2007 Annual Report

Barcelona Supercomputing Center
Centro Nacional de Supercomputación

The 2007 Annual Report of the Barcelona Supercomputing Center - Centro Nacional de Supercomputación (BSC-CNS) summarizes the center's activities for the year and provides a short description of the organization.

GOBIERNO DE ESPAÑA
MINISTERIO DE EDUCACIÓN Y CIENCIA

Generalitat de Catalunya
Departament d'Innovació, Universitats i Empresa

UPC UNIVERSITAT POLITÈCNICA DE CATALUNYA

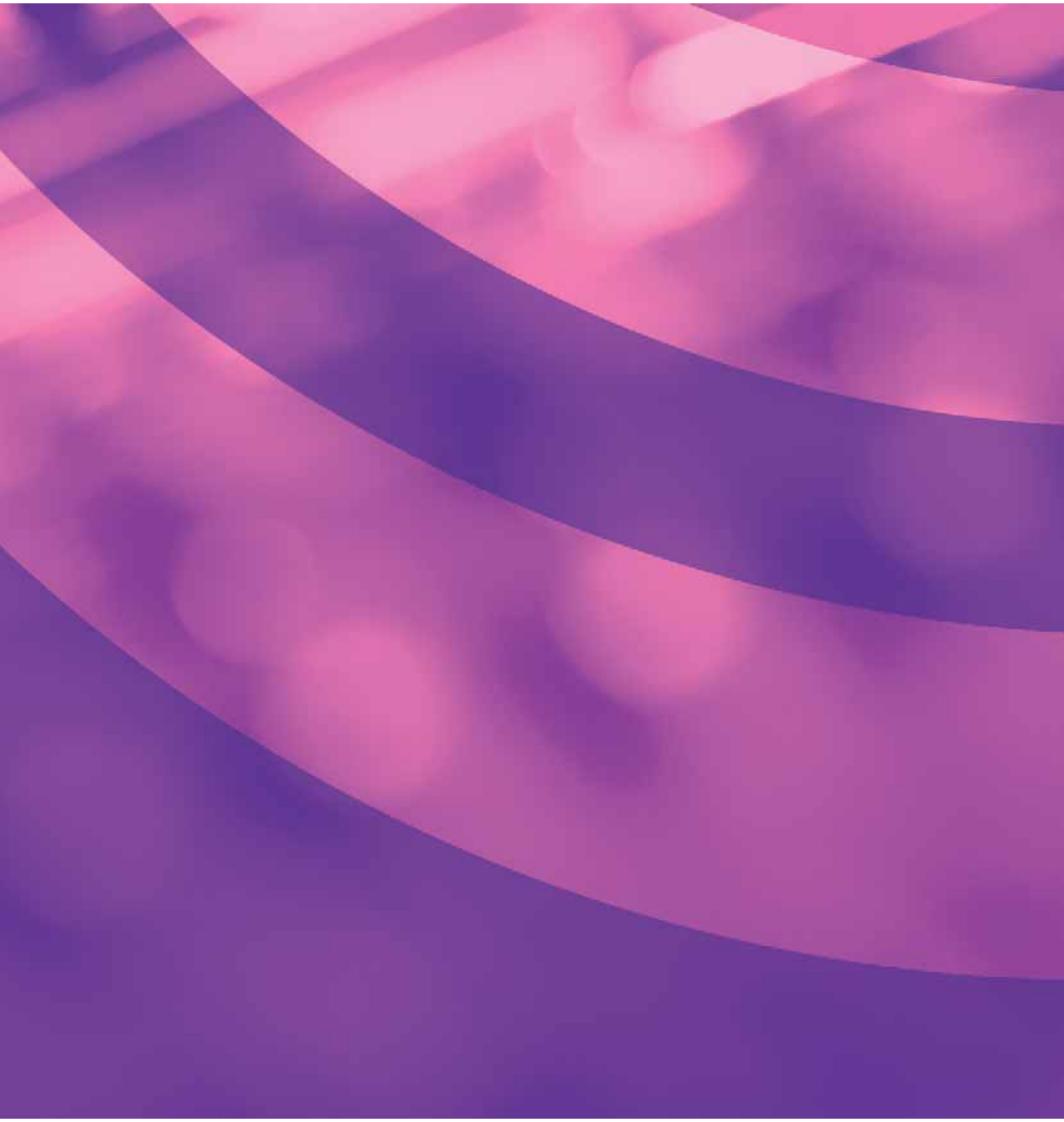
2007 Annual Report

Barcelona
Supercomputing
Center
Centro Nacional de Supercomputación


BSC

Table of Contents

1 The Year in Perspective



2007 was a year of consolidation for BSC-CNS: consolidation of people, both at research and support level, consolidation of projects, both public and in collaboration with private companies, and consolidation of systems, with the Spanish Supercomputing Network running at full speed.

2007 saw BSC-CNS continue with its strategy to attract the most skilled people from around the world. The centre increased its staff from 137 at the end of 2006 to 200 at the end of 2007, with 23 different countries being represented: Argentina, Belgium, Brazil, Bulgaria, Canada, Chile, Colombia, Cuba, France, Germany, India, Ireland, Italy, Jordan, Lebanon, Mexico, Poland, Russia, Serbia, Turkey, United Kingdom, United States and Spain.

Consolidation also took place at organisational level and in January 2007 BSC-CNS created CASE, the Computer Applications in Science and Engineering department. CASE was designed to be a key link between the BSC-CNS, the Scientific Community and the High-Tech Industry with strong needs in High Performance Computing (HPC). CASE develops its own codes and optimizes scientific applications for the most efficient use of supercomputers. The Management department was also created in 2007 by bringing together the existing Administration, Finance, Projects, Technology Transfer, Marketing and Communication teams.

The Computer Sciences, Earth Sciences and Life Sciences Departments continued to build upon their strong foundations in 2007 in their research fields. Computer Sciences in both Hardware and Software research for the development of the supercomputers of the future; Earth Sciences through its research in Air Quality Forecasting and Earth System Modelling; and Life Sciences advancing the understanding of Molecular Biology and evolution of living organisms.

The work carried out by the scientists at BSC-CNS resulted in above 200 publications in leading journals in the different research areas covered by the Centre, such as: Proceedings of the National Academy of Sciences, Journal of the American Chemical Society, Public Library of Science Computational Biology, Journal of Geophysical Research, Geophysical Research Letters, Environmental Modelling & Software, IEEE Transactions on Computers, IEEE Micro, IBM Journal of Research & Development or Physical Review Letters.

BSC-CNS income in 2007 was 12 M€. 6.7 M€ corresponded to the ordinary budget coming from the Spanish and Catalan Governments, BSC-CNS owners; and 5.3 M€ from competitive projects. In 2007, BSC-CNS also increased its participation in collaborative research projects and participated in 11 projects funded under the EU 7th Framework Programme and 10 projects funded by the Spanish Government. National project highlights include the Consolider project "Supercomputación y e-Ciencia" where 21 best of breed Spanish research teams collaborate to design supercomputing applications to efficiently use HPC architectures. BSC-CNS continued too its close collaboration with key industry leaders, including the MareIncognito project with IBM, focused on building the supercomputers of the future; exploration of future chip designs for the personal computer mass market with Microsoft, and the Kaleidoscope project on next generation seismic imaging technology with REPSOL.

The Spanish Supercomputing Network (Red Española de Supercomputación, RES) reached full development in 2007. RES is a project lead by the Spanish Government that consists in the creation of a distributed supercomputing infrastructure to enhance supercomputing support to Spanish research groups, in a way which is transparent to the users. RES members are, in addition to BSC-CNS, the Centro de Supercomputación y Visualización de Madrid (CeSViMa), the Instituto de Astrofísica de Canarias and the Universities of Cantabria, Málaga, Valencia and Zaragoza. RES has a single Access Committee, composed of prestigious Spanish scientists, which determines the projects that can enter the RES supercomputers. More than 600 R&D projects took advantage of the RES infrastructure in 2007. These produced more than 400 publications, several of them in outstanding journals such as Nature, Journal of the American Chemical Society, Journal of Biological Chemistry, Angewandte Chemie, Journal of Cosmology and Astroparticle Physics, Astrophysical Journal, Physical Review Letters, Physics Reports or Nano Letters.

The BSC-CNS also took steps to help consolidate HPC at European level. In April 2007, 14 European countries signed a Memorandum of Understanding for the creation of a Partnership for Advanced Computing in Europe (PRACE), whose mission is the creation of a persistent pan-European HPC infrastructure, consisting of few tier-0 supercomputing centres which will provide European researchers with access to capability computers and form the top level of the European HPC ecosystem. BSC-CNS, as the representative of the Spanish government, signed as a "Principal Partner", thus expressing its interest in hosting and funding one of the main Tier0 HPC centres of the new HPC infrastructure.

BSC-CNS staff received several awards in 2007, two of which were especially relevant. Mateo Valero received the Eckert-Mauchly Award, the Computer Architecture community's most prestigious prize, and José María Baldasano (Earth Science department director) shared as a member of the Intergovernmental Panel on Climate Change (IPCC) the 2007 Nobel Peace Prize.

The people who work at BSC-CNS are the organization's key asset. It is thanks to their effort, skills and capabilities that BSC-CNS is steadily approaching its goal of becoming a European reference in HPC and e-Science.

