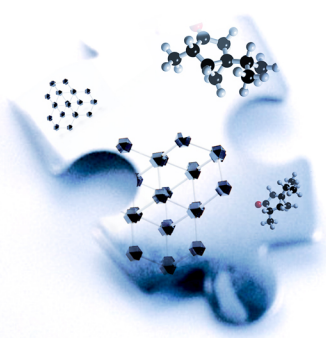


ZIENTZIA ETA TEKNOLOGIA FAKULTATEKO II. IKERKUNTZA JARDUNALDIAK

ENPRESA ETA BERRIKUNTZA TEKNOLOGIKOKO ZENTRUEN
AURKEZPENERAKO V. JARDUNALDIAK

2010
Martxoak
15 - 16 - 17
de Marzo

II JORNADAS DE INVESTIGACIÓN DE LA FACULTAD DE CIENCIA Y TECNOLOGÍA V JORNADAS DE PRESENTACIÓN DE EMPRESAS Y CENTROS DE INNOVACIÓN TECNOLÓGICA



ZTF-FCT
Zientzia eta Teknologia Fakultatea
Facultad de Ciencia y Tecnología



Euskadi

eman la zabal zazu



Universidad del País Vasco Euskal Herriko Unibertsitatea

DEKANO ANDREAREN GUTUNA

Zientzia eta Teknologia Fakultateko **Lehenengo Ikerketa Jardunaldiek** izan zuten harrera bikaina kontutan izanik, aurtengo kurtsoan **bigarren ekitaldia** egin dugu **martxoaren 15, 16 eta 17 egunetan**. Oraingo honetan lehenengo aldiz karrerako azkeneko ikasturteetako ikasleentzat **Enpresen aurkezpenen V jardunaldiak** aldi berean izan dira.

Hortaz **lortutako xedea bikoitza izan da**, alde batetik **ikasleei zein ikertzaileei** talde ezberdinek aurrera eraman duten ikerketen azkeneko nobedadeak erakutsi zaizkielako eta bestalde gure lana zein arlotan burutzen den zuzenean jakiteko interesa duten **enpresa eta produkzio arloko** arduradunei gure ikerketa ildoak ezagutzera eman dizkiegulako, eta hau etorkizunean elkarrekin lan egin ahal izateko pauso bat da.

Ekimenak arrakasta handia izan du eta **82 Fakultateko Ikerketa Taldek** SGIker Ikerketa Zerbitzu Orokorrekin eta Biofisikako Unitatearekin batera deiladiari erantzun diote. Adierazgarria da Zientzia eta Teknologia Fakultateko 2. Ikerketa Jardunaldietan aurkeztutako poster kopuru handia, honek ikastegiko jarduera zientifikoan aniztasuna adierazten du eta ikasleen artean sortu duten interesa azpimarragarria. Bestalde, Jardunaldi hauetan **Salvador Ferrer doktoreak, Espainiako ALBA sinkrotoiaren zuzendari zientifikoko** ikertzaile ospetsuak, hartu zuen parte **“Luz sincrotón: Una herramienta extraordinaria para la ciencia”** hitzaldiarekin. Horrez gain, enpresen alorretik **Koldo Saratxaga**, enpresa kudeaketarako aholkulariak, izan genuen **“Un nuevo estilo de relaciones. Para el cambio organizacional pendiente”** hitzaldiarekin.

Uste dugu Zientzia eta Teknologia Fakultateko II Ikerketa Jardunaldi hauetan geneukan xedea lortu dugula eta horrek ikerkuntza oinarritzat duen etorkizunerako ekintzak sustatzen jarraitzeko aukera ematen digu, gure ikastegiko ezaugarrietako bat. Dekanotza taldeak oraingoan ere Fakultateko langileen parte-hartze kartsua eskertu nahi du, izandako arrakasta lortzeko ezinbestekoa izan baita.

Esther Domínguez

Zientzia eta Teknologia Fakultateko Dekano Andrea

CARTA DE LA DECANA

Dada la excelente acogida que tuvieron las I **Jornadas de Investigación** de la Facultad de Ciencia y Tecnología, durante el curso actual hemos celebrado la **segunda edición** de las mismas durante los **días 15, 16 y 17 de Marzo**. Como novedad en esta ocasión se hizo coincidir con las **V Jornadas de Presentación de Empresas** a los estudiantes de los últimos años de carrera.

Así el **objetivo cubierto ha sido doble**, ya que por una parte se ha podido mostrar tanto a **alumnos como investigadores**, las últimas novedades de la investigación llevada a cabo por los diferentes grupos y por otra se han dado a conocer nuestras líneas de investigación a los agentes **del mundo empresarial y productivo**, interesados en conocer de primera mano los campos en que se desarrolla nuestra actividad, un paso más para el establecimiento de futuras colaboraciones.

La iniciativa ha sido un éxito siendo **82 los Grupos de Investigación de la Facultad** que han respondido a la convocatoria, junto con los Servicios Generales de Investigación SGIker y la Unidad de Biofísica. Es ilustrativo también el elevado número de posters presentados en estas II Jornadas de Investigación de la Facultad de Ciencia y Tecnología, representativos de la variedad de actividades científicas del centro, siendo muy destacable el interés suscitado entre los estudiantes. Por otra parte, en el marco de estas Jornadas hemos contado con la participación de un prestigioso investigador, el **Dr. Salvador Ferrer, Director Científico del Sincrotrón Español ALBA** que disertó sobre: **“Luz sincrotrón: Una herramienta extraordinaria para la ciencia”**. Además, desde el ámbito empresarial tuvimos la colaboración de **Koldo Saratxaga**, consultor de gestión empresarial, cuya conferencia versó sobre: **“Un nuevo estilo de relaciones. Para el cambio organizacional pendiente”**.

Creemos que se ha cumplido el objetivo marcado en estas II Jornadas de Investigación de la Facultad de Ciencia y Tecnología, lo que representa un incentivo para seguir apostando por acciones futuras que tengan como eje la investigación, una de las señas de identidad de nuestro centro. El Equipo Decanal desea una vez más, agradecer la entusiasta participación del personal de la Facultad, que ha sido la clave del éxito alcanzado.

Esther Domínguez

Decana de la Facultad de Ciencia y Tecnología

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Elevated CO₂ and plant physiology: plant contribution to climate change mitigation

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KEY WORDS: Bioenergetic crops, climate change, CO₂ sinks, plant physiology and production.

Climate change raises important scientific challenges for plant physiologist. Firstly we need to expand and broad our knowledge about the responses of plants to the environment, so that we can predict the impact of climate change on the growth of the crops and natural ecosystems. Secondly, the understanding of the response of the plants to climate change takes us tools and knowledge to minimize the negative impact.

The rise of CO₂ may alter the global climate rising temperature and modifying the rainfall pattern exacerbating even more the risk of drought and salinity, specially in the Mediterranean region, reducing drastically the productivity of the crops. In consequence, one of the main uncertainty when analysing the global impact of climate change in the productivity of agroforestry and of ecosystem is the response of the plants to elevated CO₂ in combination with other environmental stresses.

Plants through photosynthetic activity function as excellent sinks of environmental CO₂ reducing the effects of climate change and contributing to the Kyoto compliance. On the other hand, the produced biomass could have an energetic use. However, those perspectives can be altered by factors such as limitation of nutrients and water, temperature rise, salt stress and/or other factors related to the rise of CO₂ that can affect physiology and productivity of the plants.

Thus, the objective of this research group is focused on the analysis of different factors that affect physiology, growth and productivity of the plants in the nowadays changing environment such as atmospheric CO₂, water availability, soil salinization, NO₃⁻ availability, as well as interactions within them.

At the same time, we intend to take advantage of the capacity of the own plants for kidnapping the excess of environmental CO₂ permitting that way a longer period of C retaining, eventually using plants as biomass source for utilization as renewable bio-fuels.

Saloña Bordas, Marta I. PhD, Beatriz Díaz Martín MSc, Maite Gil Arriortúa MSc, Patricia Valbuena Lacarra MSc
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KEY WORDS: Insects, Forensics, Pest diagnosis and control, PMI estimations.

1.- Concept

Forensic Entomology applies the knowledge about the structure and dynamics of insect communities and other arthropods to assist in legal matters resolution, such as judicial (abuses, neglect, crimes o deaths) or economic problems (infestations or plagues), where the correct interpretation of the information provided by entomologic evidences can play a valuable or even crucial role, particularly, in Court proceedings.

2.- Applications

- ❖ Evaluation of the insect activity in a sample to estimate
 - Postmortem Interval (PMI) in cases of murder, suicide or natural death.
 - Data, origin and type of contamination, abuses o neglects involved in myasis of animals and dependent people (sick or elderly people and children), infestation of stored food, real property and other legal aspects.
- ❖ Detection of toxics and/or drugs in corpse remains in case of impossibility to carry out toxicological routine analysis; larvae incorporate and bioaccumulate chemical metabolites of drugs from the corpse and other remains into their own tissues.
- ❖ Molecular identification of human cadavers, in cases of suspected homicide without corpse, it is possible to carry on the identification of human DNA using gut contents from entomological evidences.
- ❖ Maggot therapy; larvae activity of some species can remove only the necrotic tissue and promote wounds healing.
- ❖ Illegal species deal; the use of insects as geographic indicators provides information to solve illegal traffic of cars and goods deal.
- ❖ Identification and estimation of damages to areal property, personal property and other kind of properties.
- ❖ Population control, to prevent sanitary and economics problems that some insects can cause (pest, disease vector, etc.)
- ❖ Biologic waste treatment; the high metabolic activity that necrophagous species present can be useful as an effective tool with applicability to reduce organic residues.

4.- Main Objectives that are being developed by the research group

1. To cooperate with different group of professionals including forensic pathologists and police to ensure common guidelines and standards protocols for best practice in forensic entomology that guarantee the future collaborations.
2. To increase our knowledge about the necrophagous fauna in the Basque Country (C.A.P.V.) with:
 - a) Morphological identification of the main infesting species.
 - b) Molecular tipification of the most relevant entomofauna for forensic purposes.
 - c) Estimation of their developmental rates in our latitudes.
 - d) Establishment of the faunal succession patterns on corpses in our biogeographical environment.
3. To develop different control strategies for the insect populations that cause damages in transported or stored food, livestock, areal properties and other material damages.
4. To apply the knowledge about the developmental biology of necrophagous species suitable to an efficient waste management as a possible tool to reduce residues of organic fraction.

Genomics and Animal Health: interactions of exogenous and endogenous retroviruses with the host.

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KEY WORDS: genomics, candidate genes, infectious disease, disease resistance, bioinformatics

The main research line of the group **Genomics and Animal Health** of the Genetics, Physical Anthropology and Animal Physiology Department is the analysis of the genetic basis of infectious diseases with viral aetiology. We have two main scientific goals: The search for functional polymorphisms affecting the immune response and the study of the influence of host genetics in the pathogenesis of infectious diseases and cancer. Currently we seek to contribute to the clarification of some aspects of the pathogenesis of two viral diseases, Ovine Pulmonary Adenomatosis and Maedi-Visna. We are analyzing candidate genes of both the innate and adaptive immunity with different markers and techniques (Sequence Based Typing, Microsatellites, SNPs). Association between markers and disease development is tested employing logistic regression, taking into account marker type, sample size and structuration. We hope that our research will open new channels for the elimination of infectious diseases affecting livestock.

On the other hand, the endogenous retroviruses (ERVs) can have both beneficial (resistance to infectious counterparts and a role in placentogenesis) and adverse effects (they may cause disease) in the host. Given the amount of genomic information currently available following the complete sequencing of various genomes, we are carrying out a multi-species genomic analysis to identify retroviral elements inserted in these genomes. We are also characterizing their evolutionary dynamics and their possible expression and functional role, using bioinformatics methods. Currently, an *in silico* analysis is being carried out to see which genes are located close to bovine ERVs and to quantify the ERVs' expression. The next step will be the analysis of their effect on the host's genome.

Finally, we also considered a technological objective, such as the development of tools for the detection and analysis of polymorphisms that can be used as markers for disease progression. This point we carried out both at laboratory reagents and protocols and bioinformatics software for storage and analysis.

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KEY WORDS: Huntington's disease, CAG repeat, huntingtin, age of onset, candidate gene, association analysis.

BACKGROUND: Huntington's disease (HD) is a rare, neurodegenerative, monogenic and hereditary disorder caused by the expansion of the CAG repeat which is located in the first exon of the IT-15 gene. IT-15 or HD gene codifies a protein called huntingtin (HTT). When the length of the CAG repeat of the huntingtin reaches 35 or more trinucleotide repeats, it produces a pathological form of the protein.

The pathological features of the disease are the motor symptoms (the most common and characteristic of the disease is the chorea), cognitive decline (dementia) and psychiatric and behavioural abnormalities (anxiety, irritability, aggressiveness...). Usually these symptoms occur in the middle 40s, but they can appear before 20 years old (juvenile onset) or after 60s.

The CAG repeat length and the age of onset (AOO) are strongly correlated, but the CAG repeat does not explain only by itself the AOO. It was observed that individuals with the same number of CAG repeats can develop the disease at very different ages. Then, it was described that between 40-72% of the variability of the AOO is explained by the CAG repeat length, which means that other factors are involved and as it was reported later, that factors can be environmental and genetics.

The variability of the genome is studied analysing the genetic markers (polymorphisms). One way of studying the relationship between a genetic character and a disease is the genetic association analysis. This is based on the candidate gene's polymorphism testing and it informs whether an association between a polymorphism (in our case an Single Nucleotide Polymorphism, SNP) and the character you chose (AOO) is statistically significant or not.

OBJECTIVE

Our aim is to identify genetic factors, other than the CAG repeat length, that modify Huntington's disease age of onset (AOO) using candidate gene association analysis. As this disease has not yet any cure, the identification of the age of onset's modifier genes could lead to the identification of possible therapeutic targets.

MATERIALS AND METHODS

- Samples: neurologists of 5 of the main hospitals from the Basque Country have collected biological samples and clinical data from 140 individuals belonging to 42 HD families. 85 of the 140 individuals are carriers of the mutant HTT and 51 of those individuals are symptomatic.
- Association analysis: We chose to test the SNP for being the most common polymorphism in the human genome. This methodology compares the frequency of one SNP between pairs of groups (classified, taken into account their AOO and CAG repeat length, into cases and controls).
- AOO: was established by each neurologist who collaborates in this study. By consensus it is considered that the disease starts when the first motor symptoms are noticed.
- CAG repeat length: in each person we have to carry out a DNA extraction (from blood), DNA amplification (fluorescent-PCR), an analysis of the length of the amplified fragment and sequencing (with the Abi Prism 3100 automatic sequencer).
- SNPs genotyping: to genotype the SNPs we used the SNPlex technique which is available in the "Sequencing Service" of the UPV/EHU.

R+D+I services offered by the CBET research group: assessment and monitoring of environmental pollution and chemical toxicity testing

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KEY WORDS: CBET consolidated research group, R+D+I services, assessment and monitoring of environmental pollution, toxicity testing, histopathological diagnosis, advising, formation, facilities for aquaculture.

Since 1985 the group of "Cell Biology in Environmental Toxicology" of the University of the Basque Country develops research and teaching activities within the Environmental Toxicology field. The group is recognized since 2001 as a consolidated research group. The main field of expertise is in the development and application of early warning cell and molecular markers of pollution. The group has experience in the assessment and monitoring of biological effects of pollution (North Iberian Peninsula, Mediterranean Sea, North Sea), including accidental oil spills (Prestige) and industrial and urban wastes. The group promotes the Marine Station of Plentzia.

We offer the following **R+D+I services**:

- Assessment of environmental quality (marine, estuarine, and terrestrial environments).
- Monitoring programmes of environmental pollution.
- Toxicity testing (REACH legislation).
- Determination of biological activity of chemicals.
- Histopathological diagnosis of fish and shellfish diseases.
- Scientific and technical advising. Areas: pollution, accidental spills, environmental toxicology, use of biomarkers, cell culture and in vitro systems, microscopy, molecular, cell and tissue organization of animals.
- Scientific formation: Masters, postgraduate courses, specialization courses, PhD programme, laboratory training.
- Estabulation and maintenance of experimental animals. Marine aquaria. Zebrafish facility. Facilities to run chemical exposures.
- Processing of samples for histology, light and electron microscopy, cryotechniques.
- Quantification of levels of specific proteins, enzyme activities, gene expression, immunolabelling, cell structure.

Examples of recent collaborations-contracts with enterprises are given below:

- PETRONOR S.A.: contract for biomonitoring of the waste discharge site (Punta Lucero, Bizkaia) of the petrol refinery (2000 up to now).
- NORSK HYDRO and NIVA (Norway): contract for biomonitoring of the North Sea (Water Column monitoring 2003, 2004-2005 and 2008).
- IHOBE S.L.: contract to make an inventory of affections in the Basque Coast after Prestige oil spill (2003-2004).
- CIS S.L. (Galicia): contract for monitoring of the impact of the Prestige oil spill on the Cies and Ons islands (2004-2006).
- LE CEDRE (France): EU contract "Pollution monitoring and ecological impact assessment following accidental oil and other chemical spills in marine waters" (2007).
- IRIS (Norway): EU project PRAGMA "A pragmatic and integrated approach for the evaluation of environmental impact of oil and chemicals spilled at sea: input to European guidelines", 2006-2007.
- DEAD SEA LABORATORIES (Israel), INTRINSIQ (UK): EU project NANORETOX "The reactivity and toxicity of engineered nanoparticles: risks to the environment and human health" (2008-2012).
- AZTI Foundation (Sukarrieta), INBIOMED FOUNDATION (San Sebastian) and BIOBIDE S.L. (San Sebastian): work together in the Spanish technological platform DareNet to promote the use of zebrafish in research. Support the Spanish MSI project NANOCANCER "Determination of genotoxic and carcinogenic potential of metal nanoparticles using alternative methods in vitro and in vivo with zebrafish and invertebrates" (2010-2012).
- FULCRUM (Leioa): Spanish Ministry of Environment project VERTITOX "Development of procedures for the integrated operative control of urban and industrial effluents into the coastal area" (2008-2010).

Subcellular localization and function of human deubiquitinases

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KEY WORDS: DUBs, deubiquitinases, ubiquitin, siRNA screening, nuclear transport, signaling pathways.

Ubiquitination is one of the most common postranslational modifications of proteins. Depending on the number of ubiquitin molecules attached, and the type of chain formed, ubiquitination may either alter the localization and function of a protein, or induce its degradation by the proteasome. Ubiquitination is a reversible process, and the removal of ubiquitin from target proteins is carried out by a group of functionally and structurally related enzymes termed deubiquitinases (DUBs). 95 DUB-encoding genes have been described in humans.

Similar to reversible phosphorylation/dephosphorylation, reversible ubiquitination/deubiquitination regulates many aspects of cell physiology, including the activity of several proteins and signal transduction pathways involved in cancer development. Given their role as regulators of these pathways, and their importance for the maintenance of cell homeostasis, proteins involved in the process of ubiquitination/deubiquitination, including the DUBs, are viewed as potential targets for the development of novel anticancer therapies. Following the lead of kinase inhibitors, a next wave of targeted antitumor agents might well be DUB inhibitors. The development of therapeutic approaches based on DUB targeting, however, is seriously hampered by the limited information available on the function of these enzymes. In fact, although a subset of human DUBs is relatively well characterized, our knowledge about most deubiquitinases is virtually non-existent. In this regard, our group has set up two research projects to explore two different aspects of DUB biology that are still poorly understood.

Our first project focuses on how the subcellular localization of the DUBs is regulated. The nuclear envelope defines two main compartments within a eukaryotic cell: the nucleus and the cytoplasm. The nucleocytoplasmic transport and localization of proteins is a major determinant of how their activity is regulated within the cell. Using *in vivo* transport assays, fluorescently-tagged proteins, and immunofluorescence techniques, we are studying the mechanisms and signals that regulate the nucleocytoplasmic transport of the human deubiquitinases. We have already identified several functional transport signals in a subset of DUBs, and we are addressing now the functional consequences of these signals.

The aim of our second project is to identify new cancer-related proteins and signaling pathways that are regulated by DUB activity. In order to assess the role of human DUBs on the regulation of several cancer-related signaling pathways, we will carry out a RNA interference-based functional screening. Each DUB gene will be systematically silenced in cells, and the phenotypic effect of DUB knockdown will be evaluated by using a series of markers. These markers are GFP-tagged proteins whose cellular localization is dependent on the activity status of a determined signaling pathway. Our first functional screening will evaluate the effect of DUB down-regulation on the activity of the PI3/Akt pathway, the Ras/Raf/MAPK pathway, the JAK/STAT pathway, and the NFAT pathway.

Besides these functional studies, we have established a collaboration with the Genetics Service of the Hospital de Basurto in order to assess the expression of several human DUBs and evaluate its correlation with the clinicopathological characteristics of these tumors.

We expect that the novel basic and preclinical information derived from our work will contribute to improve the functional characterization of human deubiquitinases, a first and necessary step to exploit their potential in cancer therapy.

Bacterial response to stress

Identification of cellular factors controlling responses of autochthonous and allochthonous bacteria to environmental stresses in aquatic systems

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KEY WORDS: Bacterial stress responses, aquatic systems, viable but nonculturable bacteria, proteome and transcriptome profiling.

Prokaryotes are ubiquitous, although specific abiotic and biotic conditions are required for each species' optimal growth. The natural environment, in which prokaryotes live, often undergo great seasonal and circadian changes, such as temperature variations, changes in levels of solar radiation and in the availability of nutrients. These changes are particularly pronounced in aquatic systems.

When environmental conditions become adverse, bacteria must be able to withstand stress and to implement strategies which permit them to survive until suitable conditions for growth and development are re-established. Thus, the acquisition of the stress-resistant phenotype ensures survival and even proliferation of prokaryotes in a restrictive or unfavourable environment.

For many years our group has been using *Escherichia coli* as a microbial model organism to study how bacteria respond to different adverse conditions, such as, starvation, visible and UV light, suboptimal temperatures and salinity. These conditions resemble the environment that bacteria face in natural aquatic systems, for example, in marine ecosystems, coastal zone, *etc.* Our results show that *E. coli* responses to such adverse conditions depend on the nature of stress and that all these responses have a common denominator: the acquisition of the viable but non culturable state (VBNC). Although these studies revealed a number of important physiological and phenotypic characteristics associated with the acquisition of the VBNC state, still very little is known about the molecular mechanisms that control the response to these adverse conditions. Similarly, the mechanisms, which are responsible for the exit from the VBNC state (e.g. when the environmental conditions become favorable again) are mainly unknown.

Therefore, the aim of our current work is to learn more about the molecular aspects that regulate the response of the autochthonous and allochthonous bacteria (i.e. *E. coli*, *Vibrio harveyi*) in aquatic systems to some environmental stresses. Several techniques (such as proteomic tools, RNA profiling and molecular genetics approaches) will be used to discover the key cellular factors that are expressed to regulate cell adaptation under various adverse conditions.

In addition to revealing the cellular factors and molecular mechanisms that bacteria need for their survival under stress, the results of this study can also have implications in industry (e.g. water and food quality control) and biomedicine (e.g. development of new strategies for control and monitoring the presence of pathogenes).

Besides these studies of basic investigation we realize others more applied that develop in two slopes:

- field of the waste water treatment (Wastewater treatment plant of Crispijana)
- development of antimicrobial for cosmetic and food products (IDOKI SCF TECHNOLOGIES, S.L.)

Post-transcriptional control in bacteria

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KEY WORDS: RNA processing and decay, RNA degradosome, antisense RNAs, bacterial stress responses.

By catalyzing RNA decay, cellular ribonucleases counterbalance transcription and are thus essential to the control of gene expression. Recent progress in our understanding of RNA processing and decay in *Escherichia coli* is largely attributable to the characterization of RNase E, a site-specific endoribonuclease that cleaves in A/U-rich regions of structured RNAs. This enzyme initiates the decay of many, if not most, messenger RNAs as well as being involved in processing of ribosomal and transfer RNA. Our recent work revealed a number of sequence determinants that could either facilitate or impede RNA cleavage by this enzyme and by other members of the RNase E family of ribonucleases. We also found that RNase E could serve as a platform for the assembly of a multi-enzyme complex (the 'degradosome') that is arguably the major center for RNA processing and decay in *E. coli* and likely in many other Gram-negative bacteria including human pathogens. As the nature and evolutionary conservation of the RNA-protein interactions that underlie the specificity and efficiency of RNase E cleavages are still poorly understood, our current efforts are aimed at using multi-disciplinary approaches to (i) map essential amino acid residues of this endoribonuclease and (ii) investigate their contribution to the RNase E-mediated catalysis and enzyme's interactions with the major sequence determinants of RNase E cleavage sites. Apart from gaining fundamental insights into the nature of RNA-protein interactions, this work will also open new avenues for the rational design of RNase E variants with altered and highly specific activities. Furthermore, this study is likely to have direct implications for development of nucleotide-based inhibitors of RNase E that can potentially be used as specific antimicrobial drugs.

Another line of research is focused on post-transcriptional mechanisms that are mediated by *trans*-encoded small RNAs (sRNAs), a recently emerging and continuously growing class of non-coding antisense RNAs that play important regulatory roles in bacterial adaptation and survival under numerous stress conditions. We have recently characterized two different mechanisms, by which the *trans*-encoded antisense RNAs RyhB and DsrA as well as *E. coli* ribonucleases control the fate of their target mRNAs. The main goal of our current studies is to attain a broader view of biological functions and post-transcriptional mechanisms regulated by sRNAs. We are particularly interested in characterizing new stress-related non-coding RNAs and examining their regulatory functions. Moreover, given that the post-transcriptional mechanisms controlled by sRNAs have been characterized in detail only for a limited number of transcripts, we are also planning to further clarify how the formation of sRNA/mRNA complexes affect the fate of different sRNAs and their targets, and investigate the contribution of the RNA chaperone Hfq and cellular ribonucleases to the rate-limiting and subsequent steps in disassembly and processing of these complexes. It is anticipated that this study can significantly add to our understanding of the global regulatory networks that coordinate physiological adjustments in microorganisms facing environmental challenges.

