywords: Geoarcheology; Organic matter; Deforestation; Py-GC/MS

Indirect ecological interactions in the rhizosphere

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Abstract:

We are interested in identifying indirect ecological interactions in the rhizosphere: Direct rhizosphere interactions have been studied extensively, but little attention has been given to indirect interactions. We are also interested in soil food webs and their consequences for the composition and structure of plant communities. To examine this, we use a combination of fatty acids signatures of microorganisms, soil animals and plants, as well as detection of 13C isotope ratios as an indicator of trophic levels. Soil microorganisms consume significant amounts of plant assimilated carbon, but this carbon-flow has been difficult to quantify. 13C pulse labelling of fatty acids not only allows us to define C allocation, but to quantify the flow of plant assimilated carbon to microorganisms. We measured the dynamics of the flow of newly assimilated C into AM fungi and rhizosphere bacteria and examined whether this differs between microbial communities from the rhizospheres of plants from different functional groups.

Keywords: Indirect interactions; Rhizosphere; Microorganisms; 13C isotope

Proton beam dynamic study for the high-intensity Linac 4 project

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Abstract:

Linac4 is a new accelerator complex that is under study at CERN. It is designed to accelerate H- to 160 MeV of energy for injection in the existing Proton Synchrotron Booster. The accelerator complex is composed of different accelerating structures: Radio Frequency Quadrupole, Drift Tube Linac, etc. At the transition between structures, a line containing focusing element and buncher cavities adapts the beam to the optimized condition for the next stage of acceleration. If not, we loose efficiency in the acceleration or we loose the beam. The first part of my Marie Curie Fellow is the study of the beam dynamic in the Linac4: I have worked on the dynamic in the Chopping line. It's a device between the RFQ and the DTL. The aim of this device is twofold. Firstly to modify the beam time structure and, secondly, matching to the DTL structure.

The chopper line is composed of 11 quadrupoles, three bunchers and two deflecting plates. I have worked out a solution for transporting the beam with minimum losses, adapting to the next acceleration structure, removing unwanted bunches and controlling the trajectory of the beam.

This poster will present the challenges of designing the line as well as the computer simulation of the full beam of particles performed with three different computer codes: Trace Win, Trac3D and Path Manager.

Keywords: Beam dynamics; Accelerator physics; Particles; Linac; CERN

A search for proteins involved into the pathogenesis of rheumatoid arthritis

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Abstract:

Rheumatoid arthritis (RA) is a chronic autoimmune disease. Certain autoantigens have been implied to contribute to the induction and maintenance of inflammatory reactions against the host tissue(s). Therefore the identification of novel autoantigens in RA appears to be very important for a better understanding of specific disease mechanisms.

SEREX (Serological Analysis of Recombinant cDNA Expression Libraries) is a valuable tool widely used in searching for autoantigens. The method is based on screening gene expression libraries constructed from tissue samples to find potential proteins triggering the production of autoantibodies. We used a modified SEREX method with synovial fluid from RA patient as source of antibodies.

We found numerous novel autoantibodies. There were reports that fibromodulin is a newly defined autoantigen in RA. We were also able to identify decorin, vimentin, aldolase A and eEF1A-1 as autoantigens in RA which have been previously identified to be involved into the immune response in rheumatoid arthritis.

Our results confirm the validity of results obtained using the SEREX system and that the SEREX technique is useful for the identification of novel autoantigens that play a potential role in the pathogenesis of the disease. Such proteins identified as autoantigens might help to better understand the pathophysiology of RA.

Keywords: Rheumatoid Arthritis; autoimmunity; SEREX; autoantigenes

Myristoyl CoA: Protein *n*-myristoyl transferase: A target for structure-aided design in the development of a novel anti-malarial drug

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Abstract:

Malaria, an illness caused by protozoan parasites of the genus *Plasmodium*, continues to be a key global health issue; around 40% of the world's population are at risk and more than 1 million people are killed each year. It is transmitted via bites of infected female mosquitoes (*Anopheles*) and its severest form, *falciparum* malaria, can cause blocked blood vessels, cerebral malaria, coma, and death if left untreated. There are a variety of drugs available to counter malarial infection, however effective malarial treatment is complex due to interweaved factors such as drug resistance and socioeconomic development. We have identified an enzyme from the parasite, myristoyl CoA:protein *N*-myristoyl transferase (NMT), which if inhibited will lead to parasite death. NMT catalyses the co-translational transfer of myristic acid to an N-terminal glycine of certain substrate proteins and it is known that this enzyme is essential for viability of these protozoa. Initial screening using in vitro tests of enzyme activity as well as *P. falciparum* infected erythrocytes has allowed us to identify a series of specific benzothiazole compounds that act as inhibitors of *P. falciparum* NMT. It is known that these benzothiazoles compete with binding of the peptide substrate within the NMT enzyme binding cleft. We are currently following a strategy of structure-based drug design where we will exploit slight differences in the peptide binding pockets of *P. falciparum* and human NMTs to produce selective and potent inhibitors, which we hope will lead to effective new anti-malarial treatments.

Keywords: Malaria; Rational drug design; *Plasmodium falciparum*; *N*-Myristoyl Transferase (NMT); Benzothiazole

Gold nanoparticles on silicon substrate

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Abstract:

Specific applications of bionanotechnology require the controllability of density and distribution of nanoparticles on inorganic surfaces. In order to attach nanoparticles to such substrates, functionalization via self assembly technique is employed. We investigate several approaches to develop self assembled monolayers of 1-mercapto propyl trimetoxy silane (MPTMS) on silicon wafer (100) to immobilise 15nm hydrophilic gold nanoparticles. On the one hand these techniques all involve the same steps (i.e. cleaning and oxidization of the silicon surface, MPTMS silanisation via self-assembly); on the other hand they differ in the chemicals and operative conditions employed. Our AFM data show that the techniques lead to appreciable differences in the quality of the monolayer and consequently in the controllability of the nanoparticle concentration on it. In order to generalize our results, we aim at extending these approaches by varying substrate (e.g. glass) and nanoparticle properties (e.g. size, affinity for solvents).

Keywords: Gold nanoparticle; Self assembly

Advanced study on biofilm systems in waste water

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Abstract:

In the waste water treatment industry, process optimization and performance stabilisation are prime objectives in order to achieve more effective, reliable, and economically feasible treatments of municipal, agricultural, and industrial waste streams. Through improved understanding of general waste water dynamics and from increased knowledge about how microbial community structures in biofilms are affected by waste stream composition and operational conditions, such advances can be realised to great benefit for the environment. Three biofilm reactor systems for waste water treatment have been developed at NUI, Galway, which include a Vertically Moving Biofilm Reactor (VMBR), a Pumped Flow Biofilm Reactor (PFBR), and a Horizontal Flow Biofilm Reactor (HFBR). These different reactor systems have been especially designed for local treatment of small waste streams and demonstrate very good properties for the removal of nitrogen, phosphorus, and organics. The main project aim is to study reactor biofilm dynamics by using a scientific approach that combines advanced microbial techniques. Detailed information about kinetics, micro-scale distribution of chemistry and processes, and microbial community structures in biofilms, will be obtained through the application of microsensors for a broad range of chemical species (e.g. O_2, NO_3^-, and NH_4^+) and through the use of molecular techniques like Fluorescence In-Situ Hybridization (FISH), Polymerase Chain Reaction (PCR), and Denaturizing Gel Gradient Electrophoresis (DGGE). The information gathered from these studies will subsequently be used for process optimization and for the development of advanced models to describe the function of the reactor systems under different operational conditions.

Keywords: Biofilm; Waste water; Microsensors; Molecular analysis

Advanced Laser techniques to Investigate Carbon isotopE discrimination during decomposition: The ALICE project

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Abstract:

Methods involving stable isotopes have been successfully applied since decades for various application fields (astronomy, geology, geochemistry, microbiology, community and ecosystem ecology). Tracing and measuring ^{13}C natural abundance in ecosystem compartments greatly enhanced understanding of the carbon (C) fluxes along food webs and in the plant-soil-atmosphere C exchange when compartments present different C isotopic signatures (i.e. atmospheric CO_2 *vs* photosynthetic leaves, C_3 *vs* C_4; etc.), with minimum disturbances of the system. However, the assumption that no isotopic discrimination occur during respiration is commonly made in numbers of C isotope-based ecological studies (Subke *et al*., 2004). But verifications of such assumption are sparse and not enough reliable.