Mateo Valero, Director

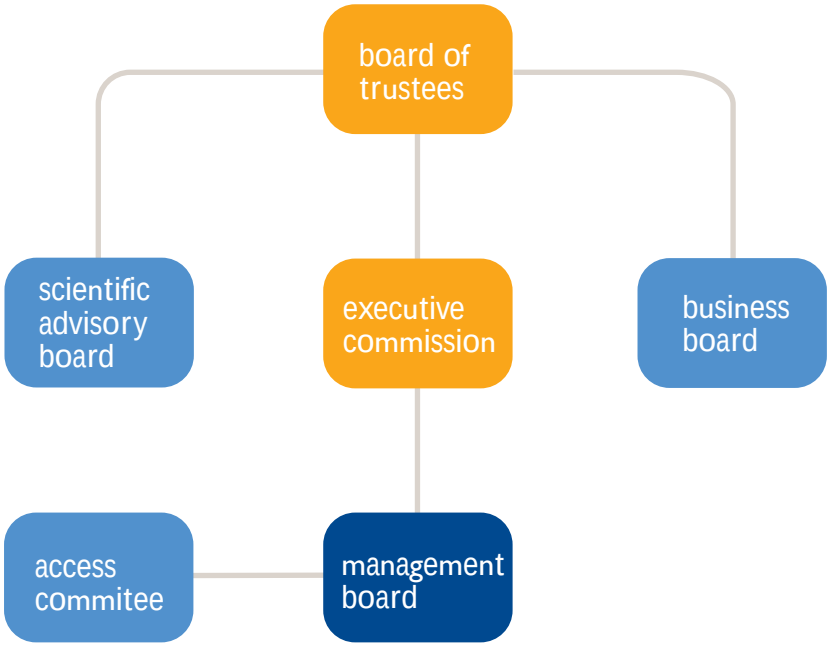
Francesc Subirada, Associate Director

2 Organizational Structure

Description of the main governing bodies and departments of BSC - CNS

Governing Bodies

The figure below describes the different governing bodies and departments that constitute the Barcelona Supercomputing Center – Centro Nacional de Supercomputación (BSC-CNS).



Board of Trustees

The Board of Trustees serves as the main governing body of the BSC-CNS Consortium and consists of representatives from each of the three shareholder institutions in the Consortium: the Ministerio de Educación y Ciencia (MEC), the Departament d'Innovació, Universitats i Empresa of the Generalitat de Catalunya (DIUE) and the Universitat Politècnica de Catalunya (UPC).

Chairman of the Board
Francisco Marcellán Español
Secretary-General of Policies on Science and Technology, MEC

Vice Chairman of the Board
Blanca Palmada
Commissioner of Universities and Research, DIUE

Members (MEC)
Carmen Andrade
Director-General of Policies on Technology

José Luís Martínez
Deputy Director-General of Research Projects

José Ignacio Doncel
Deputy Director-General of Promotion and Technology Infrastructures and Large Installations

Members (DIUE)
Joan Majó,
Director-General of Universities

Ramon Moreno,
Director-General of Research

Iolanda Font de Rubinat,
Deputy Director-General of Research

Members (UPC)
Antoni Giró,
Rector

Josep Casanovas,
Vice-Rector of University Policies

Sebastià Sallent,
Director of Fundació I2Cat

BSC-CNS Director:
Mateo Valero
Director, Barcelona Supercomputing Center

Secretary of the Board:
Francesc Subirada
Associate Director, Barcelona Supercomputing Center

Executive Comission

The Executive Comission is responsible for executing on the plans of the BSC-CNS and monitoring center progress.

Commission Chairman:
José Ignacio Doncel
Deputy Director-General of Promotion and Technology Infrastructures and Large Installations, MEC

Comission Vice-Chairman:
Ramon Moreno
Director-General of Research, DIUE

Member (MEC):
Ramon López de Arenosa
Department Head, Department of Production Technologies and Communications

Member (DIUE):
Iolanda Font de Rubinat
Deputy Director-General of Research

Member (UPC):
Xavier Gil
Vice-Rector of Research

Member (UPC):
Josep Casanovas
Vice-Rector of University Policies

BSC-CNS Director:
Mateo Valero
Director, Barcelona Supercomputing Center

Comission Secretary:
Francesc Subirada
Associate Director, Barcelona Supercomputing Center

Management Board

The Management Board is resposible for executing the guidelines defined by the Board of Trustees and Executive Commission. This board is leaded by the Director and Associate Director and it includes the directors of both research and support activities of the center.

The members included at the Management Board are:

Management Board Chairman:
Mateo Valero, *Director*

Management Board Vice-Chairman:
Francesc Subirada, *Associate Director*

Members:
Jesús Labarta,
Computer Sciences Director
Eduard Ayguadé,
Computer Sciences Associate Director
José María Baldasano,
Earth Sciences Director
Modesto Orozco,
Life Sciences Director
Sergi Girona,
Operations Director
José María Cela,
Computer Applications in Science and Engineering Director
Ernest Quingles,
Management Director

Management Board Secretary:
Mercè Calvet,
Administration and Finance Department

Scientific Advisory and Business Boards

The Scientific Advisory Board and the Business Board are intended to offer advice on scientific and business matters. The Scientific Advisory Board consists of a select group of prominent international scientists while the Business Board consists of representatives from companies that currently collaborate with and fund the Center.

Access Committee

The Access Committee is responsible for all decisions concerning the scientific use of MareNostrum. The members of the Access Committee are selected by the MEC and the Agencia Nacional de Evaluación y Prospectiva (ANEP). The Access Committee is composed of a Core Team and four Expert Panels of prestigious Spanish scientists (external to BSC-CNS).

The four Expert Panels are based on the four-group classification system employed by the

Spanish Foundation of Science and Technology (FECYT - Fundación Española de Ciencia y Tecnología): Astronomy, Space and Earth Sciences, Biomedicine and Health Sciences, Physics and Engineering and Chemistry and Materials Science. The Expert Panels are composed of high caliber scientists that also have experience in the management of research projects. Each of the four Expert Panels consists of 10 experts and is chaired by a coordinator with the help of an assistant. The Experts Panel can request an ANEP peer review of a project when required.

The Expert Panels prioritize the activities of each of their respective areas and send their recommendations to the Core Team who publishes every four months the list of approved users of MareNostrum on the BSC-CNS website.

In 2007, the members of the Access Committee included:

Core Team
Victoria Ley Vega de Seoane
Agencia Nacional de Evaluación y Prospectiva
Pedro de Miguel Anasagasti
Universidad Politécnica de Madrid
Ramón López de Arenosa
Ministerio de Educación y Ciencia
José María Cela
Barcelona Supercomputing Center-Centro Nacional de Supercomputación

Biomedicine and Health Sciences Expert Panel
Coordinator: Alfonso Valencia
Centro Nacional de Investigaciones Oncológicas
Assistant: Manuel Palacín
Universidad de Barcelona

Chemistry and Material Sciences Expert Panel
Coordinator: Agustí Lledós
Universidad Autónoma de Barcelona
Assistant: José Maria Pitarke
Universidad del País Vasco

Physics and Engineering Expert Panel
Coordinator: Pablo Ordejón
Instituto Ciencia Materiales Barcelona
Assistant: Rodolfo Bermejo
Universidad Politécnica de Madrid

Astronomy, Space and Earth Sciences Expert Panel
Coordinator: José Maria Ibáñez
Universidad de Valencia
Assistant: Vicente Caselles
Universidad de Valencia

BSC-CNS Departments

Computer Sciences Departament
Computer Sciences Director:
Jesús Labarta
Computer Sciences Associate Director:
Eduard Ayguadé

Autonomic Systems and e-Business Platforms
Head: Jordi Torres

Researcher: Vicenç Beltran
Researcher: David Carrera
Researcher: Jordi Guitart
Researcher: Kevin Hogan
Researcher: Mario Macias

Resident Student: Iñigo Goiri
Resident Student: Ferran Julià
Resident Student: Ramon Nou

Computer Architecture
Head: Alex Ramírez

Senior Researcher: Francisco Cazorla
Senior Researcher: Adrian Cristal
Senior Researcher: Roberto Gioiosa
Senior Researcher: Osman Unsal

Researcher: Daniel Jiménez
Researcher: Miquel Pericas
Researcher: Francisco Javier Vera

Technical Support: Josep Oriol Prat

Resident Student: Hilal Alaa
Resident Student: Vladimir Cakarevic
Resident Student: Paul M. Carpenter
Resident Student: Maximiliano Combina
Resident Student: Vladimir Gajinov
Resident Student: Gokçen Kestor
Resident Student: Vladimir Marjanovic
Resident Student: Milos Milovanovic
Resident Student:: Marco Paolieri
Resident Student: Cristian Perfumo
Resident Student: Petar Radojkovic
Resident Student: José Carlos Ruiz
Resident Student: Suthirta Sanyal
Resident Student: Nehir Sonmez
Resident Student: Srdjan Stipic
Resident Student: Vladimir Subotic

Resident Student: Sasa Tomic
Resident Student: Augusto Vega
Resident Student: Ramzi Younes
Resident Student: Ferad Zyulkyarov

Visiting Student: Carlos Santieri Boneti
Visiting Student: Roger Codina
Visiting Student: Kamil Kedzerski
Visiting Student: Cornelis Meenderinck
Visiting Student: Paolo Meloni

Grid Computing and Clusters

Head: Rosa M. Badia

Researcher: Julita Corbalán
Researcher: Marc de Palol
Researcher: Jorge Ejarque
Researcher: Francesc Guim
Researcher: Luis Martinell
Researcher: Josep M. Pérez
Researcher: Ivan Rodero
Researcher: Raúl Sirvent

Student Researcher: Enric Tejedor

Resident Student: Pieter Bellens
Resident Student: Maja Etinski

Visiting Researcher: Michael Parkin

Performance Tools

Head: Judit Giménez

Researcher: Xavier Aguilar
Researcher: Marc Casas
Researcher: Juan González
Researcher: Pedro Antonio González
Researcher: German Llort
Researcher: German Rodríguez
Researcher: Eloy Martínez
Researcher: Xavier Pegenaute
Researcher: Harald Servat

Visiting Student: Gladis M. Utrera

Programming Models

Head: Xavier Martorell

Researcher: Jairo Balart
Researcher: Juan José Costa
Researcher: Álex Duran
Researcher: Montserrat Farreras
Researcher: Roger Ferrer
Researcher: Marc González
Researcher: David Ródenas
Researcher: Javier Teruel
Researcher: Jorge Vaquero