Marine and estuarine plankton: bioindication and trophic ecology

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Department of Plant Biology and Ecology

KEY WORDS: Plankton, Bioindication, Climate change, Pollution, Ichthyoplankton, Trophic ecology, Estuaries, Shelf waters.

Our team is currently working on the following research areas:

▪ ***Plankton as bioindicator of short, medium and long-term environmental change:***

We are analysing time-series obtained from a monitoring programme initiated in 1997 in the estuaries of Bilbao and Urdaibai (Bay of Biscay) to investigate the relationships between changes in zooplankton composition and abundance, phytoplankton biomass, characteristics of water masses (temperature, dissolved oxygen, transparency), and climate variables such as temperature, rainfall, irradiance, as well as large-scale climate indices, e.g. the North Atlantic Oscillation (NAO) index. The main aim is to determine if plankton from these systems shows a response to climate changes and to anthropogenic perturbations that can be measured and modelled.

In the case of the estuary of Bilbao an additional aim is to use plankton as an indicator of the recovery process of this polluted system following the implementation of the Wastewater Treatment Plan for the area. In this context, we are also making the zooplankton monitoring for the Bilbao-Bizkaia Water Authority, in collaboration with AZTI-Tecnalia.

▪ ***Trophic ecology of fish larvae:***

In collaboration with research groups from AZTI-Tecnalia and ICM (Institut des Ciències del Mar) of Barcelona, we are carrying out several projects with the aim of establishing the diet of various commercially important fish larvae (anchovy, sardine, hake etc.), the relationship between food availability and condition of larvae and the spatial coupling between the distribution of larvae and their preferred preys.

The origins of the European gene pool

José Ángel Peña García¹, Luis Gómez Pérez¹, Ibone Espinosa Carcabilla¹, Miguel Ángel Alfonso Sánchez, Susana García Obregón, Ana María Pérez Miranda y Grupo Consolidado BIOMICS
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KEY WORDS: European gene pool, Last Glacial Maximum, Neolithic, cline, bovine cattle.

Most of the current Europeans are descendants and heirs of a series of human groups that colonized and recolonized in successive migratory waves this western appendix of Asia. The major milestones of human demographic history in this region of the world were the following:

1. An early colonization originating from Eastern and Southeastern Europe.
2. Retreat and concentration of human groups in the South of the continent during the Last Glacial Maximum.
3. Resettlement of Europe from the Southern refuges after the end of the glacial period.
4. Diffusion from the East of Neolithic peoples.
5. Generalization of the bovine cattle from Northern Europe.

Our investigations has helped, to a certain extent, to gaining insights on the perception that we have of this chapter of the human adventure.

ENAF: Efficiency of Nitrogen in Agro-Forest systems. Effect of mycorrhization, production, quality and minimization of environmental impact.

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KEY WORDS: agro-forest systems, fertilization, forest stands, global change, nitrogen efficiency, nitrogenous gaseous emissions, mycorrhization, plant N metabolism.

The name of the group **ENAF** stands for “Efficiency of Nitrogen and the effect of mycorrhization in Agro-Forest systems: production, quality and minimization of the environmental impact”. This group has as objectives to study in depth the fundamentals of metabolic, biochemical and physiological aspects in plants in order to help decide agronomic measures in relation to the rational use of phytochemicals (fertilizers and phytosanitary products). These advances will contribute both to the high quality agronomic and forest production, and simultaneously to reduce the environmental impact.

Some environmental problems of high importance coming from agricultural management are the pollution of waters due to the nitrate leaching and the contribution to global warming due to the emission of nitrogenous gasses derived from fertilization. A promising strategy to avoid this contamination is the use of ammonium-based fertilizers stabilised with nitrification inhibitors. These inhibitors slow down the nitrification of ammonium to nitrate in soils, maintaining the soil N as ammonium for a longer period of time. However, using these products will require that plants are adapted to ammonium nutrition, opening the research field in several ways. Our first objective is to evaluate to what extent the nitrification inhibitor itself changes its properties and efficiency under different environmental soil temperatures and water status, going in depth into the microbial populations responsible for the nitrogen gaseous emissions to the atmosphere. A second objective is to investigate how the different plant species are able to grow under ammonium nutrition and to render a high-quality natural food. A better understanding and knowledge of the physiological, biochemical and molecular mechanisms responsible for the ammonium tolerance will allow to progress in the fertiliser management and the selection of plant markers linked to a higher nitrogen use efficiency.

A strategy of high importance for the mitigation of climate change is fostering the capacity of forests as CO₂ sinks. In this regard, two lines are open to evaluate, on one side, the contribution of different forest stands to the N₂O emissions budget under our edafoclimatic conditions and, on the other side, their contribution to carbon sequestration, by producing morphologically and healthy forest seedlings with different capacities for adaptation to edafoclimatic conditions of Northern Spain. The effect of mycorrhization on the production and health of forests in relation to environmental stressing conditions is also considered by our research group.

Colaborations: Universidad Pública de Navarra (UPNa), Escuelas Técnicas Superiores de Ingenieros Agrónomos de la Universidad Politécnica de Madrid y de la Universidad de Córdoba, SERIDA (Organismo Público de Investigación del Gobierno del Principado de Asturias, NEIKER-Tecnalia, BASALAN (Diputación Foral de Bizkaia), Helmholtz Centre for Environmental Research-UFZ (Alemania), Universidade de Lisboa (Portugal), Red RUENA (Red para el Uso Eficiente del Nitrógeno en la Agricultura), BC³ Basque Centre for Climate Change, COMPO-Agricultura (Grupo K+S), Timac-Agro (Grupo Roullier), IGER-Institute of Grassland and Environmental Research (Reino Unido), INRA-L’Institut National de la Recherche Agronomique (Francia).

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Relationships between oribatid mite communities and temporal, ecosystem and climatic variables

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KEY WORDS: Oribatid mites, Climate Change, forest ecosystems, climatic zones, temporal variation.

The alterations induced by changes of climatic factors (mainly temperature and precipitation) cause changes in the structure of soil biotic communities. In the context of 'Basque Plan against Climate Change 2008-2012' and within the governmental strategic project ETORTEK, our research team is studying the edaphic oribatid mites communities of different ecosystem types in different climatic areas.

The aim of the work was to identify species and/or groups of species that define the ecosystems and the climatic zones within a temporal variation (from 20-30 years old samples to present ones).

In 2008 there were sampled 19 ecosystems (15 of them also sampled in the past, 19, 24 or 28 years ago) belonging to 6 different types of vegetation. The area shows an ombrothermic gradient distinguishing 5 climatic zones of the Autonomous Community of the Basque Country. In each sample point, 3 replicates of a litre composite soil sample were taken; each litre was made up of 4 discrete subsamples. Soil fauna was extracted with the funnel method of Berlese-Tullgren.

There were identified 8088 individuals belonging to 189 species of oribatid mites, of which 3 are possibly new species for science, 2 new records for the Iberian Peninsula and 9 new records for the Autonomous Community of the Basque Country.

The analysis of 2008 data showed that there were differences due to the ecosystem type (CCA, p-value=0.002) and also due to the climatic zone (CCA, p-value=0.002), sharing both a variability of 6.06% (p-value=0.004). There were also observed differences when comparing communities diversity between current data with the past ones (p-value=0.002), explaining 76.50% of the whole variability. A loss of diversity (species and individuals) from the past ecosystems to those of the present was observed.

Microbial communities in marine ecosystems

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KEY WORDS: Prokaryote, Protist, Dissolved Organic Matter, Particulate Organic Matter, Marine system.

The main objective of our research is to analyze the flux of the matter and energy through the microbial loop in marine food webs.

The main objectives of our research line “**Abundance, structure and activity of the attached and free-living prokaryotic communities**” are:

- to analyze the composition of L- and D-amino acids in marine systems, their utilization and release by prokaryotes, and their role as indicators of biodegradability of organic matter.
- to analyze the prokaryotic decomposition of diverse types of particulate organic matter (marine particles and macroaggregates)
- to analyze the prokaryotic heterotrophic utilization of the dissolved organic matter (enzymatic hydrolysis on polymers and the velocity and efficiency of uptake of the monomers resulting of that activity) and its variability in relation to ambient factors.
- to determine the abundance, biomass and composition of the marine prokaryotic communities and their relation with the function of the communities.
- to analyze the production, respiration and growth efficiency of prokaryotes in marine systems and asses their variability as a function of environmental factors.

The main objectives of our research line “**Interrelations between protists and prokaryotes in marine systems**” are:

- to analyze the abundance and structure of the communities of protists in different marine microhabitats: aggregates, liquid phase and interphase.
- to analyze the function of heterotrophic planktonic protists in the carbon cycle in marine systems by measuring their grazing activity.
- to investigate the chemotactic response of bacterivorous protists towards dissolved and particulate cues derived from bacterial prey.
- to analyze the function of heterotrophic planktonic protists in the control of prokaryotic communities by differential grazing depending on the size, the cell wall and the nutritional characteristics of prey.
- to analyze the resistance mechanisms developed by the marine prokaryotes generated during the successive stages of the prokaryotic-protist interaction (detection, encounter, capture handling, ingestion and digestion).

And we use the following **techniques and facilities**:

- Quantification of organic carbon by combustion at high temperature and determination of enantiomeric composition of free and combined dissolved amino acids by HPLC.
- Spectrophotometric quantification of dissolved carbohydrates and photosynthetic pigments.
- Fluorometric detection and quantification of microbial hydrolytic activities.
- Uptake of radiolabeled compounds to quantify prokaryotic heterotrophic activity and production.
- Epifluorescence, direct and inverse microscopy for microbial counts and identification.
- Image analysis for microbial biomass estimations.
- Amperometric micro-respirometry with microelectrodes to estimate microbial respiration rates.
- CARD-FISH (Catalyzed Reported Deposition-Fluorescence In Situ Hybridization) to determine biodiversity and detect phylogenetic groups of *Bacteria* and *Archaea*.
- Assays of attraction/repulsion to quantify the chemotactic response of protists.
- FLB (Fluorescently Labelled Bacteria) uptake to quantify grazing activities by planktonic protists.

Development and application of proteomic technology

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KEY WORDS: proteomics, E2F2, phosphorylation

Proteomics refers to large-scale analysis of proteins, including protein identification, expression analysis, post-translational modifications and protein-protein interactions, with the aim of elucidating a general and integral view of protein networks and cellular and pathological processes. Our group is involved in proteomics studies in two aspects. On one hand, we develop methodology in order to provide the Proteomics Facility with new services to offer. On the other, we use established proteomics approaches to tackle biological issues such as the ones related to the transcription factor E2F2.

- Protein identification is the basis of proteomics. A search engine uses data obtained by mass spectrometry (MS) to identify proteins from a sequence database. A strategy based on tandem MS allows the identification of proteins from mixtures. At the beginning, and somehow restricted by the technology we had in hand, we were able to identify proteins from purified samples and to analyse components of protein complexes and protein-protein interactions. As the result of the acquisition of new instrumentation we have extended our capabilities and can analyse complex protein mixtures, such as cell compartments and total cell extracts from which we are able to identify a few hundred proteins. Nevertheless, more in deep analysis, identifying a few thousands of proteins, has been shown to be feasible and we are trying to reinforce our methodology in order to reach those values.
- Very often, the protein contents of a number of samples need to be compared, for instance disease/normal or treated/non-treated. In order to do that, proteins need to be quantified as well as identified. The pioneer technique for this purpose has been based in two-dimensional electrophoresis (2DE) and although it is still a powerful everyday methodology new MS-based approaches are being developed and are nowadays confirmed as reliable methods for either relative or absolute quantification. Among these new methodologies label-free quantification is certainly standing out. We are applying this technology in our laboratory and the quantitative results are being very satisfactory.
- Phosphorylation has an important role in protein function. MS analysis of protein phosphorylation is not trivial due to low stoichiometry and ionisation efficiency issues. Therefore, phosphopeptides need to be enriched prior to MS analysis. Our group works on phosphopeptide enrichment methods based on titanium dioxide.
- We are applying all the technological developments mentioned above to the analysis of the E2F transcription factors. This work is being carried out in collaboration with Ana Zubiaga's Group (Genetics Department). E2F2 interacts with other proteins to carry out its function. Identifying those interacting partners may help us have a better understanding of the role of this transcription factor. Thus, immunoprecipitation with E2F2 specific antibodies or oligoprecipitation using sequences recognised by E2F2 is performed and the outcome is analysed by LC-MS/MS.

DNA variation: Genomic analysis

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KEY WORDS: Genetic markers (SNP, Microsatellites, Sequences and CNV), Population genetics, Genetic association studies

Our research group is focused on the analysis of DNA variation in animal, plant and human species.

Although the final objective could be different, all DNA variation studies performed in our research group share a similar methodology: 1) DNA purification from several tissues (blood, muscle, hair, semen, spit,...); 2) molecular biology techniques for sequencing and genotyping different genetic markers (microsatellite *loci*, single nucleotide polymorphisms or SNP and copy number variations or CNV,...), such as polymerase chain reaction (PCR), restriction fragment length polymorphisms (RFLP), SNPlex, SNaPshot, TaqMan Open Array SNP genotyping technologies and Quantitative PCR; and 3) fragment detection processes by agarose and acrylamide electrophoresis or automated capillary electrophoresis and specific software, and finally, 4) statistical analysis using specific software: Genepop, Haploview, Plink, R software, Structure, Cervus, FSTAT, DnaSP, PHASE, GeneClass, Toucan, Genomatix, Network, MEGA, SPSS, PhyML, Mr. Bayes, BioEdit, BEAST, jModeltest, Populations, PAUP, ARLEQUIN...

Two are the main areas we are working on:

POPULATION GENETICS

In this research area we are focused on the genetic characterization of local animal populations and individual genetic "fingerprint". In the first case, and based on several genetic markers, we try to establish population's taxonomy and evolution, their genetic structure, intra- and inter-population diversity, and hybridization and introgression processes. These types of studies contribute to different species conservation programs, providing useful information for defining management and conservation strategies. The genetic "fingerprint" is the exclusive genetic information of an individual. Genetic "fingerprint" allows carrying out parentage testing in animals and humans, the assignation of an individual to a certain species/breed/population, the identification of Genetic Modified Organisms (GMO), and the traceability of individuals and their products. These applications of DNA technology are included in different areas such as Animal Conservation and Genetic Improvement, Animal Resources Management, Plague Treatment, Food Safety and Forensic Genetics.

We have applied genetic markers in these fields successfully for human, domestic and wildlife animals and plant species, such as: *Ovis aries* (sheep), *Bos taurus* (cattle), *Equus caballus* (horse), *Apis mellifera* (bee), *Reticulitermes spp.* (termite), *Lepus spp.* (hare), *Cervus elaphus* (deer), *Canis familiaris* (dog), *Engraulis encrasicolus* (anchovy), *Thunnus spp.* (tuna fish) and *Zea mays* (corn).

GENETIC ASSOCIATION STUDIES

The general objective of this research area is the identification, by candidate gene or whole genome analysis, of genetic variants or markers such as SNP, CNV or Quantitative Trait *Loci* (QTL) involved in the phenotypic variability of several human and animal traits such as: susceptibility/resistance to autoimmune human diseases (Systemic Lupus Erythematosus and Antiphospholipid Syndrome), and economically important animal traits (resistance to bovine paratuberculosis, milk production in ovine species, and clam's growth).

These associated genetic markers are useful tools for an individualized human medicine, since diagnostic, prognostic and/or therapeutic markers could be identified for the mentioned diseases. In animals, the identified markers can be used in Marker Assisted Selection (MAS) based breeding programs, with the aim of obtaining bovine populations resistant to paratuberculosis, highly milk productive ovine populations and rapid growing clams.

Physiological basis of inter-individual differences in the energy balance and growth rate of bivalve seeds.

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KEY WORDS: Bivalve, Growth rate, detritus utilization, genotypic differences.

The growth performance of seeds (juvenile individuals) is a key trait which greatly determines economical success of bivalve aquaculture. Growth rate is the result of a balance between processes of energy gain and losses which is regulated by both endogenous (genetic) and exogenous (environmental) factors. Significant improvements in molluscs aquaculture might be obtained by applying physiological energetic to the study of two relevant questions, a) reduction of the economical costs associated with feeding of bivalve stocks by implementing alternative food sources and, b) selection of fast growing individuals for aquaculture purposes. These two research lines are currently being developed in our laboratory.

A) Feeding experiments using detrital matter elaborated from different vegetal species (ranging from saltmarsh vascular plants to marine macroalgae) showed the existence of

- Significant differences in the rate at which different detritus might be absorbed, (green macroalgae promoting the highest absorption efficiency), that are functionally linked to enzymatic digestibility of different detritus
- Seasonal shifts in the rate of absorption of detritus
- Digestive acclimation processes allowing individuals to improve utilization of detrital matter.

We are currently testing the contribution that detritus might have on the growth rates of cockle seeds fed diets of phytoplankton partially supplemented by both highly and poorly absorbed detrital matter.

B) Experiments of physiological energetics have been performed with fast (F) and slow (S) growing seeds belonging to different bivalves species (*Ruditapes philippinarum*, *Mytilus galloprovincialis* and *Ostrea edulis*). Growth rates were measured at the laboratory after keeping seeds under controlled experimental food conditions for long term (> 4 months). Two experimental approaches were tried: seeds belonging to the same reproductive event that achieved significantly different sizes (heads vs tails) and equal sized seeds corresponding to different reproductive events (different age).

Results of all experiments indicate that fast grower seeds take advantage of maintaining significantly higher clearance rates (filtering activity) without significant counterweight effects on absorption efficiency and metabolic rate.

The genetic basis underlying these physiological differences are currently being investigated.

Proinflammatory and protumoral effect of *Candida albicans* antigens

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KEY WORDS: Antigens, Cytokines, Recombinant proteins, Tumoral adhesion, Melanoma, *C. albicans*.

Candida albicans is a dimorphic fungus associated to hot blood animals as an opportunistic pathogen that is able to disseminate hematogenously and to cause serious infections in compromised patients. In recent years, the number of candidiasis has significantly increased in hospitals and one important reason for it is the immunosuppressant state generated in patients after surgery.

The first place where the microorganisms that have entered the bloodstream are retained is the endothelial cell lining of the vasculature. The hepatic endothelium cells have, among others, a mannose receptor that is implicated in the host immune response against *Candida albicans*. This receptor is responsible for the clearance of mannosylated circulating waste molecules, such as enzymes and extracellular matrix and it may also clear out infectious agents such as protozoans, bacteria or fungi as *Candida albicans*. The most important antigenic component from the cell wall of *Candida albicans* are the mannoproteins, which are also implicated in the resistance to phagocytosis and adhesion to host.

We have studied the effect that mannoproteins of *Candida albicans* produce in the B16M melanoma cell adhesion to hepatic endothelium (HSE) of mice and the proinflammatory response induced by cytokines. To know the effect of each antigenic protein they were cloned and recombinant proteins were obtained.

Different *Candida albicans* strains coming from our UPV collection were used. They were isolated from patients with candidiasis and compared with reference strains. Cells were harvested in different growth phases, blastoconidia and germ tubes, and after killed by different treatments. Crude extract were obtained and they were fractionated using Preparative Electrophoresis and Rotofor. Mannoproteins of each fraction were purified by Con-A affinity chromatography.

Cells from mice Hepatic Sinusoidal Endothelium were incubated with the mannoprotein fractions previously obtained and tumour cell adhesion was assessed by plate-scanning fluorimetry of BCECF fluorescence. Variations in proinflammatory cytokines were performed by Elisa.

The mannoprotein fractions obtained from *Candida albicans* enhanced tumour cell adhesion to HSE and induced an increase of TNF- α and IL-1 β proinflammatory cytokines. Among the five fractions, the FMN3 was the most important inductor of adhesion. Mannoprotein fractions were characterized by 2D electrophoresis and the immune response was measured by Western-blot against patient sera with different types of candidiasis.

Fifteen proteins were identified by microsequencing and used to perform recombinant proteins. We have found that several of them induced an immunogenic response and increased the adhesion of tumoral cells and the proinflammatory cytokine levels.

Areas of application are diagnostic and therapeutic of the candidiasis and tumour processes.

Understanding the pathogenicity mechanism of the pathogen *Aspergillus fumigatus* at molecular level by the use of molecular techniques as proteomics, PCR, RT-PCR, and DNA microarrays

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KEY WORDS: *Aspergillus fumigatus*, Pathogenesis, Genomics, Proteomics, Gene expression, Detection, Diagnosis.

Aspergillus fumigatus is an opportunistic fungus able to cause a wide range of diseases, being invasive aspergillosis one of the most important with high mortality. The lack of adequate diagnostic procedures leads to delayed treatments which increases the mortality of the infections. The pathogenicity of this fungus is polygenic and multifactorial and is not clear enough. The genome of the fungus has been sequenced but a lot of their proteins are hypothetical or with not clear functions.

Objective

Our goal is to go deeper into the knowledge of the molecular factors involved in the virulence of the fungus. To achieve this goal we are analyzing the *A. fumigatus* transcriptome. We use a whole genome microarray developed by TIGR (The Institute for Genome Research) in order to study the expression of genes in vitro during culture and in vivo during infection.

Techniques

- Conventional microbiological techniques for cultivation and detection of the microorganisms.
- Development of animal models through intravenous and intranasal routes
- Systems for DNA and RNA extraction and stabilization
- Gene expression through the use of whole genome microarray hybridization
- Bioinformatics for analysis of gene expression
- PCR Conventional, real-time PCR and RT²-PCR for gene expression confirmation and development of rapid techniques for detection.
- Electrophoresis of DNA, RNA, and proteins
- Proteomic techniques
- Protein and DNA sequencing
- Histological techniques

These studies will confirm some well known targets and the discovery of new pathways involved in pathogenicity and virulence of *A. fumigatus*, and the development of new antifungal therapeutics. The identification and selection of marker genes that unequivocally could be related with the pathogenicity will allow the development of diagnostic targets. These objectives will have important consequences on the patient's health in a near future.

Activity of the monoclonal antibody C7 and its derived CDRs against *Scedosporium prolificans* infection in an animal model

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KEY WORDS: *Scedosporium prolificans*, monoclonal antibodies, CDR, scedosporiosis.

In the last decades there has been a significant increase in opportunistic fungal infections, particularly in immunocompromised patients. Among them, a relatively high number of infections by *Scedosporium prolificans* have been reported in Spain. *S. prolificans* is resistant to most of the antifungals known; consequently, the patients have a poor outcome, and the mortality between them is very high. In the pre-antibiotic era, the passive administration of antibodies was very useful for the treatment of many infectious diseases. This kind of therapy was abandoned due to the success of antibiotic therapy but, as resistance to antibiotics, and antifungals in particular, is rising, new attention has been devoted to immunotherapy. Cell-mediated immunity has been considered the primary antifungal defense; however, recent reports have shown the existence of protective antibodies against fungal pathogens in serum, though they can be neutralized by non-protective and even deleterious antibodies.

Our research group has developed a monoclonal antibody (C7) with four biological activities in vitro: i) inhibits the adhesion of *C. albicans* to epithelial cells and to a variety of surfaces, ii) inhibits the germination of *C. albicans*, iii) kills *C. albicans* and other fungi (including *S. prolificans*) in vitro, and iv) has tumoricidal activity. What is more, recently we have shown that C7 protects mice against systemic infection by *C. albicans*. On the other hand, peptides with the amino acid sequences of the complementarity determining region (CDR) responsible for the antibody specificity represent a possible new generation of therapeutic agents, as they can retain the activity of the original antibody, but are easier and cheaper to produce, and easier to administer too. Besides, the advantage of passive immunization is the possibility of providing protection even in subjects with impaired immune responses.

Objectives

Our immediate goal was to prove protection by C7 and its derived CDRs, against systemic infection by *S. prolificans* in mice, and to compare their effect with the antifungals in use nowadays.

Results

We have shown that treatment with CDR-L1 extends the mean survival time (MST) of animals infected with *S. prolificans* compared to animals treated with a control peptide with a scramble amino acid sequence. The MST of CDR-L1 treated animals was higher than that of the animals treated with anidulafungin or micafungin too. The percentage of final survival was higher in CDR-L1 treated animals as well.

Future prospects

We will study the combined effect of CDR-L1 and some antifungals in order to get a better recovery of experimental animals from scedosporiosis.

Research Group on Animal Ecotoxicology and Water Quality

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KEY WORDS: Toxicity bioassays, Bioaccumulation, Environmental Risk Assessment, Groundwater Conservation, Biodiversity, Aquatic Oligochaetes

The research team has a wide experience on the study of aquatic ecotoxicity. The first projects were related to the risk assessment of industrial wastes, sponsored by the Basque Government, using both acute and chronic toxicity tests. These studies were mainly focused to **whole-effluent toxicity tests** (WET). Another set of studies were orientated toward the toxicity assessment of **river sediments**, where pollutants accumulate and persist for longer periods.

Since 1990 we have studied the sediment toxicity using two chronic bioassays (*Daphnia magna*: Crustacea, Cladocera) and *Tubifex tubifex* (Annelida, Tubificidae). We have participated in ring-tests with different laboratories for a new bioassays for soil (*Enchytraeus* species) and also proposed a new sediment test for the oligo-haline sections of estuaries (*Limnodrilus hoffmeisteri*). There is an increasing interest in the use of standardised sediment bioassays for measuring **bioaccumulation**, i.e., the concentration of toxic substances in the organism related to the environmental concentration, and **critical body residues**, i.e. the relationships of concentration in the biota related with impairment in survival and reproductive function.