Stable C isotope experiments currently rely on the conventional isotope ratio mass spectrometry (IRMS) for measuring the ^{13}C abundance. IRMS is, in spite of its high analytical precision, one of the limiting factors for experimental designs, in particular for continuous monitoring in field studies. In these last years laser spectrometry demonstrated to be a valid alternative to IRMS. Based on the fact that CO_2 absorption patterns strongly depend on isotopic substitution, highly sensitive laser spectrometers can be developed in order to measure the $^{13}C/^{12}C$ isotope ratio in gaseous samples containing carbon dioxide. In this context, at the Environmental Science Department, an innovative diode-laser-baser methodology has been recently developed, enabling continuous measurements of both CO_2 concentration and isotopic composition (Gianfrani *et al*., 2004; Castrillo *et al*., 2006). Such potentialities could certainly enlarge the possibilities of experimental settings, thus opening new fields of investigation.

The "ALICE" project, funded by the Marie Curie Fellowship for the Transfer of Knowledge Development Host Scheme, aims to implement an advanced laser spectrometry technology in order to study the isotopic composition and fractionation of respired CO_2 from various substrates and micro-organisms. The final stage of the project will lead to field applications of the laser spectrometer. The expected results from these works will represent a very significant advance in (i) the verification of the assumption of no isotopic fractionation during respiration and (ii) also in measurements that were impossible without the laser spectrometer. The poster presents two experimental settings illustrating these two aspects.

Keywords: ^{13}C; Decomposition; Diode laser spectroscopy; Isotopic fractionation; Leaf litter

Influence of the sterol biosynthesis inhibitor fungicides on the arbuscular mycorrhizal symbiosis

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Abstract:

The majority of agricultural important crop species forms naturally a symbiosis with arbuscular mycorrhizal (AM) fungi. These fungi offer several benefits to the host plant including faster growth, improved nutrition, higher drought resistance, and protection against root pathogens. Both these benefits, and the increased concern for environmental quality, supports the interest of these micro-organisms for management practices in agricultural and horticultural systems. However, the effects on AM fungi of cultural practices, such as the use of fungicide, are not often measured. Repeated doses or soil accumulation of these fungicides could have detrimental effects on plant growth by limiting the functioning of AM symbiosis. Up to date, very little information is available on the effects of fungicides, in particular of the sterol biosynthesis inhibitors (SBI) which are widely used in agriculture, on AM symbiosis. The aim of FUNGIMYC is to assess the impact of SBI fungicides on AM fungi. Based on the ROC (root organ culture) technology three complementary approaches - physiological, biochemical and molecular- will be considered in order to investigate the effects of SBI fungicides on 1) the development of a functional AM symbiosis, 2) the changes in sterol composition and 3) the regulation of gene expression in AM fungi.

Keywords: *Glomus intraradices*; Sterols; SBI fungicides; AM symbiosis

How a voltage regulator device can improve the power quality

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Abstract:

The creation of the European Research Area (ERA) has become the central axis of today's European research policy and also represents the main component of the Lisbon Strategy setting the ambitious goal for the Union to become, by 2010, "the most competitive and dynamic knowledge-based economy in the world, capable of sustainable economic growth with more and better jobs and greater social cohesion". Overall, knowledge stands out as the common reference point and the unifier of the three major areas of activity and investment, which comprise research, education and training, and innovation. It is also the key to industrial competitiveness and employment.

Today, and even more in the knowledge-based society of tomorrow, science and technology have a ubiquitous presence throughout the economy and in everyday life. If they are to realise their full potential in securing a continually increasing quality of life - in the broadest sense - for Europe's citizens, new relations and a more productive dialogue between the scientific community, industrialists, policy-makers and society at large, as well as scientists' critical thinking and responsiveness to societal concerns, will be needed.

In this context, the research project proposed in the framework of European Reintegration Grant - Marie Curie Actions, intends to intensify the interactions and exchanges between research and industry and between university and business world.

This presentation has been composed with the following contents:

1. State-of-the-art of the research topic
2. Research project description
3. Research results - progress work
4. Societal implications of the research project
5. Future trends

Keywords: Research; Voltage regulator; Implementation; Innovation; Knowledge dissemination

Coupling of water retention behaviour and mechanical behaviour in unsaturated soils

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Abstract:

In unsaturated soils, the pores are filled with two or more media, most commonly air and water. Field applications such as analysis of slope instabilities, landslides, underground disposal of radioactive waste, earth dams, embankments, highways and foundations, all require proper understanding of the behaviour of unsaturated soils. Mechanics of Unsaturated Soils for Engineers (MUSE) is a Marie Curie Research Training Network which has been established to generate an unrivalled database of experimental results on the engineering behaviour of different categories of unsaturated soils, to develop and validate improved constitutive model for unsaturated soils, to develop and validate improved numerical modelling capabilities for analyzing coupled hydro-mechanical boundary value problems and to demonstrate the application of constitutive and numerical modelling capabilities to a range of practical problems.