Resident Student: Javier Bueno
Resident Student: Víctor Jimenez
Resident Student: Lluis Vilanova
Resident Student: Nikola Vujic

Storage Systems

Head: Toni Cortés

Researcher: Ernest Artiaga
Researcher: Jesús Malo
Researcher: Jonathan Martí

Resident Student: Marta García
Resident Student: Albert Miranda

Computer Applications in e-Sciences and Engineering

Computer Applications in e-Sciences and Engineering Director: José María Cela

Senior Researcher: Rogeli Grima
Senior Researcher: Guillaume Houzeaux
Senior Researcher: Mariano Vázquez

Researcher: Mauricio Araya
Researcher: Hadrien P. Calmet
Researcher: Miquel Catalán
Researcher: Raúl de la Cruz
Researcher: Manuel Quero
Researcher: Albert Farres
Researcher: Mauricio Hanzich
Researcher: Pierre Lafortune
Researcher: Anne-Cécile Lesage
Researcher: Félix Rubio
Researcher: Xavier Saez
Researcher: Alejandro Soba

Student Researcher: Ruth Aris
Student Researcher: Ane Beatriz Eguzkitza
Student Researcher: Cristina Montañola

Visiting Student: Manuel Hasert

Earth Sciences

Earth Sciences Director: José María Baldasano

Group Manager: Santiago Gassó

Senior Researcher: Pedro Jiménez
Senior Researcher: Oriol Jorba
Senior Researcher: Carlos Pérez

Technical Support: David Carrió
Technical Support: Eugenio López
Technical Support: Albert Soret
Technical Support: Thomas Loridan

Post-doc: Patricia Güereca

Resident Student: Juliana González
Resident Student: Karsten Haustein
Resident Student: Simone Marras
Resident Student: Mª Teresa Pay
Resident Student: Angel Rincón

Visiting Student: Maria Gonçalves

Life Sciences

Life Sciences Director: Modesto Orozco

Computational Genomics

Head: David Torrents

Researcher: Carlos Quijano
Researcher: Jesús López

Technical Support: David García

Electronic and Atomic Protein Modelling

Head: Víctor Guallar

Researcher: Raúl Alcántara
Researcher: Benjamín Cossins
Researcher: Víctor Gil
Researcher: Diego Masone

Student Researcher: Kenneth Borrelli
Student Researcher: Frank Heinrich

Visiting Student: Ivan Duran

INB - Computational Bioinformatics node

Head: Josep Lluis Gelpi

Researcher: Félix Rubio
Researcher: Aida Santaolalla

Technical Support: Dmitri Reptchevski
Technical Support: Romina Royo

Resident Student: Alexis Torrano

Molecular Modelling and Bioinformatics

Researcher: Montserrat Barbany
Researcher: Marco d'Abramo
Researcher: Agnes Noy

Technical Support: Jordi Camps

Student Researcher: Carles Fenollosa

Visiting Student: Josep Ramon Goñi
Visiting Student: Alberto Pérez
Visiting Student: Julio José Ramírez

Protein Interactions and Docking

Head: Juan Fernández-Recio

Researcher: Solène Grosdidier
Researcher: Albert Solernou

Technical Support: Carles Pons

Visiting Student: Albert Antolín
Visiting Student: Tammy Mann-kuang
Visiting Student: Laura Pérez

Management

Management Director: Ernest Quingles

Project Manager: Gina Alioto
Project Manager: Toni Moreno

Project Officer: Nuria Nadal

Project Management Assistant: Valentín Lafuente

Marketing Executive: Renata Giménez

MareNostrum Visitors Manager: Oriol Riu

Mobility Program Manager: Fermín Sánchez

Mobility Program Assistant: Anna Monrós

Human Resources, Finance and Administration

Head: Mercè Calvet

Director's Assistant: Neus Jiménez

Associate Director's Assistant: Nuria Sirvent

Administration Assistant: Lourdes Cortada
Administration Assistant: Laura Gutiérrez

Account Officer: Cristina Calonge

Finance Assistant: Judit Soldevila

Human Resources Manager: Sandra Vargas
Human Resources Assistant: Lara Cejudo

Operations

Operations Director: Sergi Girona

System Administration

Head: Javier Bartolomé

Helpdesk: Fernando Fernández
Helpdesk: Jordi Inglés

Resident Student: Lucas Rullo
Resident Student: Cristian Simarro
Resident Student: Ivana Teodor

Security and Networks: Carlos Kishimoto
Security and Networks: Juan Carlos Sánchez

System Administration: Xavier Fustero
System Administration: Sergi Moré
System Administration: Jordi Valls

Performance and Planning: Asier Roa
Performance and Planning: Miquel Ros

User Support

Head: David Vicente

User Support: Pere Munt
User Support: Jorge Naranjo

Technical Support: Xavier Abellan

Project Technical Support: David Agudo

Webmaster: Silvina Rusinek

Maintenance Assistant: Albert Riera

BSC staff

3 Research and Support Activities

The internal scientific departments and their results during the year 2007

Jesús Labarta
Computer Sciences
Director

Eduard Ayguadé
Associate Computer
Sciences Director

The research activities aim at meeting computer architecture and application requirements for the design of future high-performance and supercomputing systems.

These research activities are done within internal BSC-CNS projects, in projects in the framework of the European Union and with leading-edge companies in the field. During 2007, the department participated in 6 IST FP6 projects (ACOTES, BEinGRID, BREIN, SARC, SORMA and XtreemOS), 3 networks of excellence (HiPEAC, CoreGRID and HPC-Europa) and several research contracts with companies (IBM, Microsoft and Sun Microsystems). During 2007 the department had two new IST FP7 projects approved (MERASA and Velox), the continuation of the HiPEAC network of Excelence, the continuation of the IBM project (MareIncognito) and the creation of the BSC-Microsoft Research Centre. The department also coordinated the Basic Research in Supercomputing section of the Spanish Consolider program "Supercomputing and eScience".

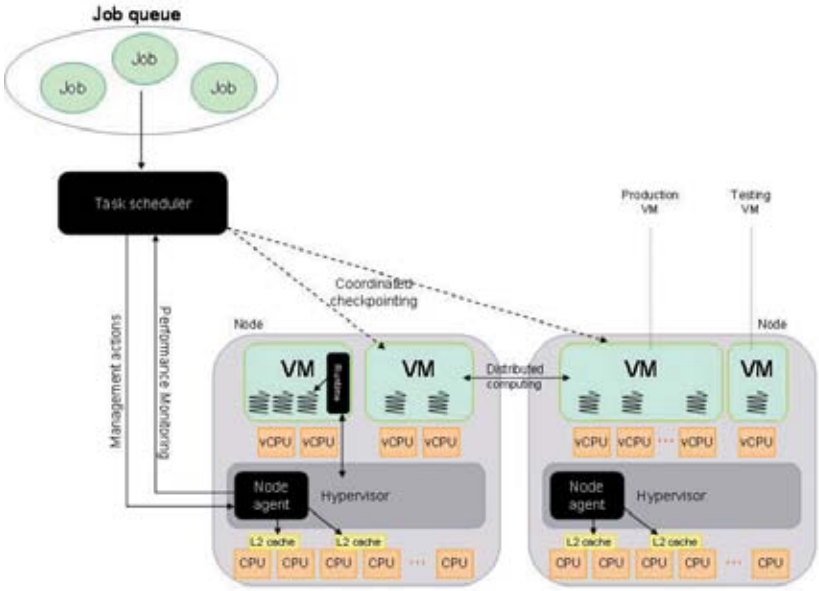
Autonomic Systems and eBusiness Platforms (eBP)

In 2007 the Autonomic Systems and eBusiness Platforms group continued its efforts to build a self-adaptive execution environment for heterogeneous workloads. The research activities of the group addressed the following main topics:

- In collaboration with IBM Watson, the group conducted research on the explicit management of heterogeneous workloads, comprising of both transactional applications and long running batch jobs, in the context of data centers. The work performed took full advantage of virtualization technologies as well as utility-based computing to achieve differentiated and comparable performance among such a heterogeneous set of workloads. This research also contributed to the LAGrid program.
- In the EU SORMA project, the group implemented an economically-enhanced resource manager (EERM), which performs resource provisioning based on economic models. In particular, this group proposed techniques used by the EERM to support revenue maximization across multiple Service Level Agreements (SLA). In the online simulation area the department successfully built a prototype which was able to increase Middleware performance. Later the group extended the collaboration with Samuel Kounev (Cambridge University) to build QoS-aware Resource management for Globus using prediction.
- In the EU BREIN project, the group participated in the design and prototyping of a semantically-enhanced resource allocator, which assigns resources depending on the information given by service providers with regard to the level of preference (according to business goals) of their customers and on the resource requirements of the tasks. The allocation process is enhanced by semantically describing the tasks and resources and using these descriptions to infer the resource assignments. Virtualization is used to provide a fully customized and isolated virtual environment for each task, which is then consolidated in order to achieve a better utilization of the provider's resources. In addition, the system supports fine-grained dynamic resource distribution among these virtual environments based on SLA.
- In collaboration with the University of Coimbra (Portugal) and ZIB Institute (Germany) a set of self-healing solutions for legacy software was developed, continuing the work started in 2006.

These approaches took advantage of virtualization concepts to improve the effectiveness and reduce the cost of the solutions; moreover, forecasting methods were proposed to predict potential failures and avoid consequences such as undesirable performance or even crashes and apply recovery actions at the best moment, reducing the time between failure and the time to recover.The group participates in CoreGRID, a network of excellence on Grid, in the area of Self-healing.

- A compressed page cache (CPC) was implemented in the Linux OS. By introducing memory compression to the operating system, a wide range of memory demanding applications can use larger working sets, reducing the amount of tasks' swapping required for their execution and improving bandwidth between the memory and I/O subsystems. Our current compressed page cache (CPC) system is the first implementation capable of making the most of traditional multiprocessor/multicore systems like the JS21 blades.The team is working to extend it to run on a heterogeneous architecture like the Cell/BE processor.
- Finally the group also participated in the EU XtreemOS project, proposing eBusiness applications for the project, whose objective is to build and promote a Linux-based OS to support virtual organizations for next generation grids.