Most recently, the research group has used the **Weight –of –Evidence (WOE) approach**, referred to the process which combines several Lines of Evidence (LOEs) for the environmental assessment of the water quality. In this approach we have incorporated data from four type of data (LOE), namely sediment chemistry, field benthic faunistic community, habitat alterations, sediment toxicity and in recent times bioaccumulation data, too. This conceptual framework requires a Reference Condition to which compare the data obtained from contaminated sites. The data base used for reference condition has been built from many different sites of the study region and it represents the unpolluted Non-Toxic condition of the river sediments in the Basque Country and Ebro River Basin. The **Reference Condition Approach** established as a general philosophy in the European Water Framework has been used in our toxicity risk assessment studies of river sediments through multivariate statistical analyses. Water Authorities yearly publish data on sediment chemistry and field invertebrate communities, measured at sites that are part of the Water-Quality Surveillance Networks, that can be very useful for the assessment of ecological status of water courses and also for future development of Sediment Quality Criteria. The aim of our actual research is to combine these data with sediment toxicity and bioaccumulation data in order to do a risk assessment using the WOE approach.

We also investigate on **Aquatic Oligochaete Systematics and Conservation** of karst regions in the Cantabrian area. Our objectives are:

- First, to contribute to the knowledge on biodiversity of aquatic subterranean fauna
- Second, to describe new taxa for Science, because the composition of the subterranean communities is mostly unknown.
- Third, to contribute to the management for conservation of groundwater through the assessment of biodiversity calculated by indexes of richness, rarity and vulnerability.
- Fourth, to develop evolutionary hypothesis based on biogeography, morphology and molecular data.

Human Genetic Evolution

Concepción de la Rúa¹, Neskuts Izagirre¹, Montserrat Hervella¹, Lara Fontecha¹, Santos Alonso¹, Isabel Smith², Saioa López¹, María Dolores Boyano³, Jesús Gardeazabal⁴, Jesús María Careaga⁵
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KEY WORDS: ancient DNA, degraded DNA, mitochondrial DNA, forensic analysis, bioanthropology, melanoma, genetic expression, human diversity, resequencing, bioinformatics.

DEGRADED DNA: RECOVERY AND ANALYSIS

Ancient DNA (aDNA) is recovered from tissues of organisms that lived in the past. The recovery of aDNA sequences is essential for forensic and evolutionary studies. The degradation of aDNA requires a complex and laborious methodology for its analysis. This process includes, taking precautions to avoid contamination with exogenous modern human DNA and the authentication of results by independent multiple analysis. The preservation state of the genetic material recovered from ancient samples limits the type of genetic markers that we can analyze. The mitochondrial DNA (mtDNA) is the best marker due to the high copy number per cell; but its maternal transmission only tells us about the demographic history of women. We could also try to analyze the Y-chromosome variability, both for individual identification and for kinship analysis.

PIGMENTATION OF THE SKIN AND MELANOMA

There are genetic and environmental factors that determine the risk to melanoma susceptibility. In particular, light-skinned individuals are less protected against photocarcinogenesis and/or photoaging after solar irradiation, especially in recent years, when UV radiation has increased due to the weakening of the ozone layer. Therefore, we are trying to identify genetic variation associated with skin pigmentation in humans, in order to infer its adaptive value and assess its biomedical implications. For that reason, we are focusing on the detection of differentially expressed genes in melanocytic cell lines from individuals with different skin pigmentation, using expression chips (Affymetrix). Subsequently, a subset of loci is selected to analyze their sequence diversity by resequencing and their variation in the copy number of their exons. The variability discovered is analyzed in collaboration with other laboratories, in melanoma patients and healthy individuals. We are evaluating the adaptive value of these polymorphisms by means of bioinformatics and trying to infer the potential biomedical implications (predisposition to cutaneous melanoma).

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Ecophysiological aspects of plant stress and soil contamination (EKOFISCO)

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Department of Plant Biology and Ecology

KEY WORDS: Environmental Stress, Biomarkers, Photoprotection, Phytoremediation, Soil contamination, Revegetation, Global Change

Since 1990 our group develops research and teaching activities on physiological and ecophysiological aspects of natural and anthropic agents causing stress in plants. The EKOFISCO group is a consolidated research group distinguish with the highest grade on the Basque Government classification for Scientific Groups in the Basque Country. The group is composed of 6 PhD and 4 PhD students.

The group has developed a variety of novel methodological tools: (i) determination of plant stress biomarkers, in particular those related to photoprotection and oxidative stress, (ii) set up of plant toxicity bioassays to determine the ecotoxicological effects of pollutants in contaminated soils, and (iii) Implementation of physiological parameters to evaluate phytotoxicity or tolerance caused by natural stress conditions as extreme temperatures, drought, light intensity, nutritional disorders, etc. Recently, in collaboration with other groups, we incorporate other genomics methodologies with emphasis in differential gene expression and in the application of DNA microarrays to assess and monitor soil health in a multidisciplinary approach.

All these methodologies has been implemented in several areas of more applied research:

- Determination of the role of photoprotective compounds and tolerance to stress conditions (natural or anthropic) of plant species of special interest for applications to agronomy, forestry and natural ecosystems.
- Use of plant biomarkers to monitor environmental and global change and genotype plant selection for tolerance to adverse climatic agents.
- Identification of environmental agents to enhance nutraceutical compounds (carotenoids and tocopherols) in crops.
- Use of plants for ecological restoration of degraded environments ,specially polluted soils through ecotechnologies as bio- and phytoremediation (Phytostabilization, phytoextraction and rhizodegradation).
- Assessment and monitoring soil health with biological indicators, during remediation processes.
- Evaluation and control of damages caused by phototrophs on infrastructures and elements of cultural heritage.

Our group is very active in the formation of PhD students (5 PhD in the last 5 years) and participate in the Official Master Environmental Agrobiology and Environmental Contamination and Toxicology.

The research indicated above is currently carry out in collaboration with relevant scientists and institutions (national and international) in a multidisciplinary approach.

Genomic and proteomic approaches to Cancer Biology

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KEY WORDS: Cancer, Cell Cycle, Cell Signaling, Gene knockout, E2F, Gene Expression, Genomics, Proteomics.

Cells receive signals for proliferation through growth factor receptors located at their plasma membrane. The signal is transduced inside the cell by signaling molecules that change the cellular state, leading to responses at the nuclear level. Cellular proliferation requires duplication of the nuclear content and physical division of the cell. This process of cell growth and division, called the cell cycle, is the fundamental means by which all living organisms propagate. It must be exquisitely controlled, because aberrant cellular proliferation may give rise to pathologies such as cancer or autoimmunity.

Our understanding of cell cycle control increased enormously with the identification of a system that coordinates the cell cycle to make it work as a clock, and that is conserved in all eukaryotes. However, two major questions remain unsolved: How does this machinery integrate and process growth-controlling signals and decide on the cell's fate? And how is this decision executed?

Research in Biomedicine has experienced an extraordinary revolution in recent years, with the development of technologies that allow the analysis of complete sets of genes and proteins in a particular cell or organism. This has led to the birth of the novel fields of Genomics and Proteomics.

We are applying genomic and proteomic approaches, together with classical methods of genetic analysis, to identify the proteins and pathways that play a key role in the control of cellular proliferation and cell fate, including the dysregulation that contributes to oncogenesis. Current areas of research in the laboratory include:

- 1. The signaling pathways that mediate cellular proliferation, with an emphasis on Ras/Rac- and PI3K-dependent signal transduction.**
- 2. The components of the cell cycle that integrate and process growth-regulatory signals. This area focuses mainly on the analysis of E2F transcription factor activities.**

Biomembranes

Biophysics Unit, Joint Centre CSIC-UPV/EHU

Itziar Alkorta¹, Alicia, Alonso¹, Gorka Basañez¹, Vadim Frolov¹, Juan Manuel González-Mañas¹, Félix M^a. Goñ¹, César Martín Plágaro¹ and Helena Ostolaza¹
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KEY WORDS: Bacterial toxins, Pore-forming toxins, Apoptosis, Membrane fusion, Lipid rafts, Biofilm formation .

The Biophysics Unit is a Joint Centre CSIC-UPV/EHU whose research is oriented towards the understanding of the structure and function of biological membranes, in an attempt to improve human and environmental health. We focus our research on the biophysical study of biomembranes and proteins, with special emphasis on the application of bioinformatics, structural genomics and other advanced methodological tools.

ROLE OF CELL MEMBRANES IN BACTERIAL PATHOGENESIS

We are interested in two bacterial toxins, hemolysin from *Escherichia coli* and adenylate cyclase from *Bordetella pertussis*, that are essential virulence factors in the pathogenesis of important human diseases. Elucidation of structural features required for interaction with host cells and the role played by the target cell membrane in such interaction are focal points in our effort to understand their mechanism of action at molecular level.

THE MECHANISM OF ACTION OF TOXIN PEPTIDES ACTING AT THE MEMBRANE LEVEL

Our research interests focus on the interaction of pore-forming toxins with cell and model membranes. In particular, we are currently studying the actinoporins, 20 kDa protein toxins produced by sea anemones.

MITOCHONDRIAL MEMBRANES, APOPTOSIS AND CANCER

During apoptosis, mitochondrial membranes undergo dramatic changes in permeability and morphology. The principal components involved in these processes are the BCL-2 family proteins, with the assistance of an increasing number of protein/lipid effectors. Our goal is to elucidate the molecular mechanisms of action of specific members of the BCL-2 family and/or their effectors at the membrane level. BCL-2 family proteins play an important role in cellular responses to chemotherapy, and the information gained may facilitate progress in the fight against cancer.

MECHANICS AND DYNAMICS OF CELLULAR AND MODEL MEMBRANES AT NANO SCALE

We study membrane fusion and fission; proteo-lipid interaction, creation and regulation of membrane shape and topology by proteins.

SPHINGOLIPIDS, "RAFTS" AND MEMBRANE DOMAINS

Our group studies, on the one hand, the characteristics of sphingomyelinases and, on the other, the changes induced by the ceramides in the physical properties of the membrane, with the aim of identifying the molecular base of the physiological activity of the ceramides. We are also analysing the tendency of diverse sphingolipids (ceramides, sphingosin) to form domains in the lipid bilayer plane.

INTER-DOMAIN RELATIONSHIP IN INTEGRAL MEMBRANE PROTEINS

More than half of drug targets are membrane proteins. In this sense, membrane protein research has always been an important research area. We study the role of membrane protein in two processes: Bacterial conjugation. It will contribute to solve the problem of antibiotic resistance. Biofilm formation. They are highly resistant to antibiotics. The study of membrane proteins involved in biofilm formation would be a solution to the problem of the majority of the nosocomial infections.

Feeding, growth and reproduction in terrestrial invertebrates

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KEY WORDS: Scope for Growth, Production, Heliciculture, Biological Plague Control, Vermicompost

Objectives:

1. We study growth and reproductive trends in wild populations of terrestrial gastropods. Results and conclusions can be given alternative uses: population management as regards to endangered species of molluscs or biological plague control on agricultural schemes.
2. We use physiological methods to determine scope for growth in the edible snail *Helix aspersa*. Our work focuses on the study of the effects of different foodstuffs (commercial or natural) on production in relation to intensive snail farming and design of commercial foods.
3. Processing Solid Urban Residuals: understanding the physiological basis of vermicompost production by *Eisenia foetida*.

Commercial snail farming requires a stable supply of concentrated and balanced food, dependence on fresh vegetables representing a potential risk for sustainable production. Practical experience derived from snail producers shows large growth differences associated to feeding procedures. A correct formulation of balanced and highly digestive foods becomes a priority if high conversion indexes and fertility are to be maintained in order to guarantee economic benefit. Available information on the influence that both quality or quantity of offered food exert upon growth of farmed snails remains scanty and this fact is actually limiting production in western Europe, meaning that market demands (foremost in France, Italy and Spain) rely on imports from third countries.

The red worm (*Eisenia* spp.) constitutes a biotechnological resource commonly used in organic waste recycling, obtaining as final products organic fertilizer and worm meat (a source of animal protein used in animal food production). *Eisenia* can be reared in a variety of substrates showing high rates of growth and reproduction when compared with other soil organisms. Nevertheless, different studies reveal the negative influence of particular waste constituents, presumably by a combination of both toxicity and feeding restrictions. Our work deals with the influence of composition and maturing times of compost produced from urban solid wastes upon individual growth and reproduction of *Eisenia* worms applying the experimental resources of physiological energetics. We determine individual growth, reproductive effort and growth rates in newborn, reared in garbage mixtures comparing results with rates obtained with a natural substrate (manure from pasture-eating horses).

Methods

1. Field surveys and sampling followed by the use of mathematical models to evaluate growth and reproduction patterns for various gastropoda populations of the species *Arion ater* and *Helix aspersa*.
2. Analysis of Biochemical composition of tissues, faeces and foodstuffs.
3. Respirometric determinations of metabolic rate in individuals and tissues.
4. Laboratory experiments in growth chambers under controlled conditions (environmental and feeding parameters). Use of SFG (scope for growth) procedures to determine potential growth: Ingestion rate, Egestion Rate, Absorption Efficiency, Metabolic Rate, Gut Capacity, Transit time.

Enzyme and Cell Technology

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KEY WORDS: Enzyme, biocatalysis, microalgae, cyanobacteria, gene-exchange, magnetic nanoparticles, hydrogels, endostatin, chiral hydroxyalkanoic acids, biodiesel, bioethanol, CO₂ sink, added-value products.

The main goal of the Enzyme and Cell Technology Group is the **use and development of nanotechnologies** which employ **biocatalysts** (isolated enzymes or microbial cells) for **industrial, environmental or biomedical applications**. The Group has experience and equipments for the production, purification and characterization of proteins and enzymes with industrial or biomedical interest. For this purpose there are available techniques to culture heterotrophic (bacteria, yeasts and fungi) and phototrophic (eukaryotic microalgae and cyanobacteria) microbial cells in orbital incubators or bioreactors (fermentors and photobioreactors). Also there are available technologies for the immobilization of biocatalysts by adsorption or covalent-linking onto solid supports, and entrapment in polymeric matrices (hydrogels) which allows their use in reactors of different design and operation modes at laboratory scale.

Recently, other nanotechnologies have been developed for the synthesis and functionalization of magnetic nanoparticles of interest in industrial biotechnology and biomedicine. Thus, lipases have been immobilized to catalyze the transesterification reactions to produce biodiesel as well as polyhydroxyalkanoate depolymerases, enzymes capable to degrade bioplastics in order to obtain chiral monomers for the synthesis of bioactive compounds of interest in pharmacy or other functionalized bioplastics. Also intensive cultures of microalgae showing remarkably tolerance to CO₂ are being investigated as components of new biological CO₂ sinks of utility to mitigate the release to the atmosphere of industrial gas effluents. The resulting cell biomass will be evaluated as a source of biotechnological added-value products and of reserve oils or polysaccharides of interest to produce biodiesel or bioethanol, respectively.

Among the available analytical or preparative techniques are remarkable the use of VIS/UV spectrophotometry, preparative (LPLC y FPLC) and analytical (HPLC) chromatographies, and electrophoresis (isoelectrofocussing, native PAGE, SDS-PAGE, 2D-PAGE) for the separation and characterization of proteins and nucleic acids. Moreover, the Group possesses facilities and experience to carry out techniques for protein isolation and characterization, enzyme assays, protein cross-linking, image analysis, and the design and operation of lab-bench bioreactors. Also molecular biology techniques for gene cloning, PCR, and for the expression, purification and characterization of recombinant proteins are available.

At present, the on-going **basic** and **applied** projects are:

- Recombinant human endostatin derivatives: a tool to improve protein stability and to study protein-protein interactions
- Immobilization of hydrocarbon-degrading bacteria in biodegradable hydrogels for the bioremediation of oil-spills in sea-shore
- Enzymic degradation of bioplastics for producing chiral monomers
- Gene exchange in thermophilic cyanobacteria
- Synthesis and functionalization of magnetic nanoparticles with enzymes and bioactive compounds
- Utilization of microalgae as a CO₂ sink and as a source to obtain biofuels and other added-value products

These researches were funded by UPV/EHU, the Basque Government (SAIOTEK), MEC (VEM), MSC, Instituto de Salud Carlos III and the European Union (Contract nº 026515-2).

Control of inflammatory processes by bioactive sphingolipids

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Department of Biochemistry and Molecular Biology.

KEY WORDS: Apoptosis, cell proliferation, migration, ceramides, Sphingolipids.

Bioactive sphingolipids play essential roles in normal cell and tissue homeostasis as well as in the establishment and progression of numerous diseases, particularly in those illnesses that are associated to inflammatory responses. Although much progress has been achieved in the last two decades, the mechanisms whereby sphingolipids exert their effects are incomplete, and in many instances unclear.

Ceramides, sphingosine and their phosphorylated forms, sphingosine 1-phosphate (S1P) and ceramide 1-phosphate (C1P), are particularly important because they are present in many inflammatory lesions, and can be generated through the action of pro-inflammatory stimuli. Whilst ceramides and sphingosine can induce cell cycle arrest and promote apoptosis, C1P and S1P promote cell growth and are potent inhibitors of cell death. Our group has long been interested in establishing the biological effects and mechanisms of action of C1P. We first discovered that C1P was mitogenic for fibroblasts and macrophages and have established some of the metabolic and signaling pathways that are involved in these actions. Specifically, C1P stimulates the mitogen-activated protein kinases (MAPK) extracellularly regulated kinases (ERK)1-2 and c-Jun N-terminal kinase (JNK), as well as the phosphatidylinositol 3-kinase (PI3-K)/protein kinase B (PKB, also known as Akt) pathway, and protein kinase C- α , all of which are implicated in the stimulation of cell growth. In addition, we found that C1P potently blocked apoptosis through mechanisms involving inhibition of sphingomyelinase or serine palmitoyltransferase activities, upregulation of the inducible form of nitric oxide synthase (iNOS) or PI3-K, depending on cell type.

At present, our studies are aimed at understanding how these bioactive molecules can control inflammatory processes. Our recent progress includes the elucidation of a new biological activity of C1P, this being the stimulation of macrophage migration. This novel action of C1P led us to identify a specific plasma membrane receptor that is coupled to Gi proteins. In addition to this, we are also investigating the effects of different synthetic analogs of C1P so as to be able to control inflammatory processes, and cell growth and death. In particular our work involves studies on chronic inflammatory illnesses (chronic obstructive pulmonary disease (COPD) and ulcerative colitis), atherosclerosis, and different types of cancer, including studies on tumor metastasis. Many of these studies are being performed in collaboration with different research groups, which are detailed below.

Collaborators:

Robert Bittman (City University of New York, USA)

Paola Bruni (University of Firenze, Italy)

Antonio Delgado, Josefina Casas and Gemma Fabriás (CSIC and University of Barcelona)

The network signaling coupled to P2X₇ is involved in CRAMP and EGF receptor modulation

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KEY WORDS: P2X₇, ATP, ERK172, Duox, Catelicina, Ca²⁺, EGFR.

Submandibular gland (SMG) has been considered a useful model for the study of the signal transduction coupled to purinergic, muscarinic, and adrenergic receptors. Some many years ago, we started to work on the signal network coupled to P2X₇ receptors, the main purinergic receptors expressed by mouse and rat SMG (Alzola, E. et al., 1998; Marino, A. et al., 1999). The main objective of our work is focused on the signal pathways coupled to the P2X₇ receptor and their physiological consequences in the SMG cells (García-Marcos, M., et al., 2009). Among the ionotropic receptors, P2X₇ presents unique properties. Structurally, it contains an intracellular C-terminus much longer than other P2X receptors, the cytoplasmic tail contains several domains for protein-protein and lipid-protein interactions which give to this receptor the ability to form a pore and provoke cell death. P2X₇ activation induces at least two permeability states; it is able to increase permeability to cations such as sodium, calcium, potassium or protons like others P2X receptors, but after a prolonged exposure to ATP it allows the entry of molecules up to 900 Da (North, R.A., 2002). This receptor is able to induce apoptosis related events like plasma membrane blebbing, DNA fragmentation, caspase activation or phosphatidylserine exposure. The P2X₇ receptor is not only expressed in blood cells such as macrophages, neutrophils or lymphocytes, but also abundantly expressed in epithelial cells. Both acinar and ductal cells from SMG express functional P2X₇ receptors. Our results with P2X₇ knock-out mice reveals that this receptor is the main purinergic receptor responsible for the ATP-mediated responses in these tissues (Pochet, S., et al 2007). We have determined the coupling of P2X₇ to a NAD(P)H oxydase and the generation of reactive oxygen species (ROS), by a mechanism independent of MAPK kinase or calcium entry in mouse SMG cells. However, in rat SMG cells, the ROS generation by P2X₇ is coupled to Duox in a calcium dependent manner. (Seil, M., et al. 2008). The ROS production mediated by the receptor seems to have a protect role on the depolarization of mitochondrial inner membrane carry out by the activation of P2X₇ (García-Marcos, M., et al. 2005). Recently, we have determined that P2X₇ receptor regulates the EGF receptor pathway in SMG cells by acting on AMPK, an enzyme responsible for the energetic balance in the cell (Fontanils, U., et al., 2010 in preparation).

Recently, in other studies, by using wild and knock-out murine peritoneal macrophages, the cathelicidin-related antimicrobial peptide (CRAMP) regulates the signal transduction mediated by P2X₇. In wild type cells, ATP increased the intracellular concentration of calcium (Ca²⁺), the uptake of ethidium bromide, the production of ROS, the secretion of IL-1 β , the release of oleic acid and LDH; and decreased the intracellular concentration of K⁺. In knock-out mice, ATP was unable to elicit any response. CRAMP, the unique murine antimicrobial peptide derived from cathelicidin inhibited all the responses coupled to P2X₇ receptors in macrophages from WT mice. CRAMP had no effect on the increase of the (Ca²⁺) evoked by a combination of ATP and ivermectin in macrophages from P2X₇-KO mice. It seems that CRAMP inhibits the responses secondary to the activation of the murine P2X₇ receptors expressed by peritoneal macrophages. This inhibition is not mediated by formylated peptides receptors (FPR) and is specific since CRAMP has no effect on the response coupled to P2X₄ receptors. We could conclude that the interaction between P2X₇ receptors and cathelicidin-derived antimicrobial peptides is species-specific, in some cases (man) positive, in others (mouse) negative and that, at least in mouse, the cathelicidin-related peptide is not the natural agonist of P2X₇ (Seil, M., et al., 2010).

Phenomenological and theoretical Cosmology

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KEY WORDS: Cosmology, Relativistic kinematics and hydrodynamics, dark matter, dark energy.

Our research in this line of work focuses on various theoretical and phenomenological aspects of the Universe at various scales, either within the framework of Einstein's theory or in the broader context of modified theories of gravity. This area of research is nowadays in a golden age, which began two decades ago with the arrival of observational data. This information has been received continuously since then and one could very well assert now that the data available is of exquisite precision. The most revolutionary aspect is that, broadly speaking, this data infers surprising conclusions about the possible components of the Universe, whose "presence" is manifested in the kinematics of the Universe both at the scale of galaxies and clusters, and at cosmic scales.

Description based on keywords from the theoretical frameworks, concepts and tools we use to achieve the general objectives (in italics) of this line of research:

- *Parametrisations for the evolution of the Universe*
Relativistic kinematics
Modifications of General Relativity due to extra dimensions (brane, DGP model, LDGP and QDGP models, model of Dvali-Turner)
Dark energy (cosmological constant vs. phantom energy)
- *Observational Tests*
Type Ia supernovae (SN), background radiation (CMB), baryon acoustic oscillations (BAO)
Equation of state of dark energy
Cosmic Complementarity
Frequentist statistics
- *Unification of dark matter and dark energy*
General Relativity, relativistic hydrodynamics and classical field theories
Description of the Universe on cosmological scales
Description of the Universe at galactic scales
- *Asymptotic behaviour of cosmological models*
Dynamical systems applied to cosmology
Initial conditions
Stability
Autonomous systems, attractors

Physical and mathematical foundations of the structure of the Universe

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KEY WORDS: General Relativity, black holes, gravitation, elementary particles.

Einstein's field equations (or modifications) are to be interpreted as the balance between the geometric properties of spacetime and the physics of non-gravitational fields, and constitute the basic framework for the study of the Universe. Moreover, in order to understand it, one must deepen into the description of the early stages, high energy regimes, and the principles that regulate the laws that govern the Universe, or the nature of its fundamental constituents. Therefore, Cosmology is closely related to the rest of the aspects concerning the structure of the Universe, that is, to the more fundamental aspects, which in general are of a more mathematical nature.

Description based on keywords from the theoretical frameworks, concepts and tools we use to achieve the general objectives (in italics) of this line of research:

- *Dynamic Horizons and geometry of trapped submanifolds*
for the description of black holes in transition from its formation to its final stationary state. Trapped (and dynamic) horizons and isolated horizons. Singularity theorems in theories with extra dimensions (eg strings) and change of signature.
- *Potentials for the curvature tensor (a new Laplacian) in Gravitation:*
potential vector of the electromagnetic field. Thermodynamics of the gravitational field.
- *Symmetric spacetimes of higher order:*
Classification, characterization and obtaining of spacetimes of arbitrary dimension with vanishing second derivative of the curvature. Generalisation to higher derivatives.
- *Physical and mathematical applications of causal tensors:*
super-energy tensor and conservation and exchange laws.
- *Description of rotating compact bodies (stars, galaxies, clusters) in General Relativity:*
Slow-roll approximation, assumptions of stationarity and axial symmetry. Perturbation theory for matching of spacetimes. Axially symmetric regions in equilibrium immersed in cosmological backgrounds: voids.
- *Principle of general covariance:*
Physical meaning, reference systems and quasi-Minkowskian coordinates.
- *Spin of elementary particles:*
Interactions between classical models of particles with spin and their quantification. Symmetry groups associated with each type of classical interaction (quantum representation). Description of bound systems of particles with spin.

Pattern recognition and speech technologies

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KEY WORDS: Speech and language technologies, pattern recognition, machine learning, spoken language processing, dialogue systems, machine translation.