It has been found that mechanical behaviour and water retention behaviour are coupled at a constitutive level in unsaturated soils. As a consequence, conventional constitutive models for unsaturated soils, which ignore this coupling, fail to predict some key features of mechanical behaviour and water retention behaviour. In order to incorporate this coupling, an elasto-plastic framework has been proposed by Wheeler, Sharma and Buisson (2003). These authors presented a simple illustrative constitutive model for isotropic stress states, to demonstrate, at a qualitative level, that key features of unsaturated soil behaviour can be represented by the new framework. Further work is however required, in order to fully validate the proposed framework and to refine the proposed constitutive model and extend it to non-isotropic stress states.

Keywords: Constitutive relation; Partial saturation; Suction; Clays; Elasto-plasticity

The evaluation of BRS based on carotid artery diameter and heart rate

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Abstract:

Introduction: Heart rate variability and baroreceptor sensitivity (BRS) are important determinants of neuronal risk factors of mortality. BRS is conventionally derived from the relationship between changes in pressure and heart rate, and recently from common carotid artery diameter and heart rate. We hypothesise that the evaluation method based on the latter provides a more selective value. Furthermore it has been reported that baroreceptor pressure sensitivity varies with posture. Method: A dedicated acquisition system was used to simultaneously record the arterial finger pressure assessed by the Finapres (Ohmeda, USA), and the R-top of the ECG signal. The Pie Medical Echo-350, active in B/M-mode using a 7.5MHz linear array transducer was used to visualise the common carotid artery. To determine BRS in a non-invasive manner, we measured the low-frequency variations (range 0.05-0.15 Hz) in various input parameters derived from the carotid artery diameter, arterial pressure and the corresponding R-R interval fluctuations, and determined the associated transfer function between the input and output parameters, under the condition of coherence (> 0.1). The BRS in a group of normotensive subjects (n = 20) in supine and upright seated position were compared. Results: The main finding is a variation of BRS peak in the two positions. Conclusions: The analysis of low-frequency fluctuations in the carotid artery diameter, and pressure demonstrates that posture affects neural control of the baroreflex.

Keywords: Baroreceptor sensitivity; Ultrasound; Distension; Heart rate; common carotid artery

Detector Control System of ATLAS

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Abstract:

The importance of using a powerful Detector Control System has much increased with the size and complexity of High Energy Physics detectors. The new generation of detectors for the LHC experiments puts further requirements onto DCS due to the inaccessibility of the equipment and the hostile environment concerning radiation and magnetic field. Techniques such as field buses for distributed input/output and Programmable Logic Controllers for closed loop control have to be employed. These represent the layer closest to the detector of a hierarchically organised multi-layer DCS.

ATLAS is one on the four main experiments of LHC, its DCS is being implemented and installed. DCS contains Front End electronics which acquire data from the different sub-systems of ATLAS, Front End computing which performs the data processing and Back End computing, using finite state machine, which allows experts and users to manage and control the whole system.

This poster will present the global structure of the DCS of ATLAS, showing how its electronics is deployed in the detector, the different computerized layers and how it is managed by the finite state machine level.

Keywords: Control; Front end; Back end; Detector

Tactile feedback in minimally invasive surgery

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Abstract:

Minimally invasive surgery or endoscopy, is revolutionising the surgical practice. Remotely controlled robotic manipulators are therefore being developed to increase dexterity and accuracy. These systems have some distinct drawbacks, preventing the fast adoption of such systems in every-day surgical practice, such as: the absence of force and tactile feedback to the surgeon's hands and lack of a natural interface with the surgeon.

It would be useful if the surgeon would have the same freedom to acquire information as he/she has in open surgery. By rubbing and palpating the tissue he gets information on texture and structure of the tissue, on blood stream pulsations through arteries, etc. Tactile information is also important for preventing tissue injury during the operation and in guiding instrument motion. Such a capability requires tactile information fed back to the surgeon. Equipping a master/slave minimally invasive surgery system with tactile perception capability is a challenge and it constitutes the essence of this project proposal.