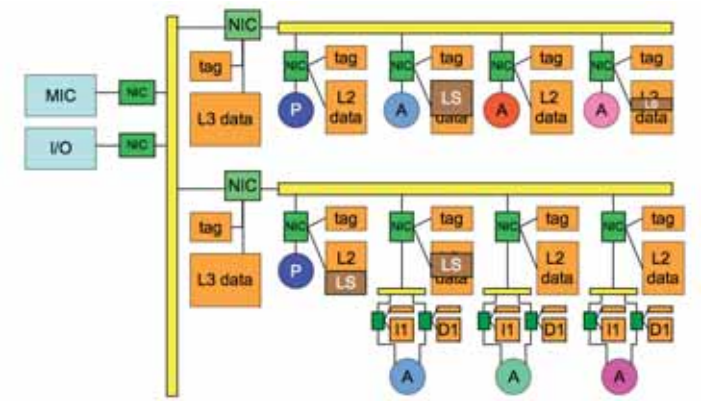
Using virtualization techniques to reduce the management complexity of large clustered data centers

Computer Architecture

In 2007, the Computer Architecture group focused its activities in four main directions: high performance heterogeneous chip multiprocessors, architecture support for novel programming models, close interaction between the architecture and the operating system, and the use of reconfigurable hardware to accelerate application kernels. In addition, the group participated in three European projects (SARC and ACOTES under FP6 and MERASA under FP7) and one network of excellence (HiPEAC). This, in addition to continuing research with Microsoft, Sun Microsystems and IBM.

Within the work on heterogeneous chip multiprocessor systems, the group tackled the following issues:

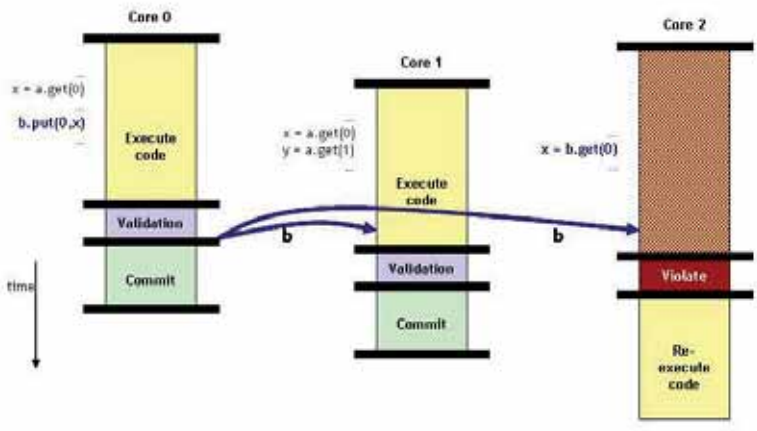
- In the SARC project the group proposed a first detailed definition of the SARC architecture: a massively heterogeneous architecture with explicit support for shared memory and programming model constructs. This architecture combines the power efficiency of heterogeneous architectures with the ease of programming of shared memory platforms. The first incarnation of the SARC architecture targets the execution of high definition media codecs, such as H.264/AVC. Also in the context of this project, the group proposed hardware extensions that would allow the processor to dynamically partition a cache shared by several processors in a CMP in order to optimize performance.
- In the ACOTES project, the group developed an analytical simulation model to predict the performance of streaming applications on massively heterogeneous platforms. This model allows the compiler to predict the performance impact of the different streaming transformations.
- In the MareIncognito project the team established a close collaboration with the Cell/B.E. processor architecture team, and performed preliminary evaluations of next generation Cell/B.E. architectures. CellSim, the execution-driven simulation infrastructure for the Cell/B.E. architecture developed in the framework of the SARC project, was used to explore different processor configurations as well as "what if" scenarios.



Scalable shared memory architecture for programmability (with memory mapped local stores for scratchpad memory) and heterogeneous accelerators for power efficiency

The group continued the research into architectural support for novel programming models. This includes:

- Transactional memory has been identified by researchers as one of the potential enabling elements of next generation programming models to facilitate development of parallel applications. The group developed different implementations of transactional memory in the framework of the Microsoft collaboration and the FP7 Velox project (to start January 2008, collaborating with other European academic partners along with AMD and Red Hat to develop TM accross the system stack). Implementations range from Software Transactional Memory (STM) implementations for C/C++ and Haskell, Hardware Transactional Memory (HTM) implementations (simulator based on M5 and PTLSim) and Hardware-assisted STM, analyzing the sources of overhead in STM implementations and features that can be accelerated/hidden with the appropriate hardware support. In the framework of the HiPEAC network of excellence, the group collaborated with University of Siena on application of TM to novel domains and in the future will contribute to the implementation of transactional memory in GCC.
- The group performed a detailed analysis of the overheads in the CellSs programming model, and determined that the task creation and management of the task dependency graph limits the scalability of the programming model. The next step is proposing specific hardware support to handle those overheads and improve scalability.



Research in transactional memory in the framework of the BSC-Microsoft collaboration agreement. Transactional memory synchronizes threads optimistally. For example, core 0 and 1 read the same memory location but do not conflict; however, core 0 writes to a memory location read by core 2, which creates a conflict that forces one of them (core 2) to abort and restart its execution

The group also continues to perform research on architecture and operating system interfaces for closer interaction, both for real-time systems and for high-performance systems:

- Collaborating with IBM, the team conducted the first quantitative evaluation of the hardware thread priorities on the POWER5 processor, the first commercial processor with this prioritization scheme. The team carried out some studies showing how the hardware thread priorities could be used to balance MareNostrum applications.
- BSC collaborated with other European universities and companies in the MERASA project, funded by the EU. MERASA aims to develop embedded processors that use multi-core technology to satisfy hard real-time constraints
- The group proposed an interface to allow the operating system to control the amount of cache allocated to each thread in a CMP architecture to optimize different of quality-of-service metrics.
- In collaboration with Sun Microsystems, the group also performed studies on the scheduling of short tasks, representative of the networking environments, on the Niagara T1, a massively multithreaded architecture.

Finally, the group initiated research activities using reconfigurable hardware to accelerate selected application kernels. A few applications from the bioinformatics domain (sequence alignment, protein docking) were ported to the Cell/BE architecture in order to identify common kernels that would benefit from hardware acceleration. The group also started with acceleration using programmable logic (FPGA), both for the acceleration of architectural simulations as well as other kernels in scientific applications.

Grid Computing and Clusters

The Grid Computing and Clusters GC group focused on two main projects in 2007: GRID superscalar and eNANOS. In addition, the group participated in the following projects funded by the European Commission: CoreGRID, BEinGRID, Brein and XtreemOS and in the international innitiative LAGrid.

GRID superscalar is a programming and execution environment for computational grids. It is able to parallelize a sequential application at runtime and the task level. Thus, it is possible to take advantage of applications that are composed of coarse grained tasks (e.g. a simulation, a program, a solver) which are common in bioinformatics, computational chemistry and other scientific fields.

In 2007, GRIDSs was first distributed as open source, and some new features were implemented:

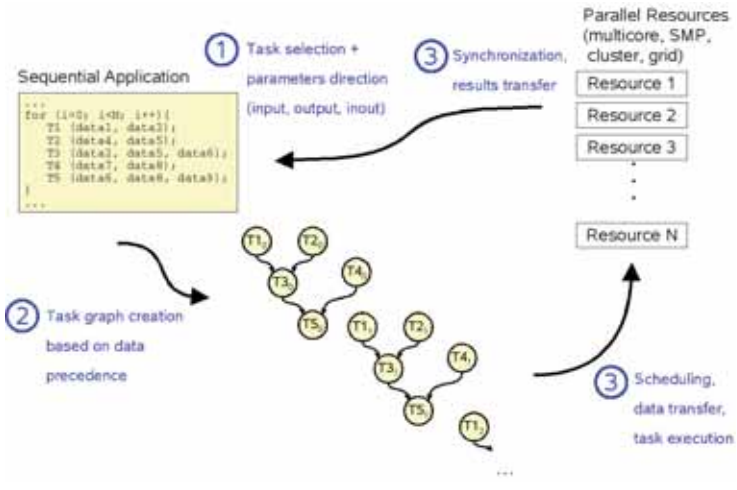
- Fault tolerance and use of task replication.
- MareNostrum supercomputer version: extensions for fault tolerance and for MPI tasks
- Implementation of a version of GRIDSs based on CoreGRID Grid Component Model (COMPSs)
- The eNANOS project is based on the idea of having strong low-level support for performing high level scheduling.The eNANOS project implementation includes: fine grain control between scheduling levels, dynamic allocation (MPI+OpenMP jobs) to improve system performance, tracking detailed scheduling and performance information that can be used for future scheduling decisions resulting in efficient scheduling (in terms of slowdown) based on performance prediction.

The group made the following progress in 2007:

- Design of prediction models to improve the performance of the scheduling policies
- Design of two new resource selection policies and a new backfilling policy
- Extension of the ISIS-Dispatcher architecture
- New Grid Resource Broker version based on Globus Toolkit 4 and Web Services.
- Development of a P2P interoperable infrastructure based on Web Services within the LA Grid project and new scheduling policies.