The aim of this research group is the development of technologies for spoken language processing. The group's early investigations were in automatic speech recognition and understanding, with contributions to semi-continuous HMMs for acoustic modelling and to stochastic finite state models for language modelling. Further work has tackled dialogue systems, mainly when they have to function in real conditions. We have also investigated the incorporation of the Basque language into our systems. For this, we have developed acoustic-phonetic models of Basque together with methods for lexical representation which take into account specifics of the Basque language. In addition we have also a line of research in machine translation. Recently we have also dealt with interactive and multimodal voice-based interfaces. Our methodological framework is pattern recognition and statistical models, specifically our contributions are mainly related with stochastic finite state models. We have proposed complete formalisms, inference algorithms and decoding strategies. In addition, we have dedicated significant effort to the design, acquisition and analysis of those linguistic resources needed for statistical model inference.

Another of our lines of investigation has been the development of prototypes and demonstrator systems. We have developed high-performing ASR systems and we have integrated into dialogue systems. This line of work culminates with projects and contracts with companies, eg. a dialogue system for an agent controlling appliances carried out together with Ikerlan and Fagor Electrodomésticos, and a dialogue system for tickets in metro Bilbao with Telvent (Abengoa Group). These projects led the principal investigator of the group to be awarded the Euskoiker Research Prize in 2004. In collaboration with the University of Zaragoza we developed a voice-based information kiosk for Softec (Ibermática). We have wide experience of joint projects with industry (Telefónica I+D, EITB, Adur Software Productions, Rosetta Testu Zerbitzuak, Scansoft, Puertas Rubio). In equal measure, we have collaborated with technology centres (Ametzgaifia, Ikerlan, Cidemco, Vicomtech) and with public bodies (UZEI, Viceconsejería de Política Lingüística del Gobierno Vasco). Special mention should be made of the effort put into the creation of resources for the Basque language under contracts from Telefónica I+D, EITB, EJIE and Scansoft.

Our current areas of research and interest are:

- Hierarchical and cooperative language models for recognition, understanding and translation.
- Multilingualism: language identification and acoustic modelling for Spanish, Basque and English.
- Specific technologies for lexical processing of the Basque language in recognisers and translators.
- Speech translation in limited domains: inference and decoding based on finite state transducers.
- Interactive systems: statistic approaches in dialogue system and management of multimodality.
- Linguistic resources: speech and text corpora, dialogue corpora, multimodal corpora.
- Doctoral training and training of technical engineers.
- Technology transfer: development of prototypes in collaboration with the industrial sector.

It is well worth mentioning a couple of ongoing projects:

- "Multimodal Interaction in Pattern Recognition and Computer Vision" CONSOLIDER-INGENIO 2010 programme (<http://miprcv.iti.upv.es>)
- "SD-TEAM : Interactive Learning, Self-Evaluation and Multimodal Technologies for Multidomain Spoken Dialog Systems" Project financed by the Ministry of Science. (<http://www.sd-team.es>)

Software Technologies Working Group (GTTS)

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KEY WORDS: Speech technologies, language and speaker recognition, multimedia searching.

Research at GTTS focuses on fundamental software technologies, in particular those related to speech processing and information retrieval. Part of our efforts are devoted to develop tools and prototypes for various applications, with emphasis on ambient intelligence environments and the Internet. We pay special attention to develop specific technologies for Basque. Finally, we offer our experience to society, either in the form of diffusion-academic training, or in the form of technology transfer for the development of commercial products.

ACTIVE PROJECTS

- National R & D (MICINN) - 2010/2012: Search and access to information contained in the speech of multimedia resources.
- Saiotek (Basque Government) - 2009/2010: Study and implementation of techniques for the identification and tracking of speakers in the search for audiovisual resources.

RESEARCH ACTIVITY IN THE LAST 5 YEARS

- **Projects:** 9 (330,000 euros)
- **Publications:** 34 (4 magazine, 3 book chapters, 27 peer-reviewed conferences)
- **Thesis:** 1 presented, 4 in progress.
- **Participation in international competitions:**
 - NIST Language Recognition Evaluation (2007 and 2009)
 - NIST Speaker Recognition Evaluation (2008 and 2010)
[NIST = National Institute of Standards and Technology (USA)]
- **Organization:** the "Albayzín 2008 Language Verification Systems Evaluation".

TECHNOLOGY TRANSFER

- **Sautrela:** software package (free access) for the development of speech processing applications.
- **Hearch:** search tool for audiovisual resources (from automatic transcriptions of speech)
- **Kalaka:** database for the development of language recognition systems.
- **Hitzaldi:** tool for audio-text alignment in parliamentary interventions.

<http://gtts.ehu.es/>
<http://gtts.ehu.es/Hearch/>
<http://sautrela.org>

Vaccination strategies for controlling some epidemic models with susceptible, infected, infectious and removed-by-immunity populations (SEIR models)

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KEY WORDS: Epidemic Models, Control Theory, Vaccination Strategies, Positive Systems.

Epidemic propagation models have nowadays a large interest and importance. One of the reasons for studying infection diseases is to develop control strategies to eradicate it from the population. In this context, the practice of vaccination constitutes one of the main techniques used to achieve such an eradication objective. Vaccination is generally applied to a large proportion of population and its main aim is to reduce the number of the susceptible individuals while increasing the number of removed-by-immunity ones.

The present project deals with epidemic propagation models from a Control Theory point of view. A SEIR model is considered for this study. Such models include population of susceptible (S), infected (E), infectious (I) and removed-by-immunity (R) individuals. This kind of models differs between the infected population and the infectious one. The former includes individuals who incubate the disease but do not still have any disease symptoms and the later is composed by individuals who do have external disease symptoms.

The project objectives can be summarized as follows.

OBJECTIVES

- 1- Analysis of mathematical SEIR models for epidemic propagation including the explicit calculation of their solutions, their positivity and stability.
- 2- Development of different control strategies based on vaccination techniques to eradicate the epidemic or to minimize its impact on the population. Several vaccination techniques are going to be considered, namely: constant, impulsive, continuous-time, discrete-time and so on.
- 3- Adaptive control strategies may also be considered in the eventual presence of uncertainty parameters in the epidemic models.
- 4- The design of observers is also foreseen with the objective of estimating the solution of all the individual populations when the model parameters are not precisely known and the initial conditions of each population are unknown.

Smart Materials for Nanopositioning

GAUDEE research group

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KEY WORDS: Nanopositioning, control, smart materials, actuators, sensors.

Smart materials are capable of responding, in a controlled fashion, to one or more different external stimuli. External stimuli can be physical or chemical, like magnetic or electric fields, and the response can, for example, be a change in dimensions. A large field of application of these materials is as sensors or actuators.

Ferromagnetic shape memory alloys (FSMAs) are a particular example of smart materials. They exhibit large strains (~6%), about an order of magnitude larger than piezoelectrics, and they have a higher frequency response than their closest related active materials, the shape memory alloys. They are also attractive because they respond to magnetic fields, meaning they don't need to be directly contacted to be actuated.

The fact that a single material acts as the active element, is an advantage, especially when trying to reduce the size of the actuators, as is the current trend. However, the hysteretic nature of the material presents a challenge to the control of the material, and requires a purpose-built controller.

From this line of research, we propose different control strategies to control FSMAs, and we have experimentally tested them out on two platforms: a home-built actuator and a commercial one. So far, very encouraging results have been obtained, and positioning accuracies of 2 nm and 25 nm respectively have been achieved.

Once the controllability of these materials in the nanometric range is fully explored, improvements to the actuators are proposed as future lines of research. Up to now, a spring has always been used as the reset force in the actuators. A new actuator with two orthogonal Helmholtz coils is proposed now. The orthogonal fields can actuate the field in the two opposite directions, and the use of a spring is no longer required. The nature of the material allows you to set a position and no longer require any input to maintain it. In addition, this new actuator could minimize the overall size and weight of the actuator. Moreover, the power supply that this new actuator required is smaller since it operates in pulsed mode, and the weight is reduced because the actuator itself has no iron yoke.

A new line of research for the group is the development of a displacement sensor with nanometric resolution based on high frequency resonant cavities.

Networked Control Systems and Applications

GAUDEE research group

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KEY WORDS: networked control systems, real-time control, monitoring, EPICS, beam diagnostics, scientific facilities.

Digital communications have changed deeply the application of automatic control systems since they allow to compute the control laws in a distributed environment. However, the network link introduces a variable time delay, which confers a partial asynchronous nature to the system. Thus, networked control systems (NCS) are a very active research topic in the automatic control community. The main advantages of NCS are the optimization of resources and a better integration of different devices, due to the advances in Information Technologies (IT). However, NCS approach involves several challenging problems related to the communications link delays and information losses. Therefore, the development of a new control theory for exploiting the possibilities of this new control approach is very attractive field of research. One of the studied solutions is based on the use of middleware strategies in order to achieve transparency in the communication stages and improve the design of large distributed systems.

In addition, event-based control strategies increase the advantages of NCS, since they can dramatically reduce the network resources requirement. However, the nonlinear nature of such schemes requires the development of control algorithms adapted to this kind of sampling methodology.

One of the most relevant characteristic of a control system is its Real-Time (RT) behavior. The research group is involved in the study of the implementation problems, from the RT point of view, of control systems in general, including NCS systems, and in comparing different technologies and solutions, including RTLinux, Labview RT, and Java RT. The main objective is the determination of applicability limits and capabilities for implementing reliable real-time control systems. In addition, this research includes the use of network links using standard technologies, such as TCP/IP.

On the other hand, the so-called Experimental Physics and Industrial Control System (EPICS) is one the main tools used in large scientific facilities for distributed control and monitoring. This middleware, which has soft real-time characteristics, is an open source initiative. The group is starting a research line around EPICS, in collaboration with ESS-Bilbao and international laboratories in the field of particle accelerators. This research line includes the implementation and study of diagnostics necessary in particle accelerators, as for example beam position monitors. This is specially focused on the design of the control system and their integration in an EPICS network.

The research group works closely with ESS-Bilbao whose proton accelerator requires an ever growing number of control and monitoring developments, leading to new research topics for the group.

Multidimensional electronic systems for Computational Intelligence applications

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KEY WORDS: Digital electronics, Computational Intelligence, FPGA.

The main objectives of the “Group of Digital Electronics Design” are: i) basic research, application and synthesis of models for nonlinear dynamic systems, ii) applied research and efficient developments of embedded electronic systems, and iii) study and development of innovative applications in the field of Computational Intelligence (mainly Neural Networks, Genetic Algorithms, and Fuzzy Systems) for all those fields of applied interest (Ambient Intelligence, Robotics and Vision, Biosystems, Intelligent Control, etc.).

RECENT APPLICATIONS DEVELOPED BY THE GROUP

Last generations of reconfigurable technologies, particularly Field Programmable Gate Arrays (FPGAs), make possible to implement a whole electronic system (e.g., processor core, memory blocks, peripherals, and application specific hardware) on a single chip with the consequent savings in size, cost and power consumption. Next, some electronic systems developed by the group with FPGA technology are outlined.

Ambient Intelligence (Aml) environments should be able to capture and process information from multiple sensors using embedded electronic systems capable of responding in real-time. The complexity and high dimensionality of these electronic environments lead to considering simplifying elements, both in modelling and in their synthesis, with the aim of improving their efficiency and performance. The group has implemented several embedded electronic systems for Aml environment control using reconfigurable hardware (FPGAs), in particular, heterogeneous hardware/software reconfigurable systems (SoPC: System on Programmable Chip).

Computational Neuroscience is the study of brain function in terms of the information processing properties of the structures that make up the nervous system. It is an interdisciplinary science that links the diverse fields of neuroscience and cognitive science with electrical engineering, computer science, mathematics and physics. A key work in this field is the “HH model” proposed by Alan Lloyd Hodgkin and Andrew Huxley in 1952. This model describes the ionic mechanisms underlying the initiation and propagation of action potentials in the squid giant axon (they received the Nobel Prize for this work in 1963). Although several hardware implementations of the HH model can be found in the literature, our group has developed the first complete digital circuit that emulates this model. The main contribution of this work consists in the use of piecewise linear approximations with variable precision to reduce the computational complexity of the neuron.

Image recognition systems are widely used in different industries such as production plants to detect faulty components on a conveyor or as surveillance systems that are capable of detecting intrusion, differentiating people or observing their motion. What all these systems have in common is the use of high performance cameras and powerful computers with few constraints in power consumption, real-time behaviour, size or cost. In autonomous mobile systems such as mobile manipulators the framework is very different. Object positions and environmental conditions have to be acquired in real-time. Visual servoing is a useful capability for both manipulator arms and mobile robots. However, fast and computation intensive tasks are difficult to implement in small and low power consumption electronic systems required in robot-like systems. The group has developed an efficient hardware/software implementation of an object recognition system for an autonomous robot based on a neural network.

Finally, as a preliminary prototyping example in the field of Automotive, we implemented a complex fuzzy controller for a vehicle semi-active suspension system composed of four parallel intelligent controllers on a single FPGA. The group is also interested in applying Model Predictive Control (MPC), the standard for complex constrained multi-variable control problems in process industry, in the field of Automotive.

Microstructural, magnetic and spectroscopic characterization of materials with high technological applications

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KEY WORDS: Magnetic Nanoparticles, Fe-Al Intermetallics, Semiconductors Optoelectronics, MSMA.

The group is comprised of six members of three different departments. They carry out different research lines:

Magnetic nanoparticles and their applications. Magnetic gold has become a reality in the XXI century. Our research group has been able to synthesize gold magnetic NPs. surrounded by organics elements, and likewise magnetic NPs of other noble metals (Ag, Cu). Our group has demonstrated for the first time, and with no doubt, that the origin of magnetism present in the gold NPs reside only in Au atoms on the surface of the NPs. Surprisingly, we also found in NPs permanent magnetism, whose origin is a mystery. There are some clear indications that make us perceive the existence of a new type of magnetic anisotropy which causes this magnetism, and our first and fundamental goal is to understand it. We also will try to extend this to other materials. Indeed, we have already obtained pure ZnO nanoparticles showing magnetic behaviour too. Regarding applications, we use the magnetic NPs in biomedicine and the first challenge we have taken is to develop a system for the ablation of cancerous tissue by means of magnetic NPs.

Materials research with potential technological applications by spectroscopic techniques. In this line we include:

- a) Compound semiconductors for optoelectronic applications, where we are currently focused on the study of ZnO because of its great potential in device applications in the region ultraviolet-blue. Our objective is to characterize the optical properties of ZnO crystals (bulk material and heterostructures) grown by different methods in order to identify the defects responsible for their luminescent properties,
- b) Magnetic Fe-Al alloys in order to understand the influence of the different parameters on their magnetic behaviour, and
- c) Shape memory materials for use in magnetic controllers-actuators capable of working at high frequencies without external temperature variation. We have recently begun working in this line with the purpose of determining the influence of atomic disorder on their properties, as well as the mechanism of fracture after fatigue induced by the cycling of the material in its use as a device.

The work above has been carried out under different financial assistance from various agencies and institutions.

MAT 2001 – 2920 ; MAT 2004 –06841 ; MAT2006-12743 ; MAT 2007 – 66129 ; MAT2009-14398.

SAIOTEK S-PE07UN35 ; SAIOTEK S-PE08UN80.

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Pressure induced complexity in solids

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KEY WORDS: High pressure, Ab initio calculations, Superconductivity, Plasmons, Phonons, Anharmonicity.

Pressure strongly modifies the properties of solids. In our group, we are trying to characterize making use ab initio theoretical techniques based on density functional theory (DFT) why pressure acts as a catalyst of complexity in the solid state and which are the unrevealed phenomena that emerge with increasing compression. Moreover, the study of matter under high pressure provides a very useful tool in the search of new materials that may be metastable at ambient conditions and, therefore, have a wide range of technological applications.

Under pressure core electrons overlap leading to an electronic complexity not expected at ambient conditions. The long lived low-energy plasmon that we have recently predicted in compressed lithium is an example of that. This plasmon is strikingly similar to the one found in the very good superconductor MgB₂. In fact, the search of new superconducting materials is one of our main goals. Pressure enhances superconductivity in lots of compounds as we have demonstrated in the group IV hydrides that may reach a T_c of 60K at high pressure. What is more, we have thoroughly studied the high pressure superconducting phases of calcium, which is the element that reaches the highest T_c.

High pressure research poses strong theoretical challenges as matter is studied under extreme conditions so that approximations valid at normal conditions cannot be applied straightforwardly. For instance, we have shown that going beyond the harmonic approximation in phonon calculations is required both in AlH₃, where anharmonic effects may suppress the large T_c predicted within the harmonic approximation, and simple cubic calcium, where the instabilities may be lifted when anharmonic contributions are included. Nonadiabaticity, electronic nesting, the enhancement of the local field effects and so on are further theoretical aspects that may become crucial under pressure in some materials.

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KEY WORDS: Crystallographic symmetry, Phase transitions, Online tools.

The Bilbao Crystallographic Server (<http://www.cryst.ehu.es>) is a web site with crystallographic databases and programs. It can be used free of charge from any computer with a web browser via Internet. The server has been operating for more than ten years, and new programs and applications are constantly being developed. The aim of the present contribution is to report on the current state of the server and to provide a brief description of the accessible databases and programs.

The server is built on a core of databases and contains different shells. The set of databases includes data from International Tables of Crystallography, Vol. A: Space-group symmetry, and the data of maximal subgroups of space groups as listed in International Tables for Crystallography, Vol. A1: Symmetry relations between space groups. There is an access to the crystallographic data for the subperiodic layer and rod groups. A k-vector database with Brillouin zone figures and classification tables of the k-vectors for space groups is also available.

The second shell contains applications which are essential for problems involving group-subgroup relations between space groups. Given the space group types of G and H and their index, the program SUBGROUPGRAPH provides graphs of maximal subgroups for a group-subgroup pair $G > H$, the different subgroups H_j and their distribution into conjugacy classes. The Wyckoff position splitting rules for a group-subgroup pair are calculated by the program WYCKSPLIT.

The next shell includes programs on representation theory of space and point groups. REPRESENT constructs little group and full group irreducible representations for a given space group and a k-vector, CORREL deals with the correlations between the irreducible representations of group-subgroup related space groups. The program POINT lists character tables of crystallographic point groups, Kronecker multiplication tables of their irreducible representations and further useful symmetry information.

Parallel to the crystallographic software we develop a shell with programs facilitating the study of specific problems related to solid state physics and structural chemistry. The program PSEUDO performs an evaluation of the pseudosymmetry of a given structure with respect to supergroups of its space group. AMPLIMODES is a computer program that can perform the symmetry-mode analysis of any distorted structure of displacive type. The analysis consists in decomposing the symmetry-breaking distortion present in the distorted structure into contributions from different symmetry-adapted modes. Given the high and low symmetry structures, the program calculates the amplitudes and polarization vectors of the distortion modes of different symmetry frozen in the structure. The program SAM calculates symmetry-adapted modes for the centre of the Brillouin zone and classifies them according to their infrared and Raman activity. NEUTRON computes the phonon extinction rules in inelastic neutron scattering. Its results are also relevant for diffuse scattering experiments.

In general, the tools located on the server can be combined to analyze, calculate and visualize problems of structural and mathematical crystallography, providing a collection of applications under the same working environment.

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KEY WORDS: Climate, meteorology, air pollution.

The EOLO group has made contributions in three main areas of research:

- Analysis of observed and modelled atmospheric and climatological data
- Use of advanced statistical techniques for classification and forecasting of different variables at the regional scale (downscaling)
- Use of mesoscale numerical models (MM5 formerly and WRF currently) for downscaling, hindcast and diagnosis of meteorological events and processes

DATA ANALYSIS

The data-analysis studies have covered diverse areas such as the variability of temperature and precipitation, SO₂ or ozone concentrations and lightning discharges. The relationship of these fields and the large-scale structure of atmospheric fields such as geopotential, wind speed, moisture, moisture transports or convective activity has been examined in detail. During the last years, these studies have also been extended to oceanic variables, such as Sea Surface Temperature (SST) and the use of reconstruction techniques to yield daily SST values despite the presence of clouds over the target area.

STATISTICAL DOWNSCALING

In this field, the members of the group have prepared methodological advances in deterministic and probabilistic (bayesian) precipitation forecasts, both at the climatological scale and also for precipitation forecasting with very short lead times. Statistical downscaling techniques have been used for practical applications ranging from operational seasonal forecast of temperature, atmospheric pollution or quantitative precipitation forecasts.

MESOSCALE NUMERICAL MODELS

The group has used the MM5 mesoscale model since 2003 and has recently (2007) migrated to NCAR's next generation model, WRF. The studies with these models have covered areas such as downscaling in climatological (long) time-scales, testing the behaviour of the different parameterizations that can be used in the model over the Iberian Peninsula. The outputs of long integrations with the mesoscale model have also been used in other practical applications, particularly covering precipitation forecasts. The model has also been used in basic research, such as the study of the atmospheric tides over the Pyrenees.

Further information on members, projects and publications can be found at the group's WEB page:

<http://www.ehu.es/eolo>

Electronic excitations and many-body effects in solids, surfaces and nanostructures

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KEY WORDS: Electronic excitations, many-body, first-principles.

Our research is devoted to *first-principles* theoretical investigations of many physical phenomena related to electronic excitations, dynamical response and many-body effects in solids. In particular, we are working on the following topics:

1. Dynamical response and friction of real solids

We study the dynamical response of metals and the energy-loss of slow ions in the framework of time-dependent density-functional theory (TDDFT) using a plane-wave basis set combined with pseudopotentials or a linearized augmented plane-wave basis set (LAPW). This enables us to study the electronic excitations which can be related to experimental measurements such as the inelastic electronic or X-ray differential scattering cross-section.

▪ Electronic and many-body properties of metallic surfaces

In order to analyse the validity of the local-density approximation (LDA) of density functional theory (DFT), we perform variational and diffusion quantum Monte Carlo (VMC and DMC) calculations to obtain the exchange and correlation energies of inhomogeneous many-body systems from the knowledge of the spherical average of the structure factor. Using the recently developed method to obtain exact expectation values of operators that do not commute with the Hamiltonian, we expect to extend the methodology to investigate the electronic response of real solids with QMC techniques.

▪ Electron and hole dynamics in solids

We investigate the lifetime of the electrons with energies a few eV above the Fermi level, which can be measured via time-resolved two-photon photoemission (TRTPPE) and tunnel spectroscopy. Lifetimes depend essentially on the electron-electron interaction, which allows understanding the dynamics of electrons and holes using many-body theory. We have performed exhaustive evaluations of the inelastic linewidth of bulk, image, and surface states in simple and noble metals using the self-energy formalism, many-body and Green function techniques. We plan to extend our research to the study of the lifetime of the surface state confined in quantum corrals on the Ag(111) surface, which have already been measured experimentally.

4. Relativistic electron structure of metal surfaces: STM images and Friedel oscillations in presence of strong Spin-Orbit

Since the rather unexpected discovery of the fine electronic structure of the Au [111] surface, the theory of the spin polarization on metal surfaces has attracted an increasing scientific interest during the last decade. Mostly due to the potential of the emerging field of spintronics and the very recently discovered topological insulators, the efforts to understand the relativistic electronic structure effects on metal surfaces has acquired a great importance. We have implemented a new method for calculating the full relativistic electron Green function based on the exact inversion of the Dyson equation. With this new method applied to surfaces with strong spin-orbit interaction (e.g. Bi110, Bi110, TI/Si(111),...), we obtain very accurate results of the electronic and spin structures in presence of impurities and also the Friedel oscillations observed with spin resolved Scanning Tunneling Microscope (STM) techniques. The results obtained so far show very good agreement with complex experimental STM images.

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KEY WORDS: Magnetic Nanostructures, Ferromagnetic Shape Memory Alloys, Thin Films, Giant Magnetoimpedance.

The Magnetism and Magnetic Materials group starts working at the Faculty 20 years ago. As a result of the research, the group is acknowledged as a consolidated research group.

The main objective of the group is to prepare and characterize new magnetic materials with outstanding applications.

Nowadays the main research lines are the following:

Nanostructured thin films magnetic materials

The study of the magnetic properties of nanomagnets is an issue of enormous interest due to their potential applications as magneto- and bio-electronic devices. The physical properties of nanostructures can be markedly different from those of bulk materials. If the reduction in size reaches a few nanometers, striking phenomena like giant magnetoresistance or magnetic coupling through non-magnetic spacers appears and plays a crucial role in determining the magnetotransport, magnetic moment and magnetic interactions.

Ferromagnetic Shape Memory Alloys (FSMA) in bulk, composite and thin film form

FSMA are active materials that undergo large deformations (up to 10% for some NiMnGa alloys) under the effect of mechanical stress and magnetic field in very short times (a few milliseconds). They present also basic aspects that are attractive for a materials scientist, as the analysis of the magnetic moment (most are typical Heusler alloys) very sensitive to atomic order, multiple structural transitions (premartensitic, martensitic, intermartensitic), large magnetoresistance, etc.

Giant Magneto Impedance (GMI) devices and thin films

The GMI effect produces huge changes in the electric impedance of a soft magnetic material and provides excellent sensitivities to small magnetic fields. It is already used in sensor devices to measure orientation (inside the Earth magnetic field) and other applications. The actual trend is to produce GMI material in the form of thin films to obtain miniaturized devices that can be integrated in microelectronic circuits.

The techniques currently employed by the group include:

- Pulsed Laser Deposition technique
- Sputtering technique
- Atomic/Magnetic Force Microscopy (AFM/MFM)
- Magneto-optical Kerr effect Microscopy
- Photolithography Laboratory
- SQUID magnetometer (SGiker facility)
- Vibrating Sample Magnetometer (SGiker facility)
- Neutron Techniques (Great European Instalation Facilities: ILL, ISIS)
- Synchrotron Radiation Techniques (Great European Instalation Facilities: ESRF, Diamond)

RF & Microwave Group

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KEY WORDS: Noise Characterization, Stability Analysis in High Power Amplifiers, LINACs.