The ultimate goal of the project is to create an Augmented Reality system for interactive image guided therapy providing the clinical user with a new generation of decision support tools. This system will integrate intra-operative and pre-operative image-information and enable the user to see beyond the organ surface to inner structures and pathology. An intuitive human computer interface consisting of 3D display systems, haptics and robotics will hide the underpinning complexity of the decision support tools.

Keywords: Tactile; Laparoscopic; Haptic; Surgery; Feedback

Modelling the role of angiogenesis and vasculogenesis in solid tumour growth

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Abstract:

Most tumours cannot grow beyond a certain size unless they acquire a blood supply. By secreting different growth factors tumours can cause nearby blood vessels to grow toward them in a process called angiogenesis. Recent evidence suggests that another kind of vessel formation, vasculogenesis, may also play an important role in tumour growth. Vasculogenesis is mobilisation of bone-marrow-derived endothelial progenitor cells (EPCs), which, once blood-borne, can home in on the tumour site and form vascular structures.

We have developed a mathematical model to describe how tumours grow when a blood supply is formed by angiogenesis and vasculogenesis. Analysis of two submodels shows that exclusively angiogenic and exclusively vasculogenic tumours exhibit similar growth dynamics. Dependent on a model parameter, there are three possible growth scenarios: the tumour remains in an avascular state, the tumour evolves to a vascular equilibrium, or unbounded vascular growth occurs. All three scenarios are also possible if angiogenesis and vasculogenesis act simultaneously. However, in that case the tumour's growth rate may increase, causing the tumour to evolve to a larger equilibrium size or to expand unboundedly.

We use the model to investigate some treatment strategies, e.g. therapies aimed at suppressing vascularisation. This investigation elucidates the need to target both angiogenesis and vasculogenesis in order to effectively reduce tumour vasculature and inhibit tumour growth.

Keywords: Tumour; Angiogenesis; Vasculogenesis; Therapy

Analysis of the bacterial community colonizing a cave containing rock art and engravings

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Abstract:

Microbial colonization causes negative effects on works of art, and specifically in painting-containing caves. At present, public awareness is demanding the preservation of these examples of the unique and scarce paintings. With that aim in mind, our group is focusing on understanding the development of microbial colonization in the Cave of Doña Trinidad (Ardales, Malaga, Spain).

The Cave of Doña Trinidad (Ardales, Malaga, Spain) contains numerous paintings and engravings some of them dated back about 20,000 years old. This study is part of a current effort on preserving this Palaeolithic art. Herein, we examined a whitish microbial colonization progressively spreading towards the interior of the cave. Knowing what micro organisms constitute the microbial community forming this colonization will represent a first step to be able to control their biodeteriorating effects.

Studying biodeterioration often implies the identification of the organisms involved in the process as well as the culturing and isolation of these micro organisms. Since only a small fraction of the micro organisms can be cultured, the application of novel molecular techniques represents a valuable complement in the study of micro organisms and their role in cultural heritage. The microbial community was analyzed based on both DNA (the total community) and RNA (the metabolically active fraction of the community).

DNA and RNA molecular surveys of the bacterial communities in different locations of the studied cave showed the presence of micro organisms belonging to different phylla, such as Firmicutes, Acidobacteria, Nitrospirae, Proteobacteria, and Planctomycetes. However, the major component of the metabolically active microbial community was an actinobacterium highly related to the genus Pseudonocardia. Among the Bacteria, Actinobacteria represent one of the most important bacterial groups in soils and subterranean environments and their role in bio deterioration processes has been frequently emphasized.

This study confirms the highly significant role of Actinobacteria in the active development of microbial colonization in subterranean environments. Further colonization by this community might threat this cave conservation if it continues its progressive spreading towards the caves interior, so there is a need for understanding the developing, and controlling the expansion, of these microbial communities.

Keywords: Subterranean environments; Rock art; Biodeterioration; Bacteria

A role for lipid rafts in ceramide-induced insulin resistance

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Abstract:

Type II diabetes is characterised by a loss in responsiveness of both muscle and adipose tissue to insulin, the main hormone that regulates the body's energy stores. Although the precise mechanisms that underlie this pathogenesis still remain unclear there is strong evidence that suggests that an increase in circulating free fatty acids may play a role in the observed reduction in insulin sensitivity in tissues such as skeletal muscle.