The GC Group also participated in several other projects:

- The group was involved in two institutes of the CoreGRID network of excellence: the Institute on Resource Management and Scheduling and the Institute on Grid Systems, Tools and Environments.
- The group contributed to XtreemOS by providing use-cases and requirements for an application based on GRIDSs and by leading the design of an application execution management environment.
- In the framework of BeinGRID, GRIDSs was integrated with the GridWay metascheduler. An application from the design of new processes and products in the chemistry sector was implemented on top of these two tools. Besides, a new grid portal was implemented that enables grid administration, project management and user GRIDSs applications deployment.
- Along with the Autonomic Systems and eBusiness Platforms group the GC group has led one of the BREIN prototypes: the Semantically Enhanced Resource Allocator. This prototype integrates semantics and ontologies, multi-agents and virtualization to perform dynamic scheduling and resource management.
- LAGrid is an IBM initiative to foster collaborative research and to offer equal opportunities to latinamerican students. Collaborative research in the framework of the Metabroker and Hurricane mitigation projects continued during 2007.



StarSs programming model enables the automatic parallelization at functional level of sequential codes taking into account the internal data dependencies of the application and independently of the target parallel architecture

Performance Tools

In 2007, the Performance Tools group focused on increasing the scalability and flexibility of their tools, introducing new automatic analysis features, enabling interoperability with other tools and exploring new strategies to extract information at execution time.

In terms of scalabilty it is important not to be limited by the trace sizes and to have the ability to efficiently process trace data to answer any question the analyst can raise. To this end, the utilities developed to work with large traces were extended with new functionalities and some of them parallelized with OpenMP. In addition, new functionalities were added to Paraver to increase the flexibility of the analysis.

Automatic analysis enables non-expert users to benefit from performance analysis. In general, it is very useful when working with large traces because it helps to drive the analysis directly to the most significant areas. The group worked on implementing two different techniques:

- One of the approaches is based on clustering algorithms to identify the structure of the trace. The clustering tool was extended to compute a CPI-Stack model at the level of the most significant computing bursts. The tool was validated with different applications such as WRF, CPMD and SIESTA.
- A second research line involved applying wavelets to identify patterns in the trace. A simple model of the performance speed-up was used to automatically detect performance bottlenecks and predict behaviour with a larger number of processes.

Different performance tools must be interoperable in order to allow building of performance analysis environments that combine their abilities and functionalities. The Performance Tools group is working on this in two directions:

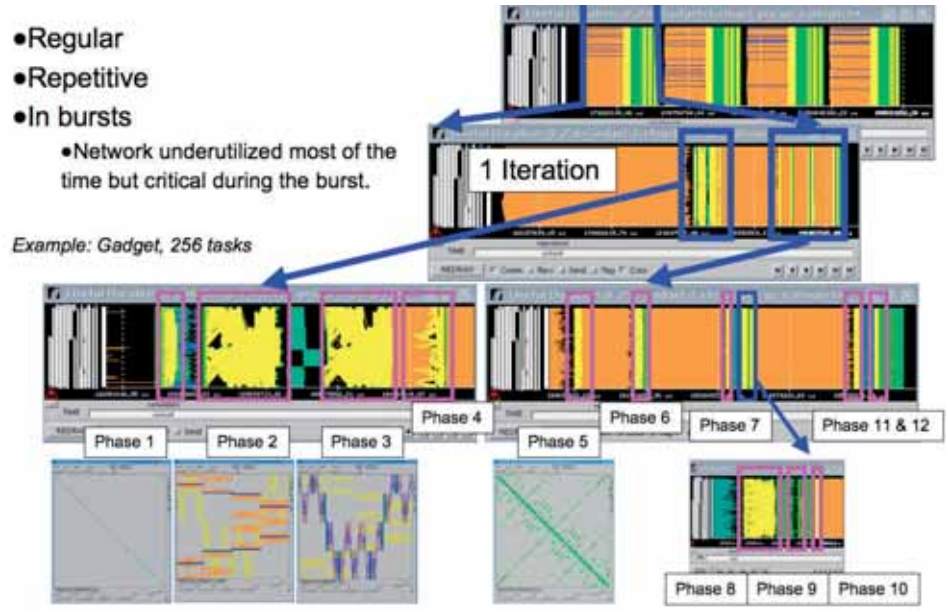
- A mix of automatic analysis with Dimemas and instruction level simulators was tested as a closing cycle to give insight on which architectural parameters have a strong impact on the performance achieved by an application.
- The integration with PeekPerf from the IBM HPC Toolkit allowed the user to compute a set of metrics from the Paraver trace and use the Peekperf visualizer to correlate them with the call tree.

The group also worked on new strategies to extract information during the execution of the parallel application:

- To focus on the relevant data and discard redundant information while the application is being executed, the group worked towards an intelligent tracing library using MRNet from the University of Wisconsin. One of the first goals was to apply the automatic analysis techniques at run time.
- To include sampling information in the trace file. Based on the mechanism of counter overflow provided by PAPI, the group implemented a version of the tracing library that periodically adds samples of hardware counters and/or call stack information.

Finally, with respect to the code maintenance, the group focused on two issues:

- Integrating the different versions of the instrumentation library
- Restructuring the Paraver code. The original code has a monolitic structure with no separation between the computing engine and the visualization. The modular engine was implemented and work started on developing a new GUI.



Scientific applications communication patterns

Explicit tasks

```
#pragma omp task
[clause[[,]clause] … ]
        structured-block

where clause can be one of:
        if ( expression )
        untied
        shared ( list )
        private ( list )
        firstprivate ( list )
        default ( shared | none )
```

Implicit tasks

```
#pragma omp parallel
```

⇒ one per thread in the team, tied

Wait on the completion of child tasks generated

```
#pragma omp taskwait
```

Example

```
void traverse(binarytree *p, bool
postorder) {
  #pragma omp task
    if (p->left) traverse(p-
>left, postorder);
  #pragma omp task
    if (p->right) traverse(p-
>right, postorder);
  if (postorder) {
    #pragma omp taskwait
  }
  process(p);
}
```

OpenMP 3.0 tasking: contribution to the standard

Programming Models

The Programming Models group focused on: OpenMP compilation and execution infrastructure, novel programming models for multicore architectures and programming models for clusters.

Regarding the compilation and execution environment for OpenMP in shared-memory multiprocessor architectures, the group worked on the following issues:

- The Mercurium source-to-source infrastructure was improved to provide better support for the restructuring of Fortran and C/C++ applications. The infrastructure supports the development of the programming models proposed in the BSC-CNS and the code generated targets the runtime libraries that support the execution of these programming models.
- Extensions to the OpenMP programming model. The group was involved in the design of OpenMP 3.0 together with the OpenMP Language Committee. BSC-CNS contributed with three extensions: tasking (also providing a reference implementation to the community), better support for nested parallelism and AUTO schedule for loops. In the context of a CAS grant from IBM Toronto, the group worked on adapting the IBM XLSMP runtime system to support tasking.

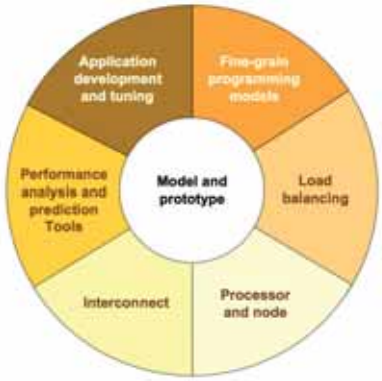
The group has continued to research into programming models for the emerging homogeneous and heterogeneous multicore architectures:

- The StarSs programming model is based on simple annotations added to sequential applications to identify tasks and their input and/or ouput arguments. StarSs is provided with two targets: CellSs for the Cell/B.E. processor and SMPSs for homegenous shared-memory multicore and multiprocessor systems. The runtime system implements an execution model that is able to dynamically (automatic parallelization at execution time) exploit the existing parallelism and to schedule work on the different cores of the architecture. For CellSs it also transparently introduces data movement between local memories and main memory. This work contributed to the MareIncognito project in collaboration with IBM Research.

- OpenMP for Cell. In the context of the collaboration with IBM Watson the group proposed a novel software cache implementation to support the compilation of OpenMP applications for the Cell/B.E. architecture. This software cache makes the data movement between the main memory and the local memories transparent, managing those memory references that the compiler is unable to optimize with prefetching. This work also contributes to the project.
- In the framework of the Microsoft collaboration, the group proposed the integration of Transactional Memory in OpenMP, trying to simplify the expression of parallelism and synchronization patterns in applications.
- In the SARC project, the group proposed extensions to the OpenMP programming model to expose the heterogeneity and memory singularities of accelerator-based multicore architectures to the programmer.
- In the ACOTES project, the group proposed a new programming model, inspired by OpenMP, to express parallelism for streaming architectures. In this approach, the programming model allows the application to be split into tasks, which are then connected using streams. A runtime library (acolib) to execute the programming model on SMPs was developed.

Finally, the group continued working on programming models for distributed memory architectures, specifically in two areas:

- The NanosDSM runtime system to support the execution of OpenMP shared-memory applications on top of clusters with distributed memory. In the context of a CAS grant from IBM Toronto, the group adapted the IBM XLSMP runtime system to work with the NanosDSM runtime system on clusters of SMPs.
- Also in the context of a collaboration with IBM Watson, the group contributed to the implementation of the runtime system for the UPC (Unified Parallel C) programming model for distributed-memory architectures, including the interaction with the compiler and the proposal of extensions to support multidimensional data layouts.



MareIncognito working packages

Storage Systems

The Storage Systems group focussed on two main topics in 2007: file system scalability and Input/Output for Grid systems. Regarding the first topic, the group worked on the following three issues:

- Cooperative caching is a well known technique used to improve the effectiveness of disk caching. The available implementations have been targeted to small-size clusters (10-100 nodes) and the implementations have always been proof-of-concept prototypes. The objective is to build a production-quality cooperative cache that is able to scale to the size of MareNostrum (few thousands of nodes). The group implemented a first version in 2007, which was able to scale and react to large changes in the number of participating nodes.
- Heterogeneous storage systems. Storage systems built from heterogeneous sets of disks are becoming a usual configuration because increasing the capacity of a storage system cannot imply the replacement of all existing disks. In previous years the group proposed a solution to this problem (AdaptRaid) that takes into account the different characteristics of each disk to build a global system. In 2007 the group worked on mechanisms to make AdaptRaid scalable by avoiding full restriping of the storage system every time new disks are added to the system.
- Composite file system. In many high-performance systems, there is a need to have different file systems (or at list different configurations of the same file system) to manage the different needs of the users. These multiple file systems force the user to know which of them is better suited for a given set of files making the user's life unnecessarily complex. During this year the group forged the concept of a composite file system. A composite file system is built on top of the existing file systems and, in an automatic and transparent way, (a) places the files into the most adequate file system (b) allows users to have a unique tree structure regardless of the underlying file systems.