- The RF & Microwave Group works in the field of high frequency circuits and systems for different applications: wireless communications, radio navigation and scientific equipment. Their basic research axes are focused on the analysis and design of microwave circuits and high frequency instrumentation. Currently, three main activities are being developed: characterization techniques of electric noise in microwave circuits, stability analysis of power amplifiers for satellite applications and RF instrumentation for particle linear accelerators (LINACs).

Electronic and optical excitations in nanostructures

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KEY WORDS: nanostructure, nanowire, nanoshell, plasmon, DFT, BEM

We study theoretically the structural and dynamical properties of metallic nanostructures, free-standing or supported on surfaces. These systems are very interesting from the basic point of view because of the emergence of quantum phenomena, which sometimes can be the basis for new applications in electronic and optical devices. We are involved in two different research topics.

One research line is focused on the electronic structure and dynamical properties of nanowires and nanoislands or thin films of a few atomic layers grown on surfaces in a controlled way. Electron confinement gives rise to quantum size effects and quantum electronic transport in metallic (as Al or Na) nanowires. At the nanometer size level electronic current doesn't follow Ohm's law but it is quantized. We are motivated by experiments with the MCBJ (Mechanically Controllable Break-Junction) technique developed in the 90s, in which the conductance is measured as nanocontacts are formed and broken. For the structure and transport study we perform quantum-mechanical self-consistent DFT (Density Functional Theory) calculations with multigrid methods and the WPP (Wave Packet Propagation) method.

Another system under study is formed by metallic islands of a few atomic layers, grown on surfaces, as Pb islands on Cu(111) surface. Experimental techniques as Scanning Tunnel Spectroscopy (STS) have proved that nanoislands of a given height are much more frequent than others. This is due to the quantum confinement of electrons in the direction perpendicular to the surface, which is the origin of the so-called quantum well states (QWS) and has consequences in different properties as superconductivity. We have studied the energy of this system and the lifetime of electrons in such states.

In this context we are also interested in the screening properties of the two-dimensional electron gas, which is a key question in order to explain the behaviour of some high temperature superconductors.

The second research line deals with the electromagnetic response of nanostructures in the interaction with electron beams or light. In this case we analyze experiments of Electron Energy Loss Spectroscopy (EELS) and optical spectroscopies, in which plasmons are excited in the nanostructures. These excitations are resonances of the electronic density, which depend on the size and composition of the nanostructure and the surrounding. Plasmonic systems give rise to large field enhancements in very localized regions, which make them very attractive in surface enhanced spectroscopy. Very recently, simultaneous measurements of electronic conduction and Raman response in molecular junctions have been reported, suggesting the possibility of sensing individual molecules. We study how the optical properties of a strongly coupled (non-touching) nanoparticle dimer are influenced by the presence of a conductive bridge between the particles. This study suggests that molecular conductance at elevated frequencies might be probed by optical means and might provide a possible path for measuring molecular conductance in the visible and near-infrared part of the spectrum. The relation between electron conduction and optical properties is also being explored in other systems as the tip of the tunnel microscope in contact with a surface or systems involving cucubiturils (CBNs), gold clusters and conductive junctions.

In these projects we collaborate with the Department of Materials Physics, DIPC and Unidad de Física de Materiales, Centro Mixto CSIC-UPV in San Sebastian.

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Technological applications of infrared radiometry

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KEY WORDS: Infrared radiation, Emissivity, FTIR, Oxidation.

It is a recently created research group (July 2002) in infrared radiometric studies and measurements. During the first years, a radiometer for direct infrared spectral directional emissivity measurements was designed, constructed and calibrated. The device, which is now fully operative, allows the measurement of the spectral emissivity of opaque samples between 1.28 μm and 25 μm , as a function of the temperature between 200 °C and 900 °C, and for emission angles between 0° and 80°. Furthermore, the emissivity can be obtained as a function of the environmental conditions: vacuum or controlled atmosphere.¹

The value of the emissivity is needed for several technological and scientific applications: radiometric temperature measurement (pyrometry), optical constant determination, low observability, high heating efficiency, thermal isolation, solar cells, etc. Additionally, depending on the specific application, low or high emissivity can be required, although, in most of the cases, a selective emissivity is desirable.

According to the possibilities of the experimental device, the following research lines are currently in progress:

- 1- Study and analysis of the measurement method with the goal of improving the radiometer performance.
- 2- Study and control of the emissivity of aeronautic alloys used in aircraft turbine engines. This project is carried out in collaboration with Industria de Turbopropulsores, S.A.
- 3- Study and characterization of the emissivity of cutting tools and some test materials used in the machining industry, so as to model and optimize the machining process. This work is done in collaboration with the Mondragon Unibertsitatea.
- 4- Application of infrared emissivity measurements to the study of in situ oxidation processes at high temperature (till 850°C). These studies lead to information about the oxidation mechanisms and the activation energy.

In the near future, it is planned to open new research areas: Optical constant determination in thin films, emissivity measurement at ambient temperatures by using both direct and indirect methods, etc.

Finally, it is important to remark that the radiometer developed in the laboratory is the only one in Spain, although there are similar and complementary ones in international reference laboratories. This permits to offer a unique service of reliable absolute emissivity measurements to other laboratories and enterprises.

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KEY WORDS: Atlantic Coast, environmental transformation, natural processes, anthropogenic impact

This research group on Coastal and Environmental Geology carries out scientific works based on a geological multidisciplinary approach (sedimentology, geochemistry, micropalaeontology, topography, radiometric datation) that allows characterization of natural and anthropogenic processes responsible for the environmental transformation of the coastal zone during the last climate cycle. In summary, its different activities can be gathered into the following main research lines:

1. Environmental transformation of polluted ecosystems through time and evaluation of environmental regeneration projects

The great variety of activities concentrated on the coastal area are making compulsory the implementation of complex management plans. Historically this area has experienced an intense human pressure that provoked its continuous physical destruction and a deep chemical and biological transformation. The development of environmental conservation and regeneration schemes on particular ecosystems makes necessary to carry out geological studies in order to evaluate their modern characteristics, their historical alteration processes, and the feasibility of environmental improvement proposals.

2. Sea-level variations as a consequence of the anthropogenic climate change

Despite an increase in the sea-level rise rate is potentially one of the most devastating impacts of the future climate change on the coastal areas, our knowledge of the climate-ocean relationship at decadal scale is very poor. Climate change influences the coastline at decadal and centennial scales, and these variations of the relative sea level are registered in the coastal sedimentary sequences. The combined study of historical records and high resolution geological reconstructions of the relative sea level is a powerful tool to fill this gap.

3. Environmental evolution during the Holocene as a consequence of natural processes

Due to the frequent, rapid and intense climatic changes that characterize the late Quaternary period, coastal environments have experienced dramatic variations. Those sediments that have accumulated on these areas contain a very complete record of the processes and events that occurred during this time interval. The high-resolution multiproxy study of this sedimentary record allows to reconstruct the past features, to understand the present conditions and to deduce the possible future environmental variability.

4. Study of sedimentary processes with social and economic consequences

Sedimentary processes in the estuarine areas are frequently altered by man-induced activities such as dredgings, which in some cases lead to undesirable repercussions (migration of meanders and sandbars, disappearance of waves, closure of channels). Sedimentological studies contribute to a great extent to understand the role of the anthropogenic influence and to establish suitable strategies for sustainable development.

5. Geological assessment of archaeological deposits

Human exploitation of natural resources has left a significant fingerprint (metal enrichments, land-use changes) in the environment from ancient times. Geochemical and isotopic analysis of sediments, combined with micropaleontological data, have been used to deal with the evaluation of the pollution levels and the ecological impacts derived from these activities in archaeological deposits.

Behaviour of B, Li, P and other rare elements in metamorphic and granitic rocks from the Central Iberian Zone (Spain and Portugal)

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KEY WORDS: tourmaline, boron recycling, lithium, phosphates, rare elements, pegmatites, Central Iberian Zone

Tourmaline bearing rocks are common, and even locally abundant, in the Central Iberian Zone (CIZ) (Spain and Portugal). The occurrence of tourmaline in different lithologies of this area suggests that B played an important role during the Variscan orogeny. This way, a good knowledge on the source of B, the processes that favoured the tourmalinization events, the possible recycling of boron from tourmaline-rich pre-Variscan rocks, and the evolution and distribution of B during the Variscan cycle, would help in the understanding of the whole Variscan orogeny. On the other hand, rare-element pegmatites (mainly rich in Li and Sn, but also enriched in Nb-Ta, Rb, Cs, B, F and P in many cases) are also common in the CIZ. In general, these pegmatitic bodies show not only a high scientific interest, but also an important economic interest, when elements and minerals associated with pegmatites are being more and more demanded by the new technologies. We are developing a global study of the pegmatites from this area, in order to obtain a valuable information not only on the geology of the pegmatites themselves, but also on the regional geology and on the geochemical behaviour of some elements (e. g. P, B, F, Li, Rb, Sn, Nb, Ta among others) during pegmatitic crystallization. In addition to the scientific aim, we can not forget the potential economic interest of such a study. The better knowledge of the mineralogical and petrogenetical features of these rocks would facilitate the knowledge and understanding of the anatomy and regional distribution of pegmatites, which is definitively helpful for the exploration and exploitation of the important mineral resources frequently found associated to the pegmatitic rocks.

RESEARCH PROJECTS DURING THE LAST FIVE YEARS

- Turmalina en la Zona Centro Ibérica: paragénesis, geoquímica y significado geológico. CICYT
- Reciclaje de boro en la corteza continental de la Zona Centro Ibérica: origen de los fluidos ricos en B e implicaciones geológicas. CICYT
- Las pegmatitas graníticas del domo gneísico del Tormes (Provincias de Salamanca y Zamora, Zona Centro Ibérica): características, distribución, petrogénesis y potencial económico. UPV/EHU
- The pegmatites from the Central Iberian Zone (Spain and Portugal): characteristics, petrogenesis, distribution and economic potential. AI/H-P
- Tipología, distribución regional, modelo petrogenético y explotabilidad de las pegmatitas de elementos raros de la Zona Centro Ibérica (España y Portugal). UPV/EHU
- Reciclaje de boro y formación de turmalina en el complejo del Álamo (Zona Centroibérica, España): implicaciones geológicas. CICYT

COOPERATION WITH OTHER INSTITUTIONS

- Dpto. Mineralogía y Petrología, Universidad de Granada
- Lab. Minéralogie et Cristallographie, Université Paul Sabatier, Toulouse, (France)
- Institut für Mineralogie und Kristallchemie, Univ. Stuttgart, (Germany)
- Lab. Cristallographie et Minéralogie, Univ. Lieja, (Belgium)
- Faculdade de Ciências, Universidade do Porto, (Portugal)
- Consejo Nacional de Investigaciones Científicas y Técnicas, (Argentina)
- Department of Earth and Environmental Science, Univ. New Orleans, (USA)

OTHER ZONES OF RESEARCH

- Pegmatites from the San Luis Range (Argentina)
- Pegmatites from New Hampshire and Maine States (USA)
- Pegmatites from the Southern Tin Belt (Namibia)

Multifunctional Systems for Environmental and Energy Applications: Microporous Materials and SOFC Components

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KEY WORDS: Microporous materials, MOF, SOFC, nanodevices, applications, energy, catalysis.

Science of Materials is especially propitious to foster multidisciplinary interactions that provide the development of new materials, including, among others, the composition, structure, properties and final use studies of these compounds. In that sense, the future applicability of the studied materials is one of the challenges of this research group.

Our research activities include the study of the zeotypic materials, such as phosphites, vanadates, selenites, arsenates and supramolecular entities (MOFs) with dipyrilidic ligands and metals of the first transition series; the study of mixed oxides with potential magnetic, conductive, catalytical, magnetoresistive or electrochemical applications and microstructural, morfological and/or thermomechanical characterization of advanced materials for potential industrial applications. In this context, the studied materials are classified in two groups:

- 1) Microporous solids that contain organic molecules bonded (hybrids) or not (templates) to the inorganic framework are potential precursors of materials with structural and/or textural porosity. These phases can be used, like zeolites, and zeotypes, in general, in industrial processes for gas separation, as molecular sieves or in catalytic processes. The mayor difference between MOFs and classic zeotypic materials lies in the structural response to the solvent removal. Zeotypes show rigid whereas MOFs have dynamic frameworks which are able to answer external stimuli, which can modify the typical properties of the metallic centres (magnetism, optic...). One emerging area into our research group is the preparation of supramolecular entities (metalloporphirins) with discrete systems based on dipyrilidic ligands and metals of the first transition series. With these compounds we are trying to obtain reservoirs of substances capable of being used as fuel, at the same time that the energy and mass transport, load and release mechanisms are analyzed and optimized.
- 2) Recent worldwide interest in building a decentralized, hydrogen-based energy economy has refocused attention on the solid oxide fuel cell (SOFC) technology as a potential source of efficient, environmentally friendly, fuel-versatile electric power. The main activity of our group is focused on the synthesis of new cathode materials in order to optimize the performance of the cell, and their characterization before, during and after operating conditions. In the long term, the goal is to achieve a cost effective processing technique and materials, to reduce the operating temperature and to prevent these materials from long term degradation in order to enable the commercial viability of this technology. One of our most important contributions, is the recently given answer to the problem showed by several mixed oxides used in SOFC, because these materials sometimes react with the electrolyte, reducing the cathode effectiveness. Therefore, we have propose the inclusion of an interlayer (protection barrier) between the cathode and the electrolyte, with the aim of reducing the solid state reactions which take place and, consequently, improving the electrochemical response of the system. In this way, the conductive properties of the cathode are substantially improved.

Our research group (IMACRIS/MAKRISI) collaborates with researchers from various universities (UC, UAB, ULL), research centres (Ikerlan, Ecole Polytechnique Fédérale de Laussane) and institutes (CSIC Madrid and Barcelona) promoting the enhancement of scientific and technological activities of great interest for research and development of new technologies.

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Palaeoenvironmental Analyses with microfossils (PAM)

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KEY WORDS: microfossils, biogeochemistry, palaeoenvironmental analyses, palaeoclimatology, environmental issues

The main objective of this research team is the reconstruction of marine, estuarine and non-marine environments of various geological contexts of late Cretaceous and Quaternary basins of the Basco-Cantabrian and Ebro regions and the North Atlantic Ocean. The methodology is based on a recent model taking into account the distribution of organisms and associated environmental parameters, besides the isotopic composition of their skeletons, and then to apply this model to the geological record. The recent model is based on the study of foraminifer, ostracod and micromammal assemblages, taking into account their taxonomy, ecology, biomineralization in cultures, geographic distribution as well as the isotopic and chemical composition of their calcitic and phosphatic skeletons, which encapsulate some chemical properties of the water. These parameters can be estimated for fossil specimens thus obtaining results on the past environments. Data for palaeoenvironmental interpretation of the marine and estuarine settings have been obtained from the study of sedimentary cores recovered from the bottom of the N Atlantic, the Basque shelf and other localities from the S Bay of Biscay as well as estuaries from Bizkaia and Cantabria provinces. After the analyses of thousands of microfossils of planktonic and benthic foraminifers and ostracods, we establish their taxonomy and distribution through the time interval represented by these sediments. The analyses of the isotopic content ($\delta^{18}\text{O}$, $\delta^{13}\text{C}$) and trace elements (Mg/Ca, Sr/Ca) of selected specimens of those microfossils provide us with an estimation of the palaeo-thermometry and trophic character of the water masses, among other parameters. Non-marine data is obtained from the sedimentary record of continental outcrops and caves where abundant fossils of ostracods and micromammals have been accumulated, among others. These assemblages are characterized taxonomically and their geochemical signals are obtained as well. Finally both kind of records, marine and non-marine, are compared using a statistical multivariate approach (based on transfer functions) providing us with a regional environmental model related to climatic variation. Detailed analyses of time evolution of these environmental modifications evidence the cyclic character of the climate change and its influence in our region. These results can be used as reports in environmental issues.

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Mass transfers through the lithosphere

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KEY WORDS: lithosphere, delamination, tectonics, structural geology, transpression, extensional collapse.

Our main research topics are the mass transfers in the continental crust, a key point for the dynamics of the lithosphere. The most important processes of mass transfer through the lithosphere are due to the motion of ductile shear zones and the intrusion of huge volumes of igneous rocks. They are mainly concerned with the links between the intrusion of plutonic rocks and the nucleation and development of ductile shear zones.

We integrate field studies of Structural Geology, rock fabric analyses, measurements of the anisotropy of the magnetic susceptibility and gravity data in order to perform 3-D models. Since this approach is concerned with geological processes rather than with regional questions, we have selected a few working areas which encompass the main steps of a complete orogenic cycle:

- **Oceanic subduction** in La Puna and the Eastern Cordillera (Salta, NW **Argentina**), with special emphasis on the Calama-Olacapato-El Toro lineament, representing a transfer zone associated to an important change in the subduction angle of the Nazca plate below the South America plate. Magmatism, recent volcanism and active seismicity related to mantle delamination of the South American plate can be also tested in this area.
- **Continental collision and transpression**, in the Central-Iberian Zone of the **Iberian Variscan belt** and in the central and western **Pyrenees**. In the Pyrenees the study analyses the evolution from continental collision to transpression during the Hercynian orogeny (Benasque and Panticosa sectors) and the superposition of the Alpine orogeny. In the Central-Iberian Zone we are mainly working in the internal structure and emplacement of granite plutons, as a way to test the influence of lithospheric delamination in old orogens.
- **Extensional collapse**, in **Betic Cordilleras**. The interest of this area is due to the presence of the **Ronda peridotites, the largest outcrops of the subcontinental mantle in the world**, which allows a unique chance to analyse the deformation of the lithospheric mantle at the Earth's surface.

All of these areas are suitable to test melt-enhanced deformation processes related to the interplay between shear zones and igneous melts. The members of the applying institutions, Universidad del País Vasco and Salamanca in Spain and CONICET in Argentina, have the methodological and regional expertise required for this type of works. The results of this research represent a significant advance in the knowledge of both, the emplacement of granite plutons and the rheological behaviour of rocks during the nucleation, kinematics and evolution of ductile shear zones. These are essential factors for the geodynamic interpretation of orogenic belts.

Fossil record and biodiversity of the vertebrate faunas from the Late Mesozoic and Cenozoic of Western Pyrenees: Evolution and environmental changes.

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KEY WORDS: Vertebrates, Cretaceous, Paleogene, Neogene, Geology, Taphonomy, Palaeobiology, Western Pyrenees.

During the last thirty years, the discovery and study of both continental and marine deposits from the end of the Mesozoic and the Cenozoic of the Western Pyrenees (mainly the Sub-Cantabrian Synclinorium of the Basque-Cantabrian Region and other adjacent areas, such as the Pamplona Basin, the Sierras of Urbasa and Andia, and the northwestern sector of the Ebro Basin), have emphasised the great palaeontological potential of this geological region in vertebrate fossils.

The activities undertaken by our research team are the geological and palaeontological study of the vertebrate assemblages from the Cretaceous, Palaeogene and Neogene, which consist of selachians (sharks and rays), actinopterygians (teleosteans and pycnodontiforms), reptiles (continental forms: dinosaurs –including birds–, pterosaurs and crocodylians; and marine: mosasaurids) and mammals (continental forms: mainly perissodactyls, artiodactyls, and rodents; and marine: sirenians).

The most relevant palaeontological sites of the studied area are the Laño quarry (Condado de Treviño), Quintanilla la Ojada (Burgos) and other Late Cretaceous localities found in Alava, Burgos and Navarra, as well as the Late Eocene site of Zambrana (Alava) and other Eocene localities from the Pamplona Basin (Navarra). Moreover, several outcrops from the Navarrese Domain have yielded ichnites of both mammals and birds of Eocene to Miocene age. Some of these outcrops are very interesting for their richness and the diversity of their fossil assemblages in the Iberian and European contexts.

This research is developed in the frame of a multidisciplinary and multi-institutional cooperation, approaching aspects of stratigraphy and sedimentology (geological context of the fossiliferous deposits), geochemistry and taphonomy (formation of the fossil vertebrate outcrops and fossil diagenesis, taphonomic biases), systematics and phylogeny, palaeoenvironmental reconstruction, evolutionary palaeoecology, palaeobiogeography and biochronology (diversity changes in space and in time). Other activities are related to the geological and palaeontological heritage, the geoconservation of the palaeontological sites and the divulgation of scientific knowledge. This project aspires to a better valuation of the studied vertebrate localities from several points of view (education, culture, fossil heritage and geotourism).

Main research lines:

- Fossil record of both continental and marine vertebrates from the Cretaceous, Palaeogene and Neogene from the Basque-Cantabrian Region and adjacent areas of the Western Pyrenees.
- Stratigraphical and sedimentological frameworks of the vertebrate fossil-bearing beds.
- Taphonomy of the vertebrate associations through the petrological, mineralogical and geochemical analyses of the fossil bones.
- Evolution and biogeography of the dinosaurian faunas from the Cretaceous of the Iberian Peninsula.
- Biodiversity, evolution and distribution of the mammalian faunas from the Eocene of the Iberian Peninsula in relation with the crisis or environmental changes at regional or/and global scale.
- Geological and palaeontological heritages. Geoconservation of the palaeontological sites from the studied area.

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Submarine hydrothermal vents rich in hydrocarbons in the mid-Cretaceous of the Basque-Cantabrian Basin: Characterization and relationship with syndepositional tectonics and magmatism

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KEY WORDS: Hydrothermal vents, hydrocarbons, tectonics, magmatism, mid-Cretaceous, Basque-Cantabrian Basin.

The Basque-Cantabrian Basin was a peri-cratonic rift during the Mesozoic oceanization phase of the Bay of Biscay. Mid-Cretaceous crustal extension and stretching caused an important increase of tectonic, magmatic and hydrothermal processes in the basin. Recently, the discovery and study of cropping out authigenic carbonate deposits and associated chemosymbiotic fauna in the basin suggest that submarine hydrothermal vents rich in hydrocarbons (oil and methane) were formed at its northern margin during Late Albian times.

According to the published model, both the syndepositional transpressive deformation and the synchronic emplacement of a high-level magmatic intrusion controlled fluid expulsion to the seabed through these hydrothermal vents. The purpose of the project herein described is to develop a multidisciplinary study of both recently discovered new hydrothermal carbonate deposits and their related units (sedimentary and magmatic) from other localities of the same margin. The physical link among the carbonate deposits, the cropping out magmatic intrusions and the syndepositional faults allows for determine the relationship between hydrothermal vents and coeval magmatic and tectonic processes. Moreover, their wide and excellent outcrops allow high-resolution studies, with a much higher resolution than that of conventional researches based on seismic profiles.

The central aims of this project are to characterize the Albian hydrothermal vents (age, internal structure, fluids composition and paleotemperatures, intensity and types of flow), establish their impact on both paleoenvironment and sedimentary facies, and determine their formation mechanisms according to syndepositional tectonics and coeval emplacement of magmatic intrusions. In order to obtain these main goals, this research project has following concrete aims:

- To date hydrothermal deposits by ammonites in order to determine the age of the fluid expulsion event (or events).
- To characterize the sedimentology, paleontology, petrology and geochemistry of the authigenic carbonates and related units.
- To carry out the structural analysis of elements which played as conduits for fluid flows (carbonate tubular concretions, syndepositional faults and dykes) as well as of growth deposits associated with both syndepositional faults and magmatic intrusion-generated forced folds.
- To identify the source rock of vented hydrocarbons by geochemical correlation.
- To create local geological models for each vent, as well a regional tectono-magmatic model which explain the Late Albian fluid expulsion event (or events) in that margin.

Finally, results from this project will contribute to a deeper understanding of the processes associated to hydrothermal vents in rift basins and particularly in the Basque-Cantabrian Basin, and they will bring new knowledge to the active petroleum exploration of its northern margin.

Acknowledgements:

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Study of the Upper Cretaceous and Palaeogene in the Basque-Cantabrian basin

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KEY WORDS: Cretaceous, Palaeogene, Stratigraphy, Micropalaeontology.

The research group, composed of palaeontologists and sedimentologists, has been active since 1988. Over these 20 years the research of the group has been focused on the study of the Upper Cretaceous and Lower Palaeogene successions from two complementary viewpoints: micropalaeontology (biostratigraphy and palaeoecology) based on planktonic foraminifers and calcareous nannofossils; and Stratigraphy and sedimentology of continental, shallow-marine and deep-marine facies.

Our research has mainly centred on the Pyrenees, more exactly in the area known as the Basque-Cantabrian Basin. In addition, sections from Tunisia, Egypt and México have also been studied.

Our particular research lines are the following:

- Palaeoclimatic-palaeoceanographic record: analysis of global climate-change events in the Palaeogene and implications for the behaviour of the present day geo-biosphere.
- Hydrocarbon reservoir models: architecture and evolution of carbonate and siliciclastic sedimentary systems.
- Marine communities and ecosystems in the Palaeogene: structure, diversity, biostratigraphy and evolution.
- Chronostratigraphy of the Palaeogene.

Among the most significant results achieved to date, the following are worth highlighting:

- (a) A notable improvement in the reconstruction of the stratigraphic architecture and of the palaeogeographic evolution of the western Pyrenees (Basque-Cantabrian Basin).
- (b) A more precise bio-, chrono and magnetostratigraphic zonation of the sedimentary succession, mainly at the Cretaceous-Tertiary boundary, the lower Palaeocene (Danian *sensu lato*), the Palaeocene-Eocene boundary and the Ypresian-Lutetian boundary.
- (c) A better understanding of the influence of tectonism, sea-level changes and climate changes on continental and marine sedimentation.

Members of the group take part in projects focused on the development of a general model for macroporosity related to ancient platform margin karst systems (Lower Palaeogene successions of the Urbasa and Andia ridges in Navarre).