We investigate the mechanisms by which fatty acids such as ceramide, a main intermediate in the sphingomyelin pathway, trigger insulin resistance and impair insulin signalling in cultured skeletal muscle cells and adipocytes. Ceramide activates an atypical Protein Kinase C zeta (PKCz) and promotes its association with the protein kinase B (PKB), a key protein in the insulin signalling, which in turn become inhibited. Whether the complex is targeted to a specific cellular compartment has been unknown. We investigated whether lipids rafts within the plasma membrane could serve to sequester and retain PKB in its inactive state. We show that lipid rafts elicit increased abundance of both PKCz and PKB following cell treatment with ceramide. Lipid rafts dispersion by cholesterol depletion of cells reduces the ceramide-mediated increase of both kinases. As a consequence the insulin-dependent activation of PKB is restored.

Our findings indicate that ceramide inhibits the hormonal activation of PKB by its association with PKCz and retention in specialised microdomains of the plasma membrane. This implies that therapeutic manipulation of PKCz activity or lipid raft composition may provide opportunities for enhancing insulin sensitivity of tissues such as skeletal muscle and fat.

Keywords: Insulin-resistance; Ceramide; Protein Kinase B; Protein Kinase Cz; Lipid rafts

SWINGOPT: Optimisation of energy integrated pressure-swing distillation processes for separation of homogeneous azeotropic mixtures

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Abstract:

Distillation in general and that of azeotropic mixtures are energy intensive processes, used to isolate a variety of chemical products. Typical examples of azeotropic from the chemical industry are the recovery of Tetrahydrofuran (THF) from THF-water mixtures, or Acetonitrile from Acetonitrile-Water mixtures. Among the possible processes, Pressure Swing Distillation (PSD) offers higher energy efficiency and simpler operating schemes.

The currently known studies in the area deal primarily with the energy efficiency and system dynamics in established operation mode. Under the project SWINGOPT, the design and dynamic operation of a two-column system for PSD are evaluated.

The core activities of the project include mathematical modelling of the start-up process, accompanied by a parallel programme of pilot plant experiments. Thus a dynamic model, capable of simulating both start-up and established operation, has been created.

Currently, optimisation of the start-up process is considered minimising duration or operating costs. The overall operating schedule is modelled using UML Activity Diagrams. As a result, the optimisation degrees of freedom can be formulated as the values of the control degrees of freedom specified in each operating period, complemented with the lengths of delays between certain discrete changes of the operation degrees of freedom such as the delay between activating the reflux stream of a column and the reduction in the column feed flow-rate.

Keywords: Process Start-up; Start-up optimisation; Heat- and mass- integration

Evaporating nanoparticle suspensions: Viscous fingering, rupture patterns and front instabilities

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Abstract:

Nanoparticle-solvent films deposited on solid substrates are associated with a rich dynamic behaviour which gives rise to a wide variety of striking self-organised patterns[1-3]. We have used a combination of optical microscopy, atomic force microscopy, and Monte Carlo simulations to study the assembly of Au nanoparticle arrays from organic solvents on silicon and graphite substrates. Simple drop deposition methods have been complemented with "meniscus-driven assembly" experiments involving the use of the wetting properties of a Teflon ring to prolong the period of solvent evaporation. The drying behaviour of the nanoparticle-solvent drops has been monitored with video microscopy. As compared to a droplet of pure (i.e. nanoparticle-free) solvent, strong dynamic instabilities occur in the dewetting front. AFM imaging has been used to study the influence of these instabilities on the local structure of the nanoparticle film. Viscous fingering patterns are also observed at both the macroscopic level (at the dewetting front) and at the microscopic scale. We have used variants of the model put forward in Ref. 2 to investigate systematically the interdependence of evaporative dewetting of the liquid and demixing of liquid and particles. Spinodal dewetting and heterogeneous nucleation are analysed in their dependence on the concentration of the nanoparticles.

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Keywords: Self-organised nanoparticles; viscous fingering; drying front instabilities; evaporative dewetting

Galaxy properties in deep cosmological surveys

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Abstract:

One of the key goals of modern cosmology is to determine how and when galaxies form. Much progress has been made in the last decade with a combination of local (2dFGRS, SDSS) and distant (DEEP-2, VVDS, ZCOSMOS) major photometric and spectroscopic surveys to study the properties of our Universe. However, our understanding of how galaxies are built up over cosmic times remains very limited.