The Input/Output for GRID systems issue is part of XtreemFS, an object-based file system for federated IT infrastructures that are connected by wide-area networks designed in the framework of the European XtreemOS project. In particular, the group contributed to the implementation of the Object Storage Device (OSD) software. Within OSD, the group worked on the implementation of striping mechanisms, as well as on management of replica updates. During the second semester, the group also started to work on the Replica Management Service (RMS) that will decide when replicas are created and/or removed. During this period, the team worked on prediction of file usage to decide which files and in which nodes files should be replicated. Although this study was performed using simulation techniques, the group plans to implement the resulting mechanisms into XtreemFS.

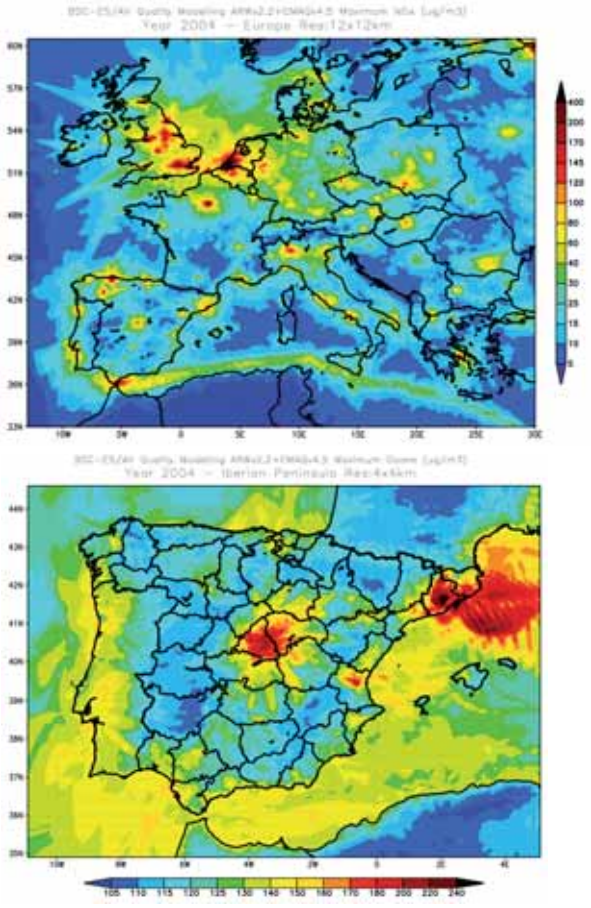
José María Baldasano
Earth Sciences Director

The Earth Sciences Department was established with the objective of carrying out research in Earth System Modelling.

The group has as main topics of research: high-resolution air quality and meteorological modelling; global and regional mineral dust modelling; and global and regional climate modelling. Currently, the group maintains daily high-resolution operational air quality forecasts for Europe and the Iberian Peninsula (http://www.bsc.es/caliope/) under the umbrella of the Caliope project funded by the Spanish Ministry of the Environment; and mineral dust forecasts for the Euro-Mediterranean region and East Asia (http://www.bsc.es/projects/earthscience/DREAM).
The group also collaborates with the World Meteorological Organisation and the Spanish Meteorological Institute for the creation of the Regional Center for Sand and Dust Warning System (SDS-WAS) covering Europe, northern Africa and Middle-East. Other research activities involve the diagnosis of the behaviour of the Earth System Modelling codes in a supercomputer framework and the improvement of the parallel versions to increase their horizontal and temporal resolution.

Air Quality

It is a challenge to forecast air pollution events in Europe and the Iberian Peninsula with very high resolution due to the complexity of the study area and the non-linearity of the processes governing the dynamics of atmospheric pollutants. In recent years, technological advances have made it possible to incorporate the latest meteorological, transport and chemical research codes into new computer platforms. Moreover, increased computational power as well as access to online data, coupled with advances in the computational structure of air quality models allow for real-time air quality forecasting.



Annual 1-hr maximum nitrogen oxides in Europe (up) and ground-level ozone for the Iberian Peninsula (down) (both in μg m^{-3}) during the year 2004

In 2007, the Air Quality Group developed a two day-hourly air quality forecasting tool based on the WRF/HERMES/CMAQ/DREAM modelling system with a high resolution (4 km) for the Iberian Peninsula and 12 km for Europe. This tool provides a better understanding of the dynamics of atmospheric pollutants and allows for early communication to the dwellers in areas that exceed air quality thresholds (Figure 1). The group offers a Spain and European Air Quality forecasting and assessment service to end-users that takes advantage of this high spatial and temporal resolution of the air quality modelling system. This forecasting service (http://www. bsc.es/caliope) offers a state-of-the-art development by depicting both the anthropogenic and natural contribution of particulate matter through the coupling of CMAQ+DREAM models. This work was developed in close collaboration with the Mineral Dust Group of the Earth Sciences Department.

The Air Quality Group carried out high-resolution annual simulations (specifically for the year 2004) for Europe (12 km, 1-hr) and nested the Iberian Peninsula simulations (4 km, 1-hr resolution; see figure) in order to describe the dynamics of air pollution and the relationship between emissions, atmospheric transport, chemistry and deposition. The results were validated against measured data from different air quality networks (EMEP, regional networks, etc.) to improve the accuracy of the forecast and to began an operational

validation. This analysis and validation was funded by an R+D Grant (CGL2006-08903) from the Spanish Ministry of Education and Science and the CALIOPE project of the Spanish Ministry of the Environment, a joint project with other Spanish (CSIC, CIEMAT, CEAM) and international research groups (University of Aveiro, Portugal; Institut Pierre-Simon Laplace, INERIS, LISA, C.N.R.S,France). The group also developed a version of the High Elective Resolution Modelling Emission System (HERMES) with very high resolution (1 km2 and 1-hr) for the Iberian Peninsula in order to address the emission needs of air pollution managing and air quality forecasting.

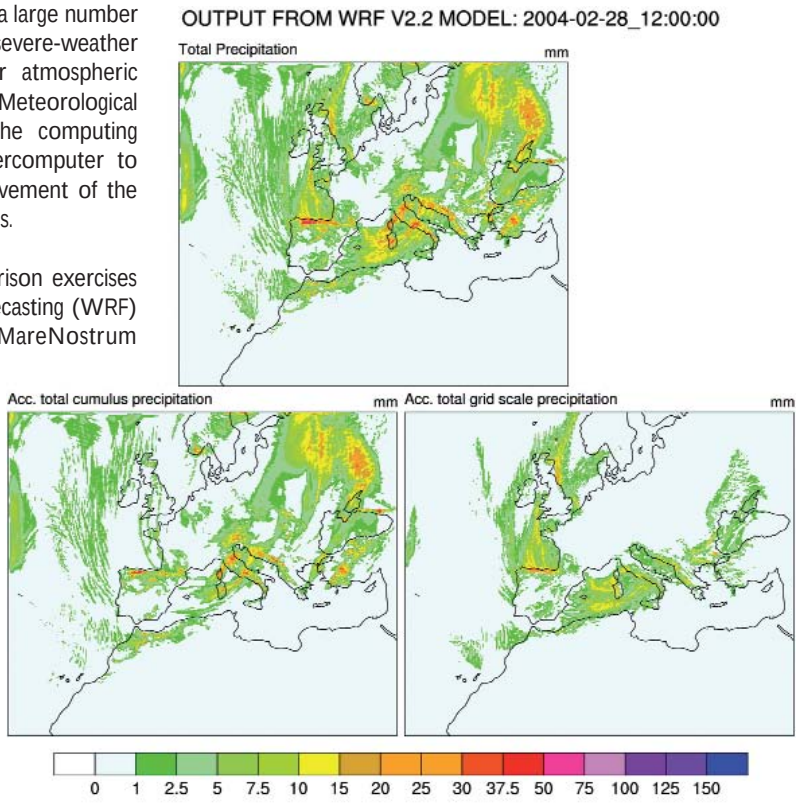
The Air Quality Group started tests for the operational implementation of the parallel version of the CHIMERE chemistry transport model as a core for air quality forecasting within the MareNostrum supercomputer. These tests included an analysis of the parallel performance of the CHIMERE and CMAQ codes when implemented in high performance supercomputing infrastructures.

The Air Quality Group was involved in technology-transfer activities for several companies and institutions (Gas Natural, Hidrocantábrico, Iberdrola, Siemens, SGS, IDOM, Ajuntament de Barcelona, Generalitat de Catalunya, etc.). The group worked on strategies for managing air pollution in large cities (Madrid and Barcelona) by measuring the impact of introducing variations in the vehicle fleets (gas natural, hybrid vehicles, etc.) or analysing the environmental impact of new industrial stacks' installations.

Meteorological Modelling

The evolution of the atmosphere governs a large number of processes that directly impact society; severe-weather situations lead to high rainfall rates or atmospheric conditions that modify the air quality. The Meteorological Modelling Group takes advantage of the computing performance of the MareNostrum supercomputer to study these areas, focusing on the improvement of the skills scores of their meteorological models.