Finally, this research group has been involved in projects that aimed to spread the social awareness of the value of geological features included in the landscape, providing knowledge and technical consultancy to the management institutions of, for example, the Ordesa and Monte Perdido National Park and the recently established Protected Biotope of the coastal transect from Deba to Zumaia, so that they can use this geological information in their twofold protectionist and pedagogic duties.

The services that the group can provide are summarized as follows:

- Theoretical-practical training in sedimentary basin analysis; advice to carry out geological mapping
- Analysis of current sediment dynamics
- Climate records: Palaeoclimatology
- Biostratigraphic and palaeoenvironmental studies
- Micropalaeontological application for resource prospecting
- Assessment of the conservation of the geological and palaeontological heritage and of its recreational and educational use and management

The Basque coast: reference sections for the Palaeogene

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KEY WORDS: Cretaceous, Palaeogene, Stratigraphy, Micropalaeontology.

The history of the Earth, since its formation about 4600 million years ago, has been punctuated by several events, most of which are recorded in the rocks that make up the planet. Geologists investigate these events “reading” the information stored in the rocky materials that crop up in different places of the Earth’s surface. The ultimate goal of this knowledge is to be able to predict the consequence of similar events that may happen again in the future. To this end, however, a referential Geological Time Scale must be constructed first. This scale is a valid global frame divided into intervals (Eons, Eras, Periods, Epochs and Stages) whose definition is based primarily on Stratigraphy, i.e., the study and interpretation of strata or layers of rocks formed by the accumulation of sediments. The International Commission on Stratigraphy (ICS) is responsible for selecting the geological sections worldwide that best represent the boundaries between unit intervals, i.e., the stages. Stage boundaries are defined by Global Stratotype Sections and Points (GSSPs).

Our group has organized several international meetings in 2006, 2007 and 2009, which showed the international community, and ultimately the ICS, the high geological quality of the Basque coastal cliffs. These are a worldwide reference to observe and study sedimentary rocks accumulated in deep-marine settings during the geological time that extends from the Early Cretaceous to the Eocene, a lapse interspersed with some of the most significant global change events.

- 1) The Cretaceous/Tertiary boundary interval is recorded in the Aitzgorri headland at Zumaia and in the Sopelana beach, reference sections of deep-marine deposits worldwide. In addition to an iridium-rich clay layer, which records the impact of a meteorite on Mexico, a complete record of the various palaeontological events that typify the transition between the two geological periods has been obtained, as well as of several magnetic polarity reversals, which are commonly used to calibrate the chronological position of the former. Furthermore, the Cretaceous/Tertiary transition at Zumaia shows spectacular, well-exposed sedimentary cyclicities that were forced by orbital fluctuations of the Earth during that time interval.
- 2) The Danian/Selandian and Selandian/Thanetian boundaries are recorded in the Itzurun beach at Zumaia and in the Sopelana beach. As a result of the International Workshop of the Palaeocene Working Group (an international team of specialists backed by the UNESCO) held in June 2007, the Itzurun beach was selected as the stratotype section for the Danian/Selandian and Selandian/Thanetian boundaries. This section contains the most complete and best-preserved record worldwide, mainly in terms of the succession of marine plankton events, polarity reversals of the Earth’s magnetic field and orbital Milankovitch cycles for both boundaries.
- 3) The Paleocene/Eocene boundary interval is recorded in the Itzurun beach at Zumaia, among other sections. It is a world-class reference section for the study of the Palaeocene/Eocene boundary in deep-marine deposits. This chronological boundary is characterized by the occurrence of a reddish marl interval. The most dramatic extinction event that affected deep-sea benthic foraminifers over the last 100 million years can be found at the base of this interval. This event and the whole marly interval record a rapid global climate warming (up to 5-6°C in less than 200.000 years), which was probably caused by a massive release of greenhouse gases from the ocean bottom sediments to the atmosphere.
- 4) The Ypresian/Lutetian Working Group of the ICS resolved, during a Workshop held in Getxo in September 2009, to define the stratotype for the Ypresian/Lutetian boundary in the Gorrondatxe beach section, at a dark marly level where the nannofossil *Blackites inflatus* first appeared approximately 48 million years ago. This section contains the most complete and best-preserved record worldwide of the succession of marine plankton events, polarity reversals of the Earth’s magnetic field and orbital Milankovitch cycles. The proposal was approved by the International Subcommittee on Paleogene Stratigraphy and will be soon submitted to be voted by the ICS and, finally, by the International Union of Geological Sciences.

Multistage Stochastic Mixed 0-1 Programming Algorithms and applications

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KEY WORDS: Branch-and-Fix Coordination, nonanticipativity constraints, Twin Node Family, scenario cluster partitioning, lagrangean decomposition, Benders decomposition.

One of the specific objectives of our activity has been to develop an exact algorithmic framework for optimizing multistage stochastic mixed 0–1 problems, so called *BFC-MSMIP*.

The uncertainty is represented by using a scenario tree and it can appear in some of the main parameters of the model, in our case, the objective function, the right hand side and the constraint matrix coefficients. The Deterministic Equivalent Model (*DEM*) of the stochastic version can be expressed by a compact representation or a splitting variable representation, where a copy of each of the 0–1 and continuous variables under each scenario appears at any stage and the nonanticipativity constraints related to the same group of scenarios in each stage are explicitly considered. An equivalent and alternative representation of the *DEM* can be given by a mixture of the compact representation (into the clusters) and the splitting representation between them. In this case, the cluster related problems are linked by the nonanticipativity constraints. We find it crucial to decide the stages where the nonanticipativity constraints are explicitly considered in the model. This information is materialized when the full model is broken down into a scenario cluster partition with smaller subproblems.

The procedure *BFC-MSMIP* cited above uses the Twin Node Family (*TNF*) concept within the algorithmic framework, so-called Branch-and-Fix Coordination, for satisfying the nonanticipativity constraints in the 0–1 variables. We present a scheme for obtaining strong bounds and branching strategies for the Twin Node Families to increase the efficiency of the procedure, based on the information provided by the nonanticipativity constraints that are explicitly considered in the problem.

Also, the procedure needs of the *LP* optimal solution for the *TNF* problems. A new computational scheme for obtaining stronger bounds based on the utilization of the Lagrangean Decomposition is being developed. We are considering four algorithmic alternatives for updating the Lagrange multipliers.

We have developed the algorithmic approach implemented in a C++ experimental code that uses the free optimization software COmputational INfrastructure for Operations Research (<http://www.coin-or.org>) for solving the auxiliary linear and mixed 0-1 submodels. Some computational experience is reported for supporting the efficiency of the new scheme. We are now working on parallel programming to improve solution times and the storage of these multistage problems in memory.

Stochastic programming has many different applications, such as production planning and distribution, energy generation, air traffic management and financial planning, for citing only a few. Actually, we are working on the adaptation and design of the implementation of the *BFC-MSMIP* algorithm for a natural gas network infrastructure design model. We are also working in the development of a stochastic model for fixed-income securities portfolio selection, by introducing two sources of uncertainty, interest rate risk and risk of default. The simplest stochastic model can be structured as a linear model, but 0-1 variables can also be included to incorporate logical constraints.

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KEY WORDS: foliated space, lamination, singular Riemannian foliation, noncommutative geometry.

Our research consists of the dynamic, metric and cohomological study of *foliated spaces*, and the analytic and K-theoretical study of the corresponding noncommutative spaces.

A (*regular*) *foliation* is a partition of a manifold by submanifolds of the same dimension, the *leaves*, arranged locally as the sheets of a book. This arrangement can be very complicated from the topological point of view, when looked globally. The influence of the ambient manifold topology on the topology and transverse dynamics of the leaves has been one of the fundamental questions in foliation theory.

Nowadays, foliation theory is a multidisciplinary field, essentially non distinguishable from the *dynamical systems theory*. It involves several and complex geometric, topologic, analytic and measurable techniques. In the last decades, the specialists in the subject have developed new fruitful research lines by removing some of the restrictions imposed to *classical foliated manifolds*. In particular, our group focuses its work in:

- 1) the study of some types of *singular foliations* (removing the *regularity conditions*);
- 2) the analysis of some *laminations* (elimination of *transverse differentiability*) and of some topological or measurable *pseudogroups* provided with simplicial structures (suppression of *tangential differentiability*);
- 3) the examination of *generic properties* in a topological and measurable sense (elimination of *totality hypothesis*);
- 4) the *noncommutative study* (*à la Connes*) of some foliated spaces (deletion of *commutativity*).

Foliation theory is playing and will play a fundamental role in the qualitative study of both the physical (cosmology and solid state physics) and biological world (molecular biology, genomics and evolution), and appears increasingly in other science fields.

Our concrete objectives can be classified in two main blocks:

- 1) *The study of metric and dynamical properties of foliated spaces* and its relations. Tilings and repetitive graphs give us examples of minimal laminations, useful in the testing of properties and relations. Moreover, noncommutative geometry gives topological and measurable tools that allow us to complete this study (see [1]).
- 2) *Cohomological study of singular Riemannian foliations*. If we classify the points following the different dimensions of the leaves, we obtain a stratification of the main manifold. We study the relation between the *basic cohomology* and the cohomology of the ambient manifold, through algebraic tools such as exact sequences and spectral sequences (see [2]).

Last publications:

- [1] F. Alcalde Cuesta, Á. Lozano Rojo, M. Macho Stadler, *Dynamique transverse de la lamination de Ghys-Kenyon*, Astérisque 323 "Differential Equations and Singularities. 60 years of J.M. Aroca" (2009).
 [2] J.I. Royo Prieto, M. Saralegi, R. Wolak, *Cohomological tautness for Riemannian foliations*, Russian Journal of Mathematical Physics, vol. 16, no. 3, 450-466 (2009).

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KEY WORDS: *L*-valued functions, (quasi-)uniformities, (quasi-)metrics, locales.

Our research focuses mainly on the study of topological problems in which ordered structures play a fundamental role. The most important aspects and objectives of our research are the following:

1. Application of the theory of lattice-valued maps to Topology.

We are interested in the study of maps taking values on sets with some kind of partial order structure, such as complete or completely distributive lattices, but specially on bounded complete domains (due to their importance in Theoretical Computer Science). The kind of problems we deal with cover the following: generation of lattice-valued maps, insertion of continuous functions between two given comparable maps of a fixed type and extension of functions (preserving continuity). The results obtained in this direction have applications in Topology and Theoretical Computer Science.

2. Asymmetric structures: Uniformities and fuzzy metrics.

Our main interest focuses on the study of the relations between (quasi-)uniform structures and certain types of (quasi-)metric structures, with emphasis on *L*-valued structures and those defined in Pointfree Topology. The previous study is fairly useful since it enables us to obtain a general theoretic framework for fuzzy (quasi-)metrics.

3. The concept of real-valued function in Pointfree Topology. Structure and applications.

Recently, we have introduced a new idea which generalizes to the field of Pointfree Topology the notion of a real-valued function. The idea is based on the work of Banaschewski on continuous real functions in Pointfree Topology. Our original contribution enables to consider maps not necessarily continuous, among which semicontinuous maps deserve a special attention. The new notion seems to be promising and up to now it has led us to many original and interesting results. These results have also applications in sections 1 and 2 above.

4. Representation of ordered structures.

This research topic is carried out in collaboration with the team led by Esteban Induráin, from the Universidad Pública de Navarra. Our main objective in this collaboration is to apply some of the techniques developed in section 1 to the representation of several ordered structures, such as interval orders or semiororders.

Methodology: Use of algebraic (order-like) tools to the solution of topological problems.

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KEY WORDS: Partial differential equations, Pseudo-spectral methods, Nonlinear Dirac equation, Stochastic differential equations, Traffic control, Isogeometric analysis, NURBS

ABSTRACT

The Numerical Analysis is a powerful tool for approximating solutions of many problems that appear in a wide range of mathematical fields. In this project we pay attention to the progress made by numerical methods in four different physical models. In particular, here there have been studied numerically a model in fluid dynamics, the nonlinear Dirac equation, the isogeometric analysis associated to the computer assisted design and the stability of the ODE systems that arise from a traffic flow model.

In this work it is presented an efficient integrating-factor method for solving a nonlinear Dirac equation (NLD). Starting with the simplest case of one space-variable, this method, unlike other approaches proposed in the bibliography, can be easily extended to problems with more space-variables.

We describe, by means of asymptotic methods and direct numerical simulation, the structure of singularities developing at the interface between two perfect, inviscid and irrotational fluids of different densities and under the action of gravity.

Isogeometric Analysis is a method for the analysis of problems governed by partial differential equations. Although this method has many features in common with the finite element method, it is more geometrically based. The main idea of Isogeometric Analysis is to use directly the geometry provided by CAD in terms of Non-Uniform Rational B-Splines (NURBS) and to approximate the unknown solutions of partial differential equations by the same type of functions.

Here it has been designed a mathematical formulation that match quite well with the dynamics of a simplified model of traffic flow. The evolution of the traffic depends on some physical parameters that can be approximated experimentally, as the time reaction or sensibility of the drivers, the security distance and the speed. We analytically deduce the conditions under which the traffic flows free or collapses by studying the stability of the equilibrium points of the system. However the addition of some stochastic interaction to the model contributes to regularize the traffic and it softens the collapse. The solutions of the corresponding SDE only can be approximated by numerical methods and due to the stiffness of the model there are recommended the implicit schemes with strong convergence as the midpoint rule.

Mathematical foundations of statistical mechanics and dispersive equations in quantum mechanics

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KEY WORDS: Partial differential equations, Fourier Analysis, Quantum Systems, Statistical Mechanics.

ABSTRACT

The past decade has seen a drastic increase in interest in ultra-cold atoms, driven by experiments on superconductors and Bose-Einstein condensates (2001 Nobel Prize in Physics) of 87Rb, 7Li, 23Na, 85Rb, 41 K, 133Cs, hydrogen, metastable triplet 4He, 174Yb, 85Rb2, etc. These quantum systems are already paving the way to a brand new technological branch (atoms lasers, atom chips, etc), and the increasing diversity of experimental situations means there is a need to better understand the theory of these complex quantum phenomena.

Rigorous quantum many-body theory is however, a notoriously difficult subject. The hurdles that have to be overcome in order to reinforce the mathematical foundations of statistical mechanics and to arrive at important new mathematical results, involve many different fields of mathematics such as probability theory, operator algebras, differential equations, functional analysis or Fourier Analysis.

In fact, a lot of new mathematical models have been created, in the last century, to describe the behavior of Quantum Systems. The research on partial differential equations, for example, had a sensible growth of interest with the appearing of the models proposed by Erwin Schrödinger and Paul Dirac (respectively in the years 1926 and 1928; both of them received the Nobel prize in 1933). The study of these models, and of the more general class of dispersive partial differential equations, deeply contributed to the development of most of the above mentioned mathematical fields. The behavior of solutions of many linear and nonlinear versions of these equations is not yet completely understood. Some deep and strong mathematical techniques, involving functional calculus and Fourier analysis (micro-local calculus, Calderón-Zygmund Theory, Fourier restriction Theorems), are involved in this project, with the aim to state new important theorems describing these phenomena in a rigorous way.

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KEY WORDS: Probability, Additive Functions, Bernstein-type Operators, Inequalities.

The group's research has focused on the interrelationships between probability theory and other mathematical fields such as number theory, approximation by positive linear operators, analytical inequalities, or combinatorics. Problems arise naturally in such fields, that either are of probabilistic nature or can be approached with probabilistic methods.

- *Number theory.* The problems of distribution of values of real additive arithmetic functions are closely connected with those of convergence of certain sums of independent random variables. These problems are the main core of what has been called probabilistic number theory, to which renowned mathematicians like P. Erdős, M. Kac and J. Kubilius, among others, have made essential contributions. Our contribution has been to extend some of the main results to additive functions with values in Banach spaces.
- *Approximation by Bernstein-type operators.* Bernstein-type operators are constructed as mathematical expectations, i.e., as integrals with respect to probability distributions, and this fact allows the use of resources of probability theory and stochastic processes to investigate many of their properties. Our contribution, in collaboration with another group from the University of Zaragoza, has consisted in the consolidation of these probabilistic techniques by obtaining many new interesting results on convergence, preservation of shape properties, best constants, etc., some of which are difficult to deal with, or even inaccessible by means of the usual analytical methods.
- *Analytical inequalities.* The probabilistic approach of some classical analytical inequalities, like Ostrowski inequality and Hermite-Hadamard inequalities, has led us to obtain results that generalize and present in a unified way most specific results founded in the literature.
- *Combinatorics.* Our research has focused on a curious phenomenon that has not received enough attention to date: many combinatorial sequences are, at the same time, sequences of moments of probability distributions. We have greatly increased the number of examples, but our main aim is still to characterize the sequences for which the phenomenon occurs and find a satisfactory explanation of the phenomenon.
- *Related problems.* The development of the ideas used in previous researches have led us also to make contributions in specific probability topics, like stochastic orderings, order statistics, majorization (in Hardy, Littlewood and Polya sense), or the properties of certain families of probability distributions. We believe this is a good illustration that the interaction between different fields often benefits and enriches all areas involved.

BIOSTATISTICS RESEARCH GROUP

Different approaches to analyze continuous and bounded outcomes: an application to health indexes

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KEY WORDS: Health-related quality of life, Patient reported outcomes, Regression models, Statistical methods

INTRODUCTION

From a probability distribution point of view, continuous and bounded outcomes are mixed random variables, having part of its probability spread out over an interval, like a typical continuous variable, and part of it concentrated on the boundaries, like a discrete variable. This is a feature that appears very often in practical research; observed values of a random variable are distributed continuously over an interval, but also concentrated on the boundaries, due to ceiling/floor effects, censoring, truncation or other reasons. Typical bounded outcomes in clinical epidemiology are patient reported outcomes (PRO).

Patient reported outcomes (PRO) are used as primary endpoints in medical research and their statistical analysis is an important methodological issue. PRO are measured with questionnaires and transformed to scores or health indexes. These scores are mostly treated as if they were from a continuous distribution and normally distributed. Nevertheless, such measures tend to generate data that have discrete, bounded and skewed distributions. Thus, standard methods of analysis that assume normality and constant variance, such as the analysis of variance or multiple linear regression, as particular cases of general linear models, may not be appropriate in this context. Theoretical assumptions of the selected methodology and interpretation of its results are issues to take into account when selecting an appropriate statistical technique to analyze data.

METHODS

We present eight methods of analysis for PRO under different assumptions that lead to different interpretation of the results. The proposed methods are: Multiple linear regression (MLR), with least square (LS) and bootstrap estimations, tobit regression, ordinal logistic and probit regressions, beta-binomial regression (BBR), binomial-logit-normal regression (BLNR) and coarsening. All methods were applied to responses obtained from a commonly used PRO, the SF-36 Health Survey, in a real data set of patients from the Galdakao Hospital in Bizkaia. Selection of an appropriate model depends not only on its distributional assumptions but also on the censoring and the continuous or ordinal features of the response.

RESULTS

The BBR approach renders satisfactory results in a broad number of situations. MLR, with LS estimation is not recommended, especially with skewed outcomes. Bootstrap estimation is preferable for continuous and skewed outcomes, although it does not perform well for ordinal responses or responses having high concentration in the boundaries. Ordinal methods are only appropriate for outcomes with a few number of categories, which is not often the case. Tobit regression is an acceptable option under normality assumptions and in the presence of responses having moderate concentration in the boundaries. The BLNR and coarsening proposals are also acceptable, but only under certain distributional assumptions that are difficult to test a priori, although computationally more challenging.

In terms of the interpretation of the results, results from the BBR, BLNR and ordinal logistic regression approaches are more convenient, especially in clinical research.

DISCUSSION

We provide general recommendations for the statistical analysis of PRO as response variables, based on the theoretical assumptions of the model and the interpretability of the results. In the specific application presented here, we recommend BBR for the analysis of the SF-36 as response variable. Other PRO, or generally speaking, other continuous and bounded outcomes, share many characteristics that make them suitable for one, or several, of the presented methodological approaches.

Mathematical technology transfer 2010

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KEY WORDS: Optimisation, Logistics, Statistics, Mathematical modelling.

In a world where quality of life depends increasingly on technology, mathematicians have a highly important role to play in advising and transferring technology to companies. Mathematics has a wide range of applications -- indeed, it can now be seen as omnipresent -- but from a corporate perspective we believe that the need for mathematics centres on the modelling of processes, in optimising and in extracting information from the data available for practical purposes of knowledge and use on the part of the company concerned.

A "mathematical model" can be defined as any form of mathematical description of part of the real world. Mathematical models are fragments of mathematics that contain all the information on the phenomena that they seek to represent. Such models are highly useful, as they enable calculations and therefore quantitative predictions to be made concerning the appearance of the phenomena considered. Once the solution to a problem is known, mathematical modelling also enables simulations to be run and strategies to be established with a view to directing the process under study towards the desired objective.

Optimisation and operational research are concerned with finding ways of obtaining the best solution to a problem that involves different types of variables which must meet predetermined conditions. They can be described in short as "the science of what is best". They can be applied to numerous problems, and more applications are emerging day by day as a result of the need for decision-making in many areas where new models need to be formulated and new algorithms developed to reach solutions.

The objectives of data-processing include exploring, summarising and detecting patterns in large quantities of data with a view to conducting more complex statistical studies and detecting isolated cases and influential observations. The problems that can be solved with statistical techniques include predicting the value of a quantitative or qualitative variable based on the knowledge of a set of observations, detecting interdependence between variables, classifying individuals or variables in blocks and summarising information in smaller, more tractable sets of variables.

The team that we present here has broad experience in collaborations with companies in the fields mentioned above. Specifically, we have conducted projects and contracts with INKOA Soluciones Agroalimentarias, Sidenor I+D, Instituto Vasco de Estadística (Eustat), Metro Bilbao, Cespa, Fundación Aguas de Barcelona, EuskoTren, Ferrocarriles de Vía Estrecha (FEVE), Cementos Pórtland Valderrivas and Eroski S. Coop among others. The most important projects of recent years have included the annual assignation of working days and rest days at railway passenger transport companies (Metro Bilbao, FEVE and EuskoTren), and the supply chain optimization in large chain stores (Eroski S. Coop.).

Mathematical applications at companies go hand-in-hand with the use of IT. In their projects with companies, the team has used various optimisation (Lingo, OSL, COIN-OR), statistics (R, SPSS) and general purpose (MATHEMATICA, Matlab) software packages. The end result of these projects has been operational IT applications.

<http://www.ehu.es/mae/grupottm/>

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KEY WORDS: Matrix Analysis, Control Theory, Linear Systems, Invariants, Perturbation

The aim of our research is to gain insight into the structure of the linear control systems and matrices and to develop mathematical techniques in order to solve problems in these areas. The following four research lines have been designed:

- a) System invariants
- b) Geometry of systems.
- c) Qualitative perturbation theory of matrices and systems.
- d) Quantitative problems on spectral perturbation of matrices.

These research lines are closely related. Nevertheless, in order to clarify the problems that we are interested in, we will state, in a general manner, some of them:

1. Pole assignment to singular systems by state feedback and output injection.
2. Study the geometry of solutions of the cover problem with stability.
3. Study the topology of the generalized partial realization problem.
4. Study the relationship between the Wiener-Hopf factorization indices and the indices given by biproper rational matrices with prescribed finite structure.
5. Clarify the meaning of Rosenbrock's theorem in the context of the theory of vector bundles.
6. Obtain reduced forms for the equations that define a bimodal piecewise-linear system and characterize structural properties such as controllability and stability for this type of system.
7. Extend the concept of controlled invariant subspace to bimodal piecewise-linear systems, studying its geometry and its potential applications.
8. Study the change of the controllability indices of a controllable pair when the elements of a column of the control matrix are slightly perturbed.
9. Find the distance from a given matrix to the set of matrices with less generic prescribed Segre's characteristic and characterize the multiple pseudospectra of normal matrices.

The methods and techniques to be used run over almost all fields of mathematics: from Linear Algebra and Matrix Analysis or Combinatorics to Differential Geometry or Commutative Algebra.

The research group splits into small subgroups according to the four research lines. Weekly seminars are kept where the progression of the subgroup's work is shown, the difficulties are discussed and other researchers' work related to our problems is explained. This and the individual study of papers are the main methodological tools. A joint research project is shared with a team of Universidad Politécnica de Cataluña. Annual meetings are held to keep track of the advances on the project. The results are published in the most important specialised journals: Linear Algebra and its Applications, SIAM Journal of Control and Optimization, SIAM Journal on Matrix Analysis and Applications, International Journal of Control, Mathematics for Control Signal and Systems, etc.

More information in: <http://www.mae.ehu.es/s0100-gigamhom/es/>.

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KEY WORDS: p-Groups of maximal class. Sylow p-Subgroups of $GL(n,q)$. Unitriangular matrices. Higman's conjecture.

The research team supervised by Prf. A. Vera López studies finite groups. Particularly, they are interested in p -groups of maximal class and in Higman's Conjecture, which asserts that the number of conjugacy classes of a Sylow p -subgroup of $GL(n,q)$ is given by a polynomial in q with integer coefficients.

In both research lines, the team has developed new computational methods that have allowed to obtain outstanding results on these two large classes of finite p -groups.

p-GROUPS OF MAXIMAL CLASS

The most important invariant parameter of a p -group of maximal class G is its degree of commutativity c . It was defined by Blackburn in 1960 and it is a measure of the commutativity among the members of the lower central series of G .

Since 1995, the problem that the team works on is to obtain the best lower bounds for c in terms of the order of G and two more invariant parameters of G . The importance of obtaining good lower bounds for c is based on the translation of these bounds into structural properties of G . For example, if there is a good lower bound for c , it is easier to obtain the defining relations of G or it is possible to give an upper bound for the number of p -groups of maximal class of given order.