In this contribution I briefly discuss the evolutionary links that must exist between the stellar mass, the environment where galaxies reside and their morphological aspect.

The growth of the fraction of massive, elliptical galaxies is accompanied by a decline in the blue star-forming galaxies in the local Universe. Thus, morphological transformation of individual galaxies, e.g. through galaxy merging, must represent a significant driver in the galaxy evolution.

In particular, as part of the VIMOS VLT Deep Survey (VVDS) -- a flux-limited I-band survey of galaxies at look-back times of 9 to 12 billion years -- the spectroscopic properties of the two main categories of galaxies are analysed: late and early-type systems at redshifts $0.4<z<1.2$. The evolution of their spectral properties and how the star formation activity depends on stellar mass are investigated.

Keywords: Astrophysics; Galaxy evolution; Stellar mass; Environment; Galaxy classification

Carbohydrates: The sweet part of chemistry and biology

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Abstract:

Carbohydrates comprise the most abundant group of compounds found in Nature. Not only do they form major components in plants (e.g. cellulose and/or starch), shells of insects, crabs and lobsters, but they are also associated to basically all cell membranes spanning from microbes to mammals. Undoubtedly, the role of carbohydrates is not only related - as it was thought in the past - to energy storage and cell protection against the outside environment. It is now well acknowledged that as messengers of biological information, they also play key roles in numerous biological processes, either normal or pathological. The investigation of carbohydrate involvement in recognition processes is, among others, the subject of Glycobiology, a rapidly expanding research area. Needless to say that the recent expansion of Glycobiology has resulted in an increased interest for synthetic carbohydrate chemistry, also termed Glycochemistry.

The close relationship between the two fields is highlighted in this contribution, which provides an overview of basic Glycochemistry with emphasis on the study of protein-carbohydrate interactions, opening the way to the design of new therapeutics.

Keywords: Glycochemistry; Glycobiology; Synthetic Organic Chemistry

Langmuir-Blodgett fullerene films on silicon substrates

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Abstract:

Fullerenes, football-shaped molecules made of pure carbon, show a diverse range of chemical and physical properties and have attracted wide interest since their discovery 20 years ago. The parent compound C_{60}, for instance, can exhibit superconductivity[1], nonlinear optical response[2], and can be used as for HIV protease inhibition[3].

A subgroup of the fullerene family, in which the carbon cage plays host to one or more atoms/ions (denoted by X), is the endohedral fullerenes[4], denoted by $X@C_{60}$ or iXC_{60}. To date, mainly rare earth-containing endohedral fullerenes have been produced in sizeable quantities and their electronic properties and applications have been studied intensively. Much less well-known are the properties of $N@C_{60}$, which is both difficult to purify and thermally unstable (above 250^{o}C). This molecule is interesting from both a fundamental and application perspective as this is the only known system in which a single, unbound nitrogen atom can be found, as was confirmed by ESR measurements on the nitrogen spin[5]. A potential application of these molecules lies in the field of quantum computing (QC). In order to produce QC devices, or study the fundamental electronic properties, thin films on specific substrates are required which in this case cannot be done via simple sublimation in ultra-high vacuum due to the thermal fragility of $N@C_{60}$. Therefore, we have instead used the Langmuir-Blodgett (LB) method to obtain homogeneous films, and here we report our results on both C_{60} and mixed $C_{60}/N@C_{60}$ films on silicon substrates produced in this way.

We used both high purity water and aqueous phenol as a subphase for the LB trough (NIMA-312D) and subsequently spread 300~400ul of a solution of C_{60} (or $C_{60}/N@C_{60}$) in benzene on the surface. Once compressed, we transfer the film onto a Si(111) substrate, which is made hydrophilic by a H_2SO_4/ H_2O_2 treatment. Our results show that homogeneous but nanostructured films are formed on the substrate. We shall discuss the morphology of these films, as investigated by AFM, in detail.