The group carried out some intercomparison exercises based on the Weather Research and Forecasting (WRF) Model implemented in the MareNostrum supercomputer. The WRF model is a next-generation mesoscale numerical weather prediction system designed to serve both operational forecasting and atmospheric research needs. It features multiple dynamical cores and a software architecture that allows for computational parallelism and system extensibility. The current WRF software framework (WSF) supports two dynamic cores: the Advanced Research WRF Model (ARW) and the non-hydrostatic Mesoscale Model (NMM). The Meteorological Modelling Group validated a simulation for the year 2004 over Europe at 12 km horizontal resolution executed with both dynamical cores of the WRF model. Several statistics were calculated to



Precipitation modelled for Europe and the Mediterranean basin with a 12km resolution (total precipitation, up; total cumulus precipitation; down-left; total grid-scale precipitation; down-right)

compare the performance of both systems at surface level (wind speed, wind direction, temperature, dewpoint temperature). The study specially focused in stagnant meteorological conditions associated with the development of air pollution episodes, and therefore was included within the umbrella of the aforementioned Caliope project funded by the Spanish Ministry of the Environment.

Also among the activities of the Caliope project, the Meteorological Modeling Group used the WRF-ARW model to provide the meteorological inputs for air quality modeling in the domain of the Iberian Peninsula (4 km resolution) and Europe (12 km). Additionally, the group performed and evaluated high-resolution meteorological simulations for a selected year (2004) for the Iberian Peninsula (18, 12 and 4 km resolution) versus European and national observations (SYNOP and METAR data, INM stations data, etc.).

The coupling of chemistry transport models with latest generation meteorological cores is demanded in order to advance the study of air pollution. Hence, among the new developments, the group also worked on the coupling between the WRF-ARW model and the chemistry transport model CHIMERE in collaboration with the Air Quality Group. The ability to couple a WRF model with CHIMERE allows users of CHIMERE to make use of the latest developments in mesoscale meteorology through the developments of the WRF project. This code is available through the website at http://www.bsc.es /plantillaH.php?cat_id=445.

The current implementations of finite-difference atmospheric models are limited in terms of scalability by the choice of computational grids and numerical methods.

Development of new supercomputer capacities required focusing on numerical techniques to break through these scalability limitations. Thus, the group (together with the Computer Applications department) started to study the steps for developing a massively parallel finite elements approach to the solution of the Navier-Stokes equations in mesoscale atmospheric dynamics. This work is based on the ALYA software developed in the CASE-BSC department and is targeted at the next generation of high-performance computers.

Finally, the Meteorological Modelling Group worked with the Computer Sciences Department of the BSC to carry out a performance study of both cores of the WRF model using the Paraver software. The purpose of the benchmark study is to analyze the computational performance and scaling of the WRF model on the MareNostrum supercomputer environment as a diagnostic of the current performance of the model under high-performance computing architectures.

Mineral Dust

The largest portion of atmospheric particulate matter is derived from arid regions and deserts of the Earth and is distributed all over the globe. The impact of mineral dust on air quality, climate, ecosystems and human health represents a major scientific and societal issue.

The Mineral Dust Group provides daily operational forecasts of mineral dust for the Euro-Mediterranean and the East Asia region based on the Dust Regional Atmospheric Model (DREAM), designed to simulate the atmospheric cycle of mineral dust. DREAM is able to deliver reliable operational dust forecasts capable of predicting all the major dust events. This service is available on the web at http://www.bsc.es/projects /earthscience/DREAM. The operational verification of the aerosol optical thickness (AOT) of the model is performed daily using Sun photometric (AERONET) observations in collaboration with international groups of research (http://www.bsc.es/plantillaH.php?cat_id=398) and MSG satellite images in collaboration with the Spanish National Institute of Meteorology (INM).

The group collaborated with the Institute for Tropospheric Research (Leipzig, Germany) providing specific 3-day operational forecasts for the German SAMUM (Saharan Mineral Dust Experiment)

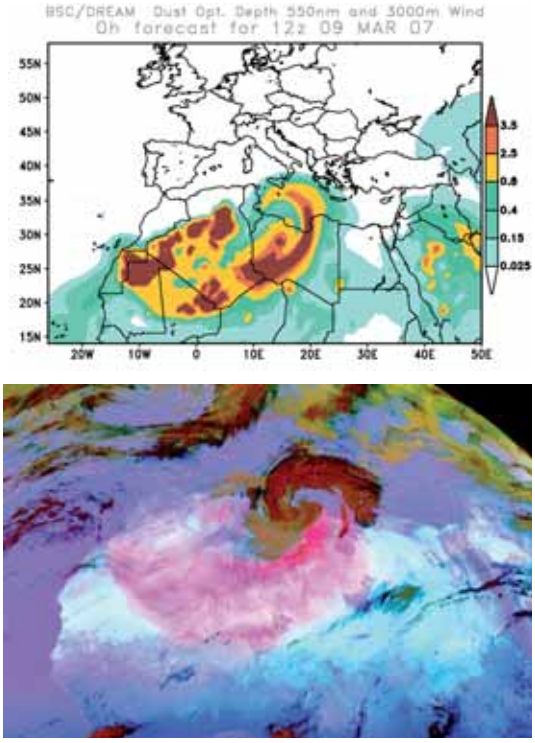
campaign (http://www.bsc.es/plantillaH.php?cat_id=415) in order to support experimentalists in planning their measurements within the context of this project. The group also participated in a dust model intercomparison with other international research groups in the context of the BodEx campaign coordinated by University College London.

The group worked together with the Meteorological Modelling Group in the compilation of the parallel Unified Model (UMO) meteorological core implemented within the Earth System Modelling Framework (ESMF) in order to introduce the atmospheric dust cycle component in a parallelized, global/regional non-hydrostatic version of the atmospheric model driver. The participation of the National Centers for Environmental Prediction (NCEP) of the United States has been active in the tasks of porting and testing the code (see figure) for the MareNostrum architecture. This work is being carried out with the support of project CGL2006-11879 funded by the Spanish Ministry of Science and Education. The project will provide the possibility of performing unprecedented global high resolution forecasts and simulations of the atmospheric dust cycle in the MareNostrum supercomputer.

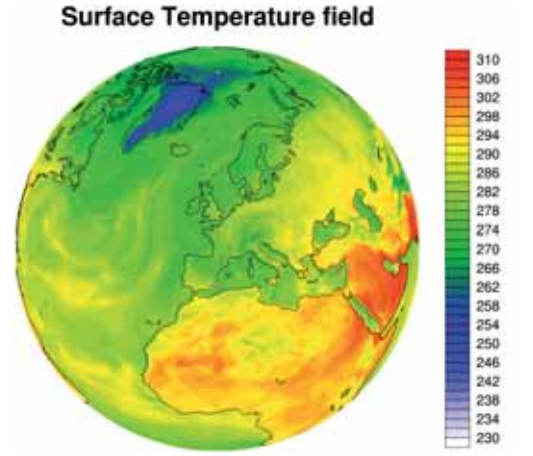
The group also worked on the establishment of dust model climatology for the Mediterranean and the Canary Islands, performing model simulations in MareNostrum for the period 1958-2006 in order to analyze the monthly, seasonal and year-to-year variation of atmospheric dust and to explore the links between simulated dust parameters and the variability of the large-scale circulation.

During 2007, the group activated a number of cross-discipline collaborations with the ocean and health research communities. In this context, the group: (1) collaborated with the World Meteorological Organization (WMO), the University of Las Palmas and the INM in order to assess the role of dust deposition into the Atlantic Ocean in the reduction of iron limitation which allows a more efficient use of macronutrients and hence of CO_2 uptake; and (2) contributed to the Meningitis Environmental Risk Information Technologies (MERIT) project to assess the role of dust storms on Meningococcal Meningitis outbreaks occurring in the Sahel region.

Finally, the group worked together with the WMO and the INM towards creating a WMO Regional Centre for Sand and Dust Warning and Assessment System (SDS-WAS) covering Europe, Northern Africa and Middle-East; and organised in Barcelona the "WMO/GEO Expert Meeting on an International Sand and Dust Storm Warning System".



Dust optical depth forecast from DREAM model and RGB dust product (pink colour) from Meteosat Second Generartion



Surface temperature field (K) obtained with the Earth System Modelling Framework-Unified Model (ESMF-UMO) by NCEP as implemented in MareNostrum supercomputer

Climate Modelling

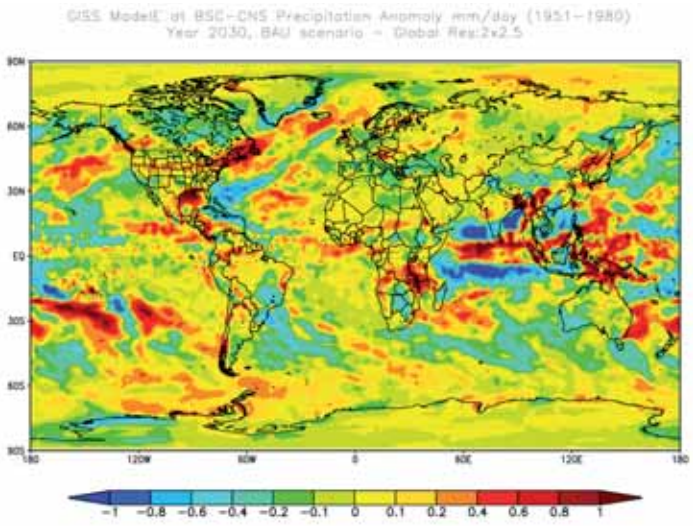
The main focus of this research line within the Earth Sciences Department is the development and testing of regional climate downscaling models for the generation of high-resolution regional climate information from coarse-resolution global circulation models (GCM) simulations.

The availability of a world-class computing facility at the BSC-CNS made it feasible to carry out global simulations at 2º x 2.5º resolution (see figure) and regional simulations at 12-20 km resolution

for Europe and the Mediterranean. This allowed the Climate Modelling Group to begin exploring connections between climate change and impacts on air quality and extreme events. Furthermore, during the year 2007 the group integrated into the *European Network for Earth System Modeling* (ENES) and collaborated with groups such as the Goddard Institute for Space Studies-NASA and the National Center for Atmospheric Research in the United States.