For particular prime numbers p up to 53, the team has checked that the obtained bounds improve, for almost all p -groups of maximal class, or are equal to the best lower bound in terms of the order of G . Also, the team has obtained these lower bounds in the particular case of a p -group of maximal class with Y_1 of class 2. The main goal of this research line is to complete the search of these bounds for any p -group of maximal class.

HIGMAN'S CONJECTURE

In 1960, Higman stated his conjecture about the number of conjugacy classes of a Sylow p -subgroup of $GL(n,q)$. By developing own computational methods, the team has verified that Higman's Conjecture is true for $n \leq 13$. Also, the team has found the conjugacy vector of the Sylow p -subgroups of $GL(n,q)$ for $n \leq 13$. Besides, the team has improved Higman's upper bound for $r(n,q)$. For $n \leq 5$, the team has calculated the canonical matrices, which are, in some sense, the simplest ones in each conjugacy class. As a consequence, the polynomials $r(n,q)$ for $n \leq 5$ have been found. The team has introduced the definition of primitive canonical matrix. The knowledge of the number of primitive canonical matrices with connected graph of size less than or equal to n should be sufficient to determine the number of all canonical matrices of size n .

On the other hand, if $U(n,q)$ is the unitriangular upper matrix of size $n \times n$ over F_q , and N_t is the conjugacy class set of $U(n,q)$, whose centralizer has order q^t , then $r(n,q) = \sum_{t=n, n+1, n+2} |N_t|$. In particular, the team has computed $|N_t|$, for $t=n, n+1, n+2$ and checked that they are polynomials in q .

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KEY WORDS: Finite p-groups, pro-p groups, characters, representations, algebraic combinatorics.

The research of this group is organised around four main areas, which we describe below:

1. Finite p-groups

In this area, we focus on the following two topics: the power structure, and the conjugacy classes, both of elements and subgroups. In the first case, our goal is to obtain families of p-groups which, as far as taking powers is concerned, resemble abelian groups (for which the identity $(xy)^n = x^n y^n$ holds for every exponent n). In the case of conjugacy classes, we investigate what properties can be deduced about a finite p-group if we fix the number of classes.

2. Pro-p groups

Currently, pro-p groups is one of the most trendy research topics in group theory. These groups provide a way of studying simultaneously a family of finite p-groups whose order grows to infinity. In this field, we are working on several problems: power structure, (co)homology, and word problems such as the width of a word and the effect of a positive law on the values of a word. In the case of the word problems, we focus on p-adic analytic groups.

3. Characters

We work on several problems related to characters and representations, mainly on finite p-groups. Even if the representations of classical groups over finite fields are well understood, there is not a satisfactory theory of the representations of their Sylow p-subgroups, and we are interested in this problem. In another direction, we are analysing how the degrees of the irreducible representations or the values taken by the characters have an influence on the structure of a finite group.

4. Algebraic Combinatorics

We look for t-designs, and more specifically 2-designs, that have nice symmetry properties, in the sense that they admit a group of automorphisms that acts regularly on its points. We are also working on the construction of combinatorial structures linked to differences in finite groups, such as difference sets, difference families, and cyclic association schemes.

Aguayo, A.T., Arandes, J.M., Ateka, A., Bilbao, J., Castaño, P., Ereña, J., Estiati, I., Gayubo, A.G., de la Hoz, A., Epelde, E., Errekato, A., Fernández, M.L., Gamero, M., González, I., Gutierrez, A., Mier, D., Remiro, A., Sierra, I., Valle, B., Vicente, J. Azkoiti, M.J.,¹ De Lasa, H.,² Sedran, U.³

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KEY WORDS: Biorefinery, wasterefinery, cracking, hydrocracking, reforming, fuels, olefins, BTX, dimethyl ether, hydrogen, CO₂ sequestration.

Aims. A sustainable refinery consists in the upgrading of: 1) Raw materials alternative to oil (coal, natural gas) and particularly vegetable biomass (Biorefinery); 2) Secondary interest streams from the refinery itself. The industrial implementation of these initiatives needs research aimed at the development of new processes and adaptation or improvement of those already implemented in order to obtain raw materials and fuels by minimizing energy requirements and environmental impact.

Methodology. The interactive study of catalytic processing steps: 1) Preparation and characterization of catalysts; 2) Kinetic modelling of the main reaction and of catalyst deactivation and regeneration, based on the experimentation at laboratory scale under similar conditions to those of industrial processes; 3) Design of reactors and proposal of process optimum conditions. Methodological contributions in these steps will be developed simultaneously.

Lines related to the Biorefinery

Catalytic processes for oxygenates valorisation. Transformation of oxygenates (methanol, ethanol, dimethyl ether) and of biomass pyrolysis liquid product (bio-oil), into fuels or light olefins (ethylene, propylene and butenes). Alternative catalysts as well as process conditions and innovative strategies for reaction operation are being used.

Hydrogen production by steam reforming of oxygenates (bioethanol, DME and bio-oil). The reforming on Ni catalysts supported on different materials is studied. An objective is the sequestration of CO₂ in situ in the reactor, which combines the reduction in the emission of this gas with the avoidance of thermodynamic restrictions in the production of H₂.

Dimethyl ether (DME) synthesis in a single reaction step from a (H₂+CO+CO₂) mixture on bifunctional catalysts. This reaction is efficient for the upgrading of CO₂ an essential for the production of fuels from raw materials alternative to oil (coal, natural gas, biomass) and a clear example of the need for process integration (synthesis of methanol and its dehydration), which involves three synergisms: 1) Combination of endothermic and exothermic processes; 2) Moderation of thermodynamic restrictions; 3) Increase in the activity of each phase (metallic and acid) in bifunctional catalysts.

Lines related to the Sustainable Refinery

Valorisation of residual feeds by hydrocracking. The integration of the two steps (hydrogenation and cracking) into one of hydrocracking gives way to a synergism between the metallic and acid functions in the catalyst and to the fact that both reactions take place simultaneously. A study will be carried out on the hydrocracking of: i) Aromatic feeds, residual feeds in refineries (pyrolysis gasoline, LCO from FCC units and the residue from the atmospheric distillation of the crude); ii) Feeds made up of used plastics (PE) dissolved in LCO and VGO and of PE pyrolysis waxes; iii) bio-oil and other biomass derived components.

Production of olefins by joint catalytic cracking of paraffins and methanol. It is a new integrated process that has advantages over the industrial processes carried out with each raw material (dehydrogenation-steam cracking and MTO process, such as energy offset and the activation of paraffin cracking by the olefins in the reaction medium).

Production of olefins from methane. The aim is the substitution of oil by natural gas, via transformation into chloromethane (which is a reactant transformed into olefins via a similar mechanism as methanol) for the production of petrochemical raw materials.

Propylene production intensification. A versatile catalytic process will be developed in order to offset the imbalance in the production of olefins concerning market requirements.

Upgrading of residues (biomass, plastics, tyres, sludges and others) by thermal and catalytic processes

Aguado, R., Alzibar, H., Amutio, M., Artetxe, M., Alvarez, S., Bilbao, J., Diaz, M.A., Elordi, G., Erkiaga, A., López, L.B., López, G., Morales, A., Olazar, M., San José, M.J., Ortiz de Salazar, A., Zabala, G.¹

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KEY WORDS: Spouted beds, fluid dynamics, gas-solid, pyrolysis, gasification, reforming, residues, biomass, plastics, tyres, sludges, olefins, hydrogen.

Aims. Fluid dynamic studies and the subsequent implementation at pilot plant and industrial scale pursue the development of applications for spouted beds in thermal upgrading (drying, combustion, gasification and pyrolysis) and catalytic upgrading (cracking and reforming) of irregular texture residual materials (biomass, paper sludge and sewage sludge) or those that are sticky or of low thermal conductivity (tyres and especially plastics). These processes are aimed at the production of values added products and fuels.

Methodology: The fluid dynamic study is carried out in a pilot-scale versatile unit provided with contactors of different geometry (conical, cylindrical of conical bottom and cylindrical) and using solids of different texture and granulometry and their mixtures. The different applications of conical spouted beds are carried out in pilot plants in order to obtain determining results for process viability: i) Suitability of material properties; ii) Production of high value added products (limonene in the pyrolysis of tyres); iii) Recovery of raw materials (monomers in the pyrolysis of polyolefins, polystyrene, PMMA); iv) Production of fuels; v) Production of components that may be integrated as raw materials in refineries, such as polyolefin pyrolysis waxes, biomass and sludge pyrolysis bio-oil and tyre pyrolysis liquid product. Based on the results and kinetic models in each process, large scale is proposed for its industrial implementation.

Lines related to Fluid Dynamics and New Applications for Spouted Beds

Gas and solid flow modelling. Experimental techniques and theoretical bases are continuously improved for the modelling of gas and solid flow. Modelling is carried out by computational fluid dynamics (CFD) in order to predict spout diameter and height, fountain height and width, average particle cycle time, gas dispersion coefficient, solid trajectories in the three regions of the bed (spout, annulus and fountain) and parameters related to segregation. Other applications require the consideration of mass, heat and momentum balances for a coupled modelling of gas and solid (essential for processes such as drying, combustion and pyrolysis).

Proposal of new applications. Fundamental studies are carried out for the implementation of the spouted bed technology in new initiatives: Drying of sand like materials and paper sludges, coating of biomedicine materials, upgrading of lignin and other residual materials and so on.

Lines related to Waste Upgrading

Combustion and thermal and catalytic pyrolysis of biomass. Pyrolysis of biomass at 450 °C gives way to a liquid (bio-oil) with reproducible yield and properties and a composition that is suitable for its use as fuel. The pyrolysis using acid catalysts improves the composition of gas and liquid products. The technological development allows operating in continuous mode under vacuum and by feeding oxygen for an energy neutral process.

Thermal and catalytic pyrolysis of plastics and tyres. A continuous process is developed for thermal and catalytic pyrolysis of waste plastics (polyethylene, polypropylene, polystyrene, poly-methyl methacrylate, poly-ethylene terephthalate and so on), scrap tyres and their mixtures.

Production of H₂ by steam catalytic reforming of waste plastics. Strategies based on the use of catalysts in situ or in line are developed and H₂ yield is improved by CO₂ capture

Selective production of polyolefins and aromatics in a thermal-catalytic process. A two-step process is being developed for an integral upgrading of bio-oil.

Polyoxometalates. Building Blocks Of Inorganic-Organic Hybrid Materials

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KEY WORDS: Polyoxometalates, Hybrid materials, ab initio calculations, Magnetic properties.

Hybrid organic-inorganic compounds have attracted an increasing interest in recent years due to the possibility of combining the different characteristics of the components to get unusual structures, properties, or applications.

A recent trend in POM chemistry has been the functionalization of polyoxometalate anions to extend their versatility and lead to new and more selective applications. The chemistry of POM-based hybrids has been significantly enriched by the inclusion of transition metal (TM) coordination complexes into the hybrid system, either to provide charge compensation or as a part of the inorganic POM framework itself. Given the importance of precise compositions and structures in all investigations focused on this class of clusters, the research toward understanding the self-assembly processes that support the formation of polyoxometalate hybrids has to be a route to enable the preparation of multifunctional materials, which take advantage of the unique physical properties associated with this class of compounds.

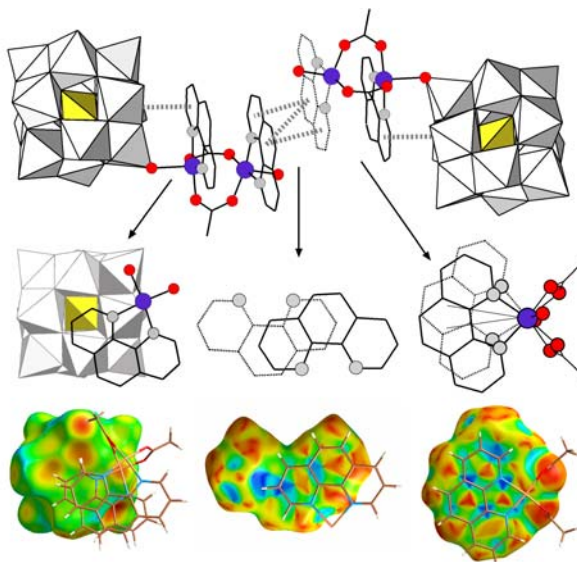
HYBRID INORGANIC METALORGANIC MATERIALS

Currently, we are interested in exploring the applicability of Keggin-POMs and TM-carboxylate cationic complexes in the preparation of new hybrid compounds. The interest of supporting TM-carboxylate complexes, which have widely been studied in magnetostructural research works, on Keggin POMs lies on the possibility of tuning the magnetic properties due to their high dependence on the nature and spatial disposition of the ligands.

Focus for the chemistry of POMs

- *Supramolecular chemistry*
- *New structural motifs*
- *Synergy*
 - catalysis
 - medicine
 - material science

The interest of our research lies on the possibility of interaction between the two sub-lattices through the organic functionalization of the POM surface or the POM framework itself. This functionalization consists in the modification of the coordination sphere of the transition metals by substituting the labile terminal water molecules with aromatic N-donor ligands (pyridine derivatives, bipyridines, phenanthrolines, terpyridines...). This substitution allows the close contact between the two sub-lattices by means of π - π interactions through the planar aromatic cations and the functionalized hybrid POMs.

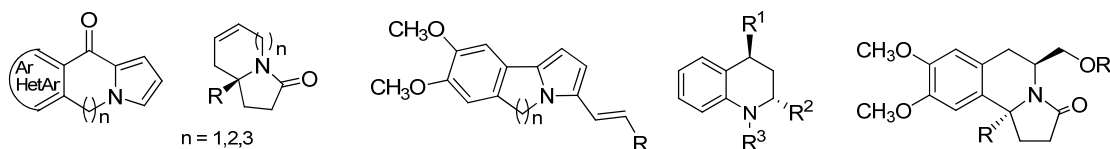


A. Gómez-San Juan, O. García-Calvo, E. Coya, I. Martín-Abraldes, E. Aranzamendi, S. Arrasate, N. Sotomayor, E. Lete

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KEY WORDS: organic synthesis, asymmetric synthesis, organometallics, heterocycles.

Our group works on Organic Synthesis, mainly in asymmetric synthesis and organometallic chemistry. Our projects are focused on the development of new synthetic methods of heterocyclic systems based on lithium, palladium, and ruthenium chemistry for the stereocontrolled formation of carbon-carbon bonds. The group has a solid background in Organic Synthesis, which allows us to face the preparation and structural determination of any kind of organic molecule.



Line 1. Metalation-cyclization sequence in the stereocontrolled synthesis of nitrogen heterocycles

The Parham-type intramolecular carbolithiation reactions for the construction of fused indolizidine and quinolizidine, and tetrahydroquinolines is explored, in order to determine the limitations and scope of the method. The diastereoselectivity of this metalation-cyclization sequence for the construction of non-planar systems, as well as its enantioselectivity, performing the reactions in the presence of chiral catalysts or ligands, is studied.

Line 2. New applications of transition metal catalyzed reactions in the synthesis of fused indolizidines, quinolines, and homologues.

We are also developing new synthetic routes to natural products and analogues, which possess interesting biological activity, via palladium and ruthenium catalyzed processes. The intramolecular C-H activation reaction or direct aryl-aryl coupling is an interesting alternative to cross-coupling reactions in the formation of biaryl bonds on (hetero)aromatic systems. Both the direct arylation and the Mizoroki-Heck reactions use similar palladium-based catalytic systems, so the control of the chemoselectivity on polyfunctionalized substrates would allow the synthesis of different heterocyclic systems with interesting biological properties. Also strategies based on carbolithiation, direct arylation and Heck cascades are developed for the synthesis of polycyclic systems in one step.

Line 3. Stereocontrolled synthesis of piperidines, azabicycles (indolicidines, pyrrolicidines,...) and fused isoquinolines

The combination of different synthetic methodologies based on organolithium chemistry, as metalation-cyclization or nucleophilic addition-intramolecular α -amidoalkylation sequences, the use of functionalized organolithiums, conjugate addition reactions, etc. has allowed the stereocontrolled preparation of various heterocyclic systems, some of the shown on the scheme. The use of chiral ligands or catalysts in these reactions is specially considered, because of its interest not only from an academic point of view, but also for the economic and environmental aspects of the catalytic methods.

For a review on our work, see: *Curr. Org. Chem.* **2003**, 7, 275. For some selected publications: *J. Org. Chem.* **2006**, 71, 6776; *Synlett* **2007**, 1101; *Tetrahedron Lett.* **2007**, 48, 2919; *Synlett* **2008**, 3188; *Org. Lett.* **2009**, 11 1237; *Adv. Synth. & Catal.* **2009**, 351 2460.

Photophysics of Molecules in Nanostructured Systems. Multifunctional Optoelectronic Materials.

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KEY WORDS: Dye Lasers, Zeolite, AIPO, Metal Organic Framework, Antenna, Sensors.

Nowadays, the design and study of hybrid systems, mainly fluorophores incorporated into solid hosts, is a booming area of research. The nanostructured materials offers a constrained environment with a high organization degree for the photoactive guest molecules, leading to versatile functional systems, which could be applied in different technological and commercial fields such as optoelectronic or photovoltaic devices. To this aim, the photophysical characterization of these nanomaterials is essential to understand the involved processes and to improve their behaviour.

In this sense, the Molecular Spectroscopy Group of the Physical Chemistry Department has a vast experience in the photophysical study of fluorophores, mainly laser dyes, with emission in the whole visible region of the electromagnetic spectrum. Indeed, in the last years the photophysical behaviour of cumarines and rhodamines in different surrounds has been deeply analyzed; i.e. solvents with a wide variety of environmental properties, polymers with different viscoelastic properties and in the interlayer space of smectite-type laminar clays. To carry out such study the laboratory is equipped with the adequate techniques; UV-Vis absorption and, steady state and time-resolved (nano- and picoseconds), fluorescence. Recently, a Fluorescence Confocal Microscopy has been acquired, which spans even more the kind of studies that can be carried out in the laboratory.

Actually, our research is focused on four main lines:

- In the last decade, and in collaboration with research groups of the CSIC, the boron- dipyrromethene (BODIPY) laser dyes has been exhaustively studied from a photophysical and quantum mechanical point of view. The aim is to know the structural and environmental properties which improve its fluorescence emission, and hence its laser performance, both in the liquid and solid state. At the same time, novel fluorescence on/off switches, based on BODIPYs, are being developed for molecular or environment sensing. These systems can be used to monitor the characteristics of the environment surrounding or to detect the presence of a specific ion or molecule.
- Recently, we have started to incorporate several fluorophores, with emission at different region of the visible, in unidimensional pores systems such as aluminosilicates (zeolite L) and aluminophosphates (AIPO-5). The technological applications are very wide, such as non-linear optics devices, light waveguide, optical sensors, antenna systems, solid-state micro-lasers and photocatalysts.
 - a) *Dye/zeolite L hybrid systems.* The idea is to have an antenna system, consisting in monomeric dyes, encapsulated in nanochannels with a specific orientation, capable of harvesting light of different energy and to transfer it to the desired place with a fixed energy. The goal is to use such devices to sensitize a semiconductor in order to develop a novel organic solar cell.
 - b) *Dye/AIPOs materials.* Other interesting purpose is to get macroscopic alignments of the photoactive entity with a preferential orientation into the nanochannels, producing a highly anisotropic response with respect to the electromagnetic radiation. Distribution and orientation of the dye along the pores are characterized by means of a confocal fluorescence microscope. This technique which provides information about the photophysical properties of the guest molecules adsorbed in single particles, thanks to the FLIM technique (Fluorescence Lifetime Imaging), polarization experiments and spectral resolution by a CCD + spectrograph coupled to the microscope.
- Finally, and in collaboration with a japanese research group (Kyoto University), luminescent properties of metal organic framework (MOF) are being studied. These materials have revealed efficient fluorescent sensors triggered by specific guest molecules.

Development of new methodologies for the synthesis of heterocyclic compounds

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KEY WORDS: Sustainable chemistry, Hypervalent iodine, Catalysis, Cross-coupling.

The two main research lines that are being conducted by our group are focused on the development of new synthetic methodologies to be carried out under sustainable conditions ("green chemistry").

• NEW METAL CATALYSTS: DESIGN AND APPLICATIONS

We plan to design and synthesize new catalysts –mainly based on palladium or copper– to be used in tiny amounts under sustainable conditions (aqueous or biodegradable media, possible reuse of the catalyst...). Our preliminary research shows excellent results for a variety of transformations as shown in *Figure 1*.

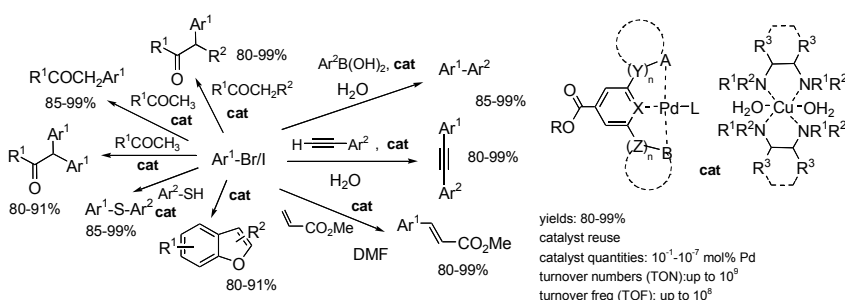


Figure 1. Selected reactions in which the new catalysts have been tested.

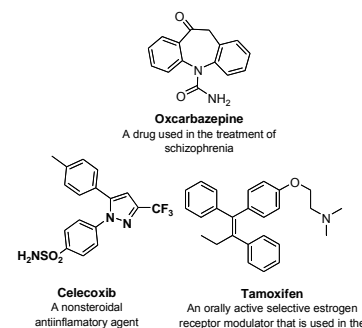
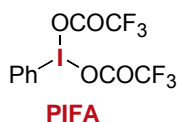


Figure 2. Target compounds prepared by the aid of the new catalysts.

The described optimized methodology has allowed us to prepare a number of polycyclic compounds of interest (see *Figure 2*) with the benefits of short synthetic sequences, economical advantages, and sustainability when compared to previous reported alternatives.

• NEW APPLICATIONS OF THE HYPERVALENT IODINE REAGENT PIFA



PIFA, [*bis*(trifluoroacetoxy)iodobenzene], has become a prominent reagent in our ongoing synthetic plans due to the soft reaction conditions that are required, its high efficiency, and its low toxicity.

One of the most attractive features of this reagent involves its ability to oxidize properly substituted amides to generate highly electrophilic nitrenium intermediates. If under such conditions our starting material contains an internal nucleophile, a cyclic compound can be formed.

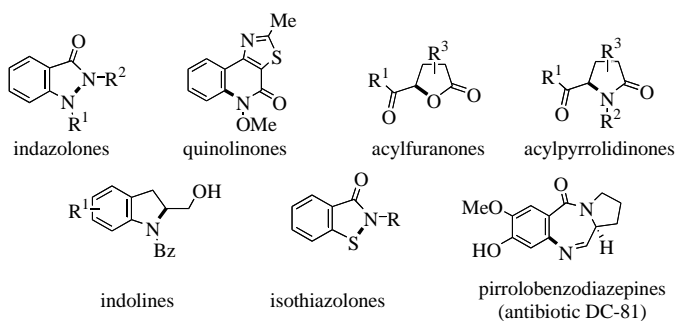
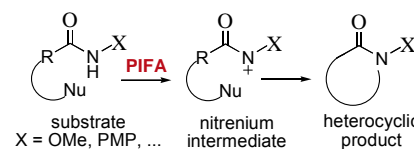


Figure 3. Selected examples of the use of PIFA in heterocyclic synthesis. The bond created by this reagent is highlighted.



The precise design of the substrates allows the preparation of a number of different heterocycles with high structural diversity (see *Figure 3*).

Transesterification. Biodiesels.

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KEY WORDS: Used frying oils, Transterification, biodiesels.

OBJECTIVE

The main objective of the project can be briefly summarized as the quantification of the amount and chemical characterization of the used oil produced in our university canteens. This oil will be methanolized under standard conditions. Among the objectives of the project is also the reuse by the university facilities of methyl esters of fatty acids (referred to as FAME) that are produced as a result of the process.

When conceptualizing the project we have taken into account the own characteristics of our university: three campuses and different learning centres distributed in different populations. Therefore, the scope project is also related to sustainability policies among the university and to promotion of renewable energies, a hot topic nowadays especially concerning to the results of the Copenhagen climate conference.

DOMESTIC USED OIL

In this regard, its worth to mention that there is still reduced information on the quantities of domestic used oil. On the contrary, there are plenty of data about used oil from other kinds of facilities like hotels, restaurants, catering companies or hospitals.

To try to quantify how much used frying oil could be picked up at our University through its students, we have requested the collaboration of the students in a pilot being carried out with our students. Students will take the domestic used oil –identifying the samples with the time it was collected and the number of people at home- to the test, and they will get the equivalent biodiesel after the experiment. This experiment will be carried out by the pupils themselves under our supervision, being the efficiency of this transesterification reaction in 1:1 used oil / biodiesel.

Extended metal-organic frameworks (MOFs)

Oscar Castillo, Antonio Luque, Pascual Román, Javier Cepeda, Mónica Lanchas, Sonia Pérez, Jíntha Thomas, Daniel Vallejo

Departamento de Química Inorgánica, Facultad de Ciencia y Tecnología, UPV/EHU.

KEY WORDS: Coordination polymers, MOFs, bioinorganic chemistry, supramolecular recognition processes, magneto-structural correlations, nanostructures, adsorption properties.

Crystal engineering is the design and synthesis of molecular solid-state structures with desired properties, based on the understanding and exploitation of intermolecular interactions. The two main strategies currently in use for crystal engineering are based on hydrogen bonding and coordination complexation. At the present, the long-standing challenge of designing and constructing new crystalline solid-state materials from molecular building blocks is just beginning to be addressed with success.