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Keywords: Fullerenes; Langmuir Blodgett; Self-assembly; Atomic force microscopy

EQCM as a suitable sensor for characterization cholinesterase immobilization and organophosphate environmental monitoring

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Abstract:

Biosensors based on the combination of mass and electrochemical sensing have been developed. Cholinesterases from different origin were immobilized on the sensor via specific ligand-enzyme interaction. Paraoxon, BZE-DADOO, propidium and carnitine were used as ligands. They interact with ChE at different binding sites. Paraoxon covalently binds to the esteratic site, BZE-DADOO is a cocaine derivative which binds to both esteratic site and peripheral anionic site (PAS), propidium is a specific PAS binder and carnitine is a substrate analog. The kinetic association and dissociation constants (k_a and k_d) and equilibrium constant (K_{eq}) were determined and used for characterization of ChE-ligand interaction. The enzymatic activity of the immobilized ChE was determined using amperometric detection of the product – thiocholine. The operational stability of ChE immobilized on the ligand modified sensor and the behaviour of native and inhibited ChEs were also investigated.

Keywords: Cholinesterase; Organophosphate; Biosensor; QCM; Amperometric

Innate and adaptive immune responses in GvL/GvHD

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Abstract:

Graft-vs-host-disease (GvHD) is a major problem in the clinical treatment of leukaemias, autoimmune diseases and other haematopoietic malignancies by transplantation of allogeneic bone marrow cells from family members and unrelated donors. High morbidity and low survival rates, leaving the patients with poor life quality and expectancy, make it a difficult therapy at present.

We use an experimental animal model for acute myelogenic leukaemia in BN rats (BNML), and inject bone marrow from the allogeneic PVG rat strain into irradiated BN recipients. T lymphocytes derived from grafted allogeneic bone marrow stem cells can recognize antigens on aberrant leukaemic as well as normal host cells, resulting in graft-versus-leukaemia (GvL) and graft-versus-host (GvH) adaptive immune responses, respectively. While cytotoxic T lymphocytes are alloreactive and cause GvHD in our rats, another subtype of T cells has been shown to suppress the activity of T effector cells (hence termed T regulatory cells), and is therefore an important candidate in prospective therapy. Natural killer (NK) cells of the innate immune system also have the ability to recognize deviating patterns of major histocompatibility complex (MHC) molecules and kill host leukaemic cells, but do not have general GvH reactivity. Furthermore, we are testing the immunoregulatory function of mesenchymal stem cells (MSC) which, however elusive at the moment, has been demonstrated by *in vitro* experiments, and was shown to alleviate GvHD *in vivo*. Transplantation of MSC should help to reveal their influence on those cells delivering the immune responses in our animal model.

The discrimination mechanisms of different cell types causing GvL and GvH effects, respectively, are currently not fully understood, but hold the key to make allogeneic stem cell transplantations a safe clinical practice in the future.

Keywords: Graft-versus-host disease; Leukaemia; Allogeneic stem cell transplantation; Innate and adaptive immunity; Animal model

Study of the mechanism of transcriptional regulation in *Bacilli* using state of the art florescence methodologies

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Abstract:

In living cells proteins perform very specialized functions, which may be essential for the survival of the organism under some environmental conditions but dispensable in a different situation. Therefore, as a means to economize, the synthesis of proteins is strongly regulated at different levels one of them being the transcription of the coding gene into messenger RNA. Transcriptional regulation is physically carried out by specific proteins called transcriptional regulators, which induce or repress gene transcription in response to different signals. We are currently studying the mechanism of transcriptional regulation of some genes belonging to *Bacillus*, one of the bacterial systems most commonly used as a model in biological studies. Two of the proteins we study, CggR and CcpN, are repressors of genes encoding key enzymes of glycolysis, one of the most important metabolic pathways in *Bacillus subtilis*, and another one, PlcR, is a pleiotropic activator of genes encoding virulence factors in different *Bacillus* species. The conditional interaction of these proteins with the corresponding operator DNA sequences is being assessed using mainly fluorescence spectroscopy methods along with other biophysical techniques. The different fluorescence spectroscopy approaches we use include steady-state and time-resolve fluorescence anisotropy, fluorescence energy transference and fluorescence correlation spectroscopy, which allows measuring macromolecular interactions at the unsurpassed sensitivity of a single molecule. As a final goal of the project, the insight into the mechanism of transcriptional regulation in *Bacilli* that this work will provide may allow identifying suitable targets to inhibit pathogenic bacteria growth and/or virulence.

Keywords: Fluorescence spectroscopy; Transcriptional regulation; Protein / DNA interactions; Single molecule fluorescence