Our research group has a long outstanding experience in the design of novel systems based on the preponderance of the bisbidentated coordination mode of the oxalato ligand to lead to a great variety of crystal structure topologies. Now, we are developing several new research lines, in which we exploit the knowledge acquired on the study of the metal-oxalato system, for example:

- We have set up a strategy for the design of one-dimensional complexes of formula $[M(\mu\text{-ox})(L)_2]_n$ containing nucleobases, such as adenine and guanine, as terminal ligands. These systems allow the study of the supramolecular interactions established by the nucleobases when they are anchored to a periodic, infinite and non-biological 1D polymer.
- We have focused on the processability of the 1D or 2D coordination polymers as nanowires and monolayers, respectively. The process is based on the reversible nature of the coordinative M-L bond. The strategy is the extraction of single molecules from bulk samples, for which there is a need to overcome supramolecular cohesive interactions and even the coordinative metal-ligand bonds. This goal is reached by means of physico-chemical methods (such as sonication or sublimation) that provide enough energy to the system to remove the cohesion within the crystals. Finally, the fragments generated are self-assembled again both in solution or on the surface to generate the same pattern as the original bulk material but on a nanometric scale.
- We are exploiting the coordination similarities among the pyrazine-2,5-dicarboxylato, pyrimidine-4,6-dicarboxylato and oxalato ligands to obtain the same structural topologies than those reported for the oxalato ligand but using the diazine ligands as connectors between the metal center. It allows the analysis of the magnetic interactions through the aromatic diazines and at the same time provides bigger voids and channels within the crystal structure that can improve the adsorption capabilities of these systems.
- We are developing new routes to afford 1D–3D coordination compounds based on secondary building units (SBUs) based on dimeric entities, in which both nucleobases and carboxylato ligands bridges the metal centers to give rise to a paddle wheel topology. The characteristics of the carboxylato and nucleobase ligands allow the control of the dimensionality and the shape of the voids and channels present within these crystal structures.
- We are also extending our research to the design of nucleobase containing halometallate complexes.

Natural products in foods, beverages and plants

Luis A. Berrueta¹, Blanca Gallo¹, Francisca Vicente¹, Diana M^a López-Márquez¹, M^a Belén Sánchez-Ilárduya¹, Miriam Romera-Fernández¹, Sergio Garmón-Lobato¹, Cristina Sánchez-Fernández¹, María Vitoria-Bernal¹, Zuriñe Rasines¹, María Ramírez¹, Adela Arranz², Carmen Iriondo³, Arantza Urkaregi⁴

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KEY WORDS: Polyphenols, anthocyanins, red wine, fruits, medicinal plants, nutraceuticals, antioxidant.

Determination of the chemical composition of foods and beverages has a huge interest from many points of view. A deep knowledge of natural products in foods can lead to improve nutritional quality or to detect geographical origins, manufacturing methods, bad practices, or adulterations.

Polyphenols are a very important group of natural products due to their ubiquity in the vegetable kingdom and their interest as a key to explaining many food properties such as flavor, astringency, aroma, and color, besides their many beneficial effects on human health as a lower risk of heart diseases and cancer.

With this aim and after successful works in ciders, apples, and edible oils, our research group is currently working in the following projects:

- Anthocyanin analysis in red txakolis of Biscay and lixiviated from freeze-dried skins after grape crushing: This analysis allows the evaluation and control of vinification procedures and quality parameters of local Origin Designation as wine color, which is one of the most important parameters directly related to anthocyanins.
- Volatile compounds analysis in txakoli by *fast* gas chromatography which are responsible for wine aroma: This feature is critical for the final quality of wine and its knowledge informs the wineries about the course of vinification.
- Development of a fast method for the determination of anthocyanins by using infrared spectroscopy, which is a fast, cheap and widely employed technique in wineries: For this purpose, chemometric tools (PCA, PLS) are employed to correlate infrared spectrum with anthocyanin contents, previously quantified by HPLC-DAD.
- Study of the polyphenolic profile of fruit derived foods, determined by HPLC-DAD and HPLC-MS/MS: This allows detecting adulterations and bad practices in the food manufacturing by using chemometrics (PCA, MLR, PLS, LDA).
- Study of anthocyanic derived pigments in aged red wine from "Rioja Alavesa" which are formed in specific reactions during the barreling. For the study of these pigments, previous wine treatments are carried out, i.e.: wine is fractionated by size-exclusion chromatography (SEC) and fractions are analyzed by HPLC-DAD-MS/MS.
- Study of Tannins in aged red wines from Rioja, which define to a great extent many properties of wine, like astringency and wine texture. Complicated multi-step separation procedures must be developed by making use of solid-phase extraction (SPE), liquid-liquid extraction (LLE) and selective evaporation of the solvent, SEC, and HPLC.
- Use of the apple by-product generated in the cider manufacture process, obtaining a high yield from bioactive molecules of very high-value-added for the food, pharmacist and cosmetic industry.
- Isolation, structure elucidation and antioxidant potential of polyphenolic compounds from plants with medicinal use.

Size Matters: From Micro to Smart Copolymeric Nanohydrogels: Synthesis and Applications

I. Katime, L.C. Cesteros, J. Veguillas, J.L. Gadea, L. Pérez, L. Agüero, A. Álvarez, M. Artetxe
Grupo de Nuevos Materiales y Espectroscopia Supramolecular
Facultad de Ciencia y Tecnología

KEY WORDS: Smart Nanohydrogels, Microemulsion polymerization, cancer and tuberculosis therapy, macrohydrogels, PEG, PVA

Hydrogels are crosslinked polymeric materials that form a three-dimensional network which can be natural or synthetic and that swell in contact with water to form soft and elastic materials. The flexibility of the polymer chains enables the entry of solvent molecules causing the hydrogel to swell, while its crosslinked structure prevents the dissolution of the hydrogel. Since the early twentieth century science advanced greatly to the point of being able to modify the structure of a large number of molecules, polymers among them, which nowadays are everyday materials and have great industrial and technological importance.

Thanks to these advances, current polymer research is centered not from the perspective of inert materials, but in developing materials for applications that are beyond its typical use.

The discovery of the microscopic world has enabled science to deepen its knowledge of materials at smaller size. The understanding of the transition from micro to nano scale will provide significant improvements in the understanding of matter and its applications. The seek for this knowledge has increased the number of investigations which, in turn, have generated a more complete knowledge about the surrounding environment and the development of new sciences that attempt to explain behavior at a microscopic scale. These new sciences have emerged due to the need for new technological breakthroughs. Nanotechnology is one of the predominant ones.

Smart targeted nanogels for cancer therapy. Smart nanogels (pH and temperature responsive) with dimensions ranging between 18 to 50 nm can be synthesized by microemulsion polymerization to be use in cancer therapy; above 50 nm the nanoparticles may cause clogging of the blood stream and below 18 nm are adsorbed by alveoli. The nanogels are vectorized to target cancer cells using a guide molecule (folic acid).

Smart nanogels for tuberculosis therapy. Smart nano-copolymeric matrixes are employed to release anti tuberculosis (anti-TB) drugs such as combined complexes of Ethambutol (EMB), Isoniazid (INH), Rifampicin (RMP) and Pyrazinamide (PZA).

Macrohydrogels. The macroscopic hydrogels under study are based on a hydrophilic polymer chemically very stable and with an excellent biocompatibility: the polyethylene glycol (PEG). This polymer has been crosslinked with the aid of cyclodextrins, molecules of great practical interest because of their ability to form inclusion complexes. The presence of cyclodextrins in this type of hydrogels makes them potential candidates for drug delivery and for the removal of water pollutants. PEG has also been used to crosslink polyvinyl alcohol (PVA), preparing hydrogels whose swelling and release properties can be regulated by the degree of hydrolysis of PVA and the PEG content of the network.

The Survey of the Cultural Heritage: Analytical Chemistry in the Field of Art and Archaeology

Aramendia J., Arana G., Arrizabalaga I., Castro K., de Diego A., Etxebarria N., Fernández L.A., Madariaga J.M., Maguregui M., Martínez-Arkarazo I., Olazabal M.A., Olivares M., Prieto N., Sarmiento A*, Usobiaga A., Zuloaga O.

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*Laboratorio Singular de Multiespectroscopias Acopladas (LASPEA), SGIKER, UPV/EHU

KEY WORDS: Environmental impact, art and archaeology analysis, non-destructive characterisation

Our research group develops innovative analytical strategies to evaluate the impact of chemical contaminants, micro-organisms and the environmental conditions on the Cultural Heritage: wall paintings, wallpapers, sculptures, historical buildings (ornamental façades), cave paintings, archaeological sites, easel paintings, stamps, lithographs, etc.

On the one hand one of the most active lines is the development of new analysis methods and strategies by using non-destructive, non-invasive and hand-held portable equipments. The use of these systems is of great importance because artworks are unique and very valuable objects and they can not be damaged nor sampled. When the artwork can not be moved to the laboratory, the equipments are moved to the objects. Techniques such as Raman and infrared (FTIR) spectroscopies, x-ray fluorescence (XRF) are of common use for this purpose

Thanks to the use of these techniques it is possible to perform a molecular speciation study in order to characterise the original components of the artworks under analysis. With the obtained results we could know, for example, if the artwork is original or fake.

However the most important know-how of IBeA research group in this field lies in the use of the same techniques not only to characterise the original components of the objects, but also to determine whether they are the promoted degradation products due to the impact of chemical contaminants or aggressive environmental conditions.

Once original and degradation products are characterised, it is possible to set the degradation pathways through the use of computerised thermodynamic studies. The knowledge of these degradation mechanisms is very important in order to establish the most risk-free as possible protocols to protect, restore, clean and preserve degraded objects in collaboration with curators and restorers.

In this sense, we have been working in the development of clean and protective technologies, essentially based on the use of ion exchange resins and modified gels. These technologies has been applied mainly on calcareous supports of several artworks (altarpieces and façades), as well as to fight against the so-called *green disease* inside tourist caves (Pozalagua)

The ongoing research activities in this field are the following:

- Study of the impact of pollutants on steel made artworks.
- Environmental pollution effects on historical buildings.
- The development of analytical methods for the characterization of the Natural and Cultural Heritage

Environmental and Food Analysis: the key for coming challenges

Alonso I.^{*}, Arana G., Arrieta N., Bustamante J., Castro K., Carrero J.A., de Diego A., Etxebarria N., Fernández L.A., Fernández S., Goienaga N., Gómez L., Gredilla A., Iparragirre A., Madariaga J.M., Martínez-Arkarazo I., Olazabal M.A., Olivares M., Omar J., Trebolazabala J., Usobiaga A., Vallejo A., Zuloaga O.

IBeA Research Group. Department of Analytical Chemistry, UPV/EHU

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KEY WORDS: Environmental sampling and analysis, environmental risk assessment, food characterization.

Our research group develops innovative analytical strategies to evaluate the effect of chemical contaminants in the environment and accommodate the design of added-value processes in the environmental chemistry and food technologies.

On the one hand one of the most active lines is the development of new sampling and analysis methods of microcontaminants (metals, organics and organometallic compounds) in natural media. There are two main goals in these research lines: the first one is to study of the mechanisms of transport and transfer among the different natural compartments, and the second one is to support the environmental risk assessment studies. In fact, we are working in a wide range of activities that go from the application of different sampling strategies (hollow-fibres, solid-phase microextraction, or supported liquid membranes) to the development and characterization of new environmental reference materials.

On the other hand, we have been working in the development of clean technologies, essentially based on the use of ion exchange resins and supported membranes, to reuse water and to recover materials. In this field we have worked with electroplating industries to design and control sewage treatment plants with high metallic content.

In addition to all those fields, we have started working in the development of analytical methods and chemical processes to implement food processing techniques in order to get added-value products such as dealcoholisation of wine, elimination of off-flavours, the transfer of food flavours and fragrances, or process monitoring.

The ongoing research activities in this field are the following:

- The development of analytical methods for the determination of emerging pollutants such as endocrine disrupters, estrogens and alike compounds, nonyl- and octylphenols, among others.
- The use of passive sampling strategies to monitor the contamination and to assess the bioavailability of key contaminants in estuaries and coast line.
- The development of analytical methods for natural flavours and fragrances and their use in food products.
- The characterization of natural food matrices to assess the quality of the product.
- Development of new food treatment techniques and products in the *haute cuisine*.

Dolores Badía,* Marisa Carrillo, Jose Luis Vicario, Efraím Reyes, Ainara Iza, Beatriz Alonso, Silvia Reboredo, Naiara Fernández, Maitane Fernández, Garazi Talavera, Jose Ignacio Martínez, Idoia Gil, Iratxe Ugarriza
*Department of Science; Organic Chemistry II.

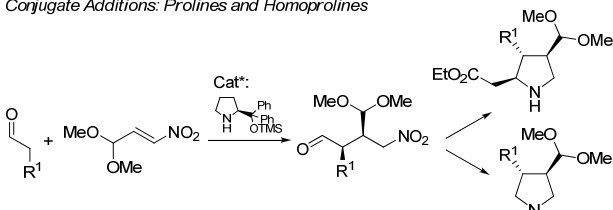
KEY WORDS: Organocatalysis, Green Chemistry, "on-water reaction", Asymmetric Catalysis

Observing how Mother Nature solves complex problems in an easy way, the human being has tried to imitate it for many centuries. Thus, the high catalytic efficiency of several enzymes in many natural asymmetric processes has inspired many researchers who have tried to understand the enzymatic activity in order to imitate its action and even to increase and improve it creating new protein-based catalysts, biocatalysts and others. However, biocatalysts show a rather narrow substrate scope due to the inherent specificity of the biologic processes. For this reason, many investigations carried out by distinguished researchers have focused in the search of new and more flexible catalyst systems which could tolerate a wider range of substrates and types of reaction.

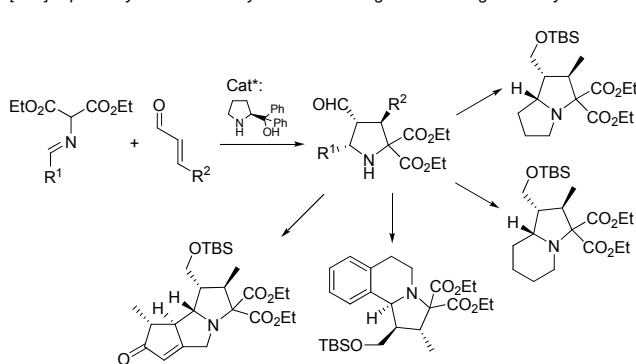
In asymmetric synthesis, not only should the catalyst of choice accelerate the reaction but it also should be very stereoselective and flexible, in order to allow its use for the synthesis of different target molecules from non-chiral precursors. In the last decade, organocatalysis has emerged as a very efficient tool in organic synthesis using small chiral organic molecules, which activate both reagents and reactants, being responsible for the stereocontrol of the reaction in the absence of any metal. These organocatalysts are stable in air, water-compatible and easily prepared in both enantiomeric forms. Furthermore, most of them are commercially available, showing a great advantage when employed by the pharmaceuticals and agrochemical industry, due to the fact that the presence of traces of contaminating transition metals is precluded, avoiding additional purification methods.

Our research in this field has prompted us to study several enantioselective organocatalytic methodologies and to the design of new catalysts which allow to carry out the reaction in water. These findings, together with the previously described advantages of organocatalysis compared to traditional metal catalytic reactions, are in accordance with the principles of *Green Chemistry*. Some of the following examples show the utility and the synthetic applications developed in our research group.

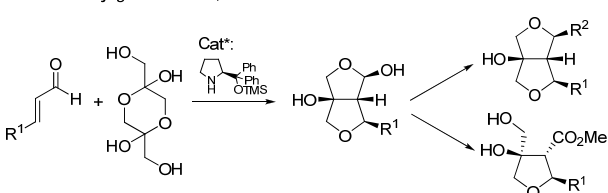
Conjugate Additions: Prolines and Homoprolines



[3+2] Dipolar Cycloadditions: Synthesis of Nitrogen Containing Heterocycles



Cascade Conjugate Addition, Aldol Reaction and Acetalization: Furofuranes



Our experience in the field of Asymmetric Synthesis is well known and internationally recognized. Our research group provides laboratory facilities for students in the last year of degree, PhD. students or post-doctoral researchers. More information can be found in the group web page (<http://www.ehu.es/GSA>) such as research projects, relevant publications, group members, available positions for students and other information.

An improved determination of Local Spin in the design of properties of Chemical Systems

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KEY WORDS:

The study of paramagnetic, ferromagnetic and antiferromagnetic substances deserves a great interest because of their special properties. Likewise, the understanding of systems containing unpaired electrons or open-shell molecules is of paramount importance due to the relevant role this kind of systems play in several areas of chemistry (catalysis and organic syntheses), biochemistry (reactive sites of enzymes), design of new materials, and other areas. However, these endeavours require the construction of adequate theoretical tools. In this sense, the Local Spin is a useful concept which allows one to characterize the spin state of an atom or a molecular fragment embedded in a molecular system, providing an important insight into electronic structures.

The decomposition of the expectation value of the N-electron spin-squared operator $\langle S^2 \rangle$ into one-center and two-center contributions has received a considerable attention in the last years, as a suitable approach to determine Local Spin. In this work we develop a spin-partitioning scheme that can be applied to any independent particle or correlated wave function. The procedure provides simpler expressions to describe local spins which are more appropriate from a computational point of view than previously described ones. To test the reliability of our methodology, we have performed numerical determinations in several molecules and radicals in triplet and doublet spin symmetries, providing results which are in agreement with the genuine chemical knowledge on these compounds.

Nanostructured Materials with Interesting Technological and Biomedical Applications

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Departamento de Química Inorgánica UPV/EHU.

KEY WORDS: Nanoparticles, fuel cells, lithium-ion batteries.

The preparation of nanometric materials involves both size decrease and a structural and electronic rearrangement; consequently, nanomaterials usually show distinctive properties that vary from the observed ones in bulk state. The aim of the present research is within this framework, focusing our effort in the optimization of synthetic methods towards the preparation of nanometric materials.

These materials would show better or different optical, conductive or magnetic properties compared to bulk counterparts, so, they could ultimately be used as cathodes or anodes in fuel cells and Li-ion batteries, both research topics of great economic and social impact. More precisely, in the project it is proposed the preparation of $\text{Ln}_{1-x}\text{A}_x\text{Fe}_{1-y}\text{M}_y\text{O}_3$ (Ln = lanthanide, A = alkaline earth metal, M = Transition metal) and $\text{LnAB}_2\text{O}_{5+x}$ (Ln = lanthanide; A = alkaline earth metal; B = Cr, Fe, Ni, Co, Cd, Mg) mixed oxides of perovskite structure and also the preparation of compounds with oxoanions like Li, transition metal or Fe, Co and Ni oxide phosphates, fluorosulfates, etc., potential candidates for Li-ion batteries.

A final goal will be the preparation and characterization of Au, Pd, Ag or Au, Pd, Ag capped Fe_3O_4 , Fe_2O_3 oxide nanoparticles, which once they are functionalized to be biocompatible they could be used as thermal agents in magnetic hyperthermia.

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¹Departamento de Química-Física; ²Departamento de Física Teórica e Historia de la Ciencia;

³Departamento de Física Aplicada I.

KEY WORDS: Quantum Mechanics

QUINST Research Lines

Quantum mechanics is at the heart of our technology and economy - the laser and the transistor are quantum devices - but its full potential is far from being realized. Recent technological advances in optics, nanoscience and engineering allow experimentalists to create artificial structures or put microscopic and mesoscopic systems under new manipulable conditions in which quantum phenomena play a fundamental role.

Quantum technologies exploit these effects with practical purposes. The objective of Quantum Science is to discover, study, and control quantum effects at a fundamental level. These are two sides of a virtuous circle: new technologies lead to the discovery and study of new phenomena that will lead to new technologies.

Our group's aim is to control and understand quantum phenomena in a multidisciplinary intersection of **Quantum Information, Quantum optics and cold atoms, Quantum Control, Spintronics, Quantum metrology, Atom interferometry, Quantum Field Theory, Superconducting qubits and Circuit QED, Quantum Technologies and Foundations of Quantum Mechanics.**

We develop multidisciplinary research in different fields around Quantum Information, Science and Technology. We contribute with theoretical models for the sake of fundamentals, experimental applications and emergent technologies.

For more information (News, Research, Events, Publications and more) visit our web page:
<http://tp.lc.ehu.es/qjst>

Analytical tools for the chemical industry

Rosa M. Alonso¹, Rosa M. Jiménez¹, Miren I. Maguregu², Magdalena Ezkurra¹, Nerea Ferreiros¹, Juan M. G. Góngora¹, G. Iriarte¹, M. Luz. Alonso¹, Oskar González¹, Nerea Ayarza¹, Estitxu Rico¹ and Itxaso Velasco¹

¹Department of Analytical Chemistry; ² Department of Painting

KEY WORDS: analytical methods, pharmaceutical, industry, environmental, art works, inks dating

FARMARTEM Group is involved in a general research line focused to the development of new methodologies applied to different fields: pharmaceutical, environmental, industrial, conservation and restoration of art works and forensic dating of written documents. The determination of analytes in complex matrixes requires the introduction of new advances in instrumental analytical techniques in order to solve sensitivity and selectivity problems, including the sustainability compromise with the use of clean technologies.

In the research topic "Monitorization of Drugs in Biological Fluids" we are developing methodologies of sample treatment, separation, characterization and determination of several drugs and their metabolites used in combined cardiovascular therapy: antihypertensive+hypolipemiant+antiplaquetelet drugs in plasma, serum and urine obtained from patients under this treatment. With this purpose, chromatographic and electrophoretic techniques with different kinds of detection are being applied, including liquid chromatography-mass spectrometry and ultra high performance liquid chromatography. These analytical methods could be utilized for stability, pharmacokinetic and pharmacodynamic studies in pharmaceutical and hospital laboratories.

The analytical methods used for the industrial applications include the use of low-resolution nuclear magnetic resonance spectroscopy of fluor (NMR-F), capillary electrophoresis and ionic chromatography with the aim of achieving more rapid and more sustainable methods, easy to implement in the quality control laboratories. Major (fluor) and minor components (anionic impurities as chloride, sulphate, nitrate, phosphate,...) are being determined in raw materials, sub and final products coming from fluor industry.

In the environmental aspect, the study of stability of different pesticides families together with the development of analytical methods for their determination in water, soils (bioremediation studies) and food are being carried out. On the other hand, new technologies for biocids fabrication with the introduction of natural products is being assayed at laboratory level, with the aim of reducing the environmental impact of pesticide active component

The chromatographic, electrophoretic and spectroscopic techniques are being also applied to establish general procedures for the identification of binding media, dyes and varnishes, traditionally used in artistic painting. We are also developing analytical methods for the identification and dating of writing inks and documents.

FARMARTEM Group works in collaboration with several European research groups as well as with different industries: Derivados del Fluor, S.A., DTS-OABE, S.L. and Lettera I+D, S.L.

The research activity of the group is being supported by Ministry of Science and Innovation (CTQ2009-11690), Basque Country Government (Projects: UE 09+/56, UE 09+/ 61 and SAIOTEK S-PE09UN44) and University of Basque Country (GIU07/02).

Chemical Technologies for Environmental Sustainability

A team of people got involved with the Sustainable Development

J.R. González-Velasco, M.A. Gutiérrez-Ortiz, J.I. Gutiérrez-Ortiz, J.A. González-Marcos, M.P. González-Marcos, A. Aranzabal, R. López-Fonseca, J.L. Ayastuy, J.I. Álvarez-Uriarte, U. Iriarte, B. de Rivas, J.M. Castresana, D. Duraiswami, N. Chimeno, U. Elizundia, M. Romero, B. Pereda, A. Blanco, E.G. Fuentes, N.K. Gamboa, C. Sampedro, I. Duque and V. Hernández

Dept. Chemical Engineering, Fac. Science and Technology ZTF-FCT, The University of the Basque Country

KEY WORDS: catalytic purification of gaseous wastes, control of automotive exhaust gases, catalysis for the production of clean energy, drinking water treatment plants, valorization of plastic wastes.

MISSION

We are actively involved in the development of knowledge and technologies for purification of waste streams by destruction and/or removal of pollutants, and their application into the industrial activities responsible for their generation. Likewise, our interest is focused on the improvement and optimization of chemical processes in order to minimise the environmental impact, resulting in cleaner production processes.

VISION

To be a Group of researchers playing an active role as a partner in International and European Frameworks, which develop innovative interdisciplinary projects in fields that generate new opportunities for improving life quality by applying the principles of Green Chemistry and Sustainable Development.

The research group is open to incorporate researchers from other groups, who can offer added value or new knowledge, or create strategic alliances. We also want to promote the formation of new researchers, helping them in developing their skills and creativity within a context of integrity, honesty and respect for people and their environment. Consequently, by addressing the great importance of Sustainability the students will improve their career perspectives and receive high personal and professional recognition.

RESEARCH LINES

1. *Development of Complex and Structured Catalysts*
 - 1.1. Manufacture of Structured Catalysts
 - 1.2. Development of Complex Catalyst
2. *Catalytic Purification of Gaseous Waste Streams*
 - 2.1. Control of Automotive Exhausts
 - 2.2. Control of Emissions of Chlorided Volatile Organic Compounds (Cl-VOCs)
 - 2.3. Control of Carbon Monoxide Emissions
3. *Catalysis for Production of Clean Energy*
 - 3.1. Purification of Hydrogen Streams for Feeding PEM Fuel Cells
4. *Recycling and Valorization of Plastic Wastes*
 - 4.1. Catalytic Depolymerization of Plastics to Monomers
 - 4.2. Catalytic Hydrogenation of Plastic Wastes
 - 4.3. Catalytic Pyrolysis of Plastic Wastes
5. *Environmental Health*
 - 5.1. Drinking Water Treatment Stations (ETAPs)
 - 5.2. Disinfection of Water in Cooling Towers
 - 5.3. New Strategies for Evaluation of Air Quality
6. *Consultancy and Transfer of Knowledge for the Industry*