The work of the Climate Modelling Group focused on the side-by-side comparison of the results from the ModelE GCM version of the NASA Goddard Institute for Space Studies (GISS) and the NCAR Whole-Atmosphere Community Climate Model (WACCM) against reanalysis products of the European Centre for Medium-Range Weather Forecasts (ERA-40), obtained by the ECMWF three-dimensional assimilation system based on satellite, radiosondes and other conventional observations. Both GISS ModelE and WACCM were implemented in a parallel high-performance computing infrastructure, the MareNostrum supercomputer. The comparison focused on the period 1957-2002, conditioned by the availability of the ERA-40 re-analysis. The main aim of this study was the definition of the degree of reliability of two specific models for use in climate prediction and to analyze their seasonal behaviour in several regions. The group studied the discrepancies between reanalysis and models for sea-level pressure, temperature, heat fluxes, total cloud cover and precipitation.

Furthermore, the group explored a new methodology applied to climate analysis, the Detrended Fluctuation Analysis (DFA). Averaging values were analyzed for different seasons and regions worldwide over distribution maps. The DFA methodology was applied for time series analysis because of its ability to filter spurious noise of unknown origin, in order to analyse the results from a different point of view with respect to that of traditional EOF or Wavelets normally used in climate sciences.



Precipitation anomaly (mm/day) for the year 2030 compared to the 1951-1980 period using the NASA GISS ModelE at 2ºx2.5º resolution implemented in MareNostrum

Regarding regional climate, the Climate Modelling group determined how concentrations of atmospheric pollutants (mainly focusing on ozone and particulate matter) responded to changes in climate over the Mediterranean by using the regional modelling system WRF-CMAQ-DREAM as implemented in the MareNostrum supercomputer. The domain of study covered an area of 4940 km x 2640 km with a horizontal resolution of 20 km and a vertical resolution of 32 layers in the troposphere. Three simulations (MareNostrum total simulation time of 108500 cpu·h) corresponding to past climate variations under summertime conditions (August months of years 1960, 1980 and 2000 - control year-) were performed and compared. Also, two future scenarios corresponding to the year 2030 SRES A1B and B1 Intergovernmental Panel on Climate Change (IPCC) scenarios were studied.

The results of the research indicated that climate variability led to an increase of the mean concentrations of pollutants in most regions from 1960 to 2000, driven by an enhanced secondary production as a consequence of the temperature increase in the period of study and the higher pressures extending towards eastern regions observed for summertime.

Modesto Orozco
Life Sciences Director

The aim of the scientists in the Life Science Department is to understand the molecular biology and evolution of living organisms using theoretical models and simulation algorithms.

The research program, led by a senior scientist, integrates different independent researchers who work in different aspects of computational biology, ranging from bioinformatics for genomics to computational biochemistry. The program is a collaborative effort with other institutions such as ICREA, IRB-PCB-UB and the National Institute of Bioinformatics. The program is coordinated with the Structural and Computational Biology Program at the Institute of Research in Biomedicine to create a Joint IRB-BSC program on Computational Biology.

When fully organized the program will have two subprograms led by two senior group leaders: i) molecular simulation and ii) bioinformatics. Four independent research groups are expected in each area. The size of each group will (in general) oscillate between 5 (junior group leader) and 15 (senior group leader). The program already has an algorithmic support unit focussed on the development of biological databases and workflows. This unit is responsible for bioinformatics support to external projects. At the time of writing this report thee group leaders (Drs. Guallar, Torrents and Fernández-Recio) plus the program director (Prof. Orozco) are already working at the BSC. The algorithmic support unit is led by Prof. Gelpí and fully supported by the National Institute of Bioinformatics. The group led by Prof. Orozco has 30 scientists, while the junior groups are smaller.

Group leaders and program director were recruited in an open-public process with advertisements in scientific journals (Nature & Science). The director of the program was hired by the BSC director advised by an international recruitment committee. The same committee advised the program director when hiring the group leaders. This process was carried out three times; the first call lead to hiring of Prof. Orozco, the second of Prof. Guallar, Fernández-Recio and Torrents, while the no group leader was recommended by the panel in the third call. A new recruitment process during 2007 was aborted before interviews since strong enough candidates were not found during pre-screening.

The major areas of interest are the following:

- Group of Molecular Modelling and Bioinformatics (M.Orozco). The group is focussed in five major areas: i) Nucleic acid simulations, ii) Protein dynamics and interactions (drug design), iii) Protein-Protein interactions (Protein docking), iv) Genomic analysis, v) Study of enzymatic reactions. This is a large group which has made important contributions to a large range of fields, especially in the Structural Bioinformatics area. This group supports the largest database of trajectories of proteins in the world (MODEL) and the most utilised database for prediction of pathological single point mutations (PMUT). It has world leadership in topics like nucleic acids simulations for drug design.
- Protein interaction and docking group (J.Fernández-Recio). This group is one of the world leaders in the development of computational tools for the prediction of protein-protein interactions. They are developing tools to predict regions of potential protein-protein interaction and algorithms that allow a fast, flexible and accurate docking of proteins. The final goal of their research is to obtain reliable three dimensional models of protein-protein complexes which can help to understand key biological process like cell signalling.
- Electronic and Protein modelling (V.Guallar). The overall objective of this lab is to explore the chemical and physical responses to local and global configuration changes in proteins, with emphasis on substrate biochemistry and ligand docking and diffusion. Such a goal may be achieved by coupling a quantum-mechanical description of the reactive process with advanced sampling techniques. This group works in two areas: i) modelling of electronic processes in hme-proteins and ii) modelling of ligand diffusion in proteins. For the first topic they use QM/MM methodologies to obtain information of how electronic fluxes along (typically) aromatic system modulate functionality of proteins. In the second area they used in-house developed software (PELE) to trace ligand exit/entry along complex channels in proteins.
- Computational genomics group. (D.Torrents). This group applies computational approaches to identify, classify and analyze functional genomic regions and regulatory associations between the components of defined biological systems. The combination and comparison of the results obtained from these approaches is allowing us to uncover and understand regulatory and metabolic scenarios and therefore to identify the basis of complex diseases and biological diversity.

- Unit of algorithmic support (J.L.Gelpi; workflows and databases). The main purpose of this group is to provide access to biological databases, both generic and project specific, and to develop web services and applications covering a broad range of analysis software. INB web services are being developed following the BioMoby standard (http://www.biomoby.org). This group consists of two teams, engineers from the external projects support team are assigned to the INB supported projects and help in the implementation and optimization of users' applications in the supercomputing environment. The Web Services and Database development team is in charge of the development of BioMoby web services and of the creation and management of biological databases.

The main program of activities during 2007 were the following:

- Group Leaders Recruitment: 2007 was the first year of normal functioning of the program. No new group leaders were appointed during this year. One call, performed during the beginning of the year ended without any strong recommendation from the external recruitment panel. A second recruitment process started in spring-summer was aborted, since no strong candidates were found. The team encountered a serious problem in attracting first class candidates to the BSC and proactive initiatives will be taken during 2008 to enrich our portfolio of top candidates for the program.
- Projects: During 2007 the department continued the collaboration with the DEISA project. The team successfully passed the evaluation of the BSC-node at the INB done by Genoma España. The group took responsibility in dealing with all the computational problems of the IMID-KIT project where BSC are working together with the National Genotyping Facility (CEGEN), different Hospitals and the INB in the determination of the genetic roots of rheumatoid arthritis. The program has also been involved in leading the Bioinformatic package in the Consolider Program coordinated by the BSC. The group is supporting the Metagenomics of the Human Intestinal Tract (MetaHIT) project leaded by the EBI-EMBL and funded by the EU, the project for the characterization of peroxysomal metabolome and the COMBIOMED (Red temática de investigación cooperativa en Biomedicina Computacional) funded by the Instituto de Salud Carlos III. Finally the program is leading one sub-workpackage within the ELIXIR project funded by the EU.

In addition to these global projects, the different Group Leaders of the program have obtained extensive support for their research projects from competitive sources.

- Joint IRB-BSC Program on Computational Biology: One key action during this period was the creation of a joint program for research in computational biology between BSC and the Institute of Research in Biomedicine. The agreement was signed during the last trimester of 2007 and will be effective beginning 2008. One of the most satisfactory consequences (from the point of view of the Life Sciences Department) is to allow access of BSC-researchers to a wet-lab which is being now equipped in the new IRB building. A lab manager was recruited and further staff are to be hired. IRB is taking care of the lab equipment and funding the laboratory manager and technician. The implementation of the Joint Resarch Program will incorporate the team led by Prof. P.Aloy and based at IRB as an associated research group.

Scientific Output

The results of the research work have been presented in a large number of scientific publications, presentations to congresses and conference lectures. For the sake of simplicity summary numbers for peer reviewed publications in scientific journal listed in ISI are presented. More detailed analysis is present in the group descriptions detailed below.

Total number of scientific articles:	35
Average ISI Impact Factor:	6.1

It is worth noting that PIs from the program are the corresponding authors of most of these papers and that several of the papers correspond to collaborations between different groups from the department. ISI impact factors of published journal papers is quite high both in absolute and relative (area-adapted) values, which suggest that work done at the Department is above average quality.

Number of papers with IF≥10	4
Number of papers with IF≥7	7
Number of papers with IF≥5	20
Number or articles in 10% best of the area	18

Molecular Modelling and Bioinformatics group

The long term objective is to understand the behaviour of living organisms by means of theoretical models, whose roots are anchored in the basic principles of physics and chemistry. With this general aim the team works with different methodologies, from mining of biological databases to classical dynamics and quantum chemistry calculations. The use of this wide range of methodologies allows the group to explore a wide range of problems, from drug design to genome analysis. Special emphasis is made in connecting basic interactions with global properties of biological systems. In general terms our work can be categorised into four major areas: i) study of small model systems, ii) analysis of stressed or unusual nucleic acids, iii) genome mining studies and iv) dynamics of proteins.

Small model systems

This group has a long history in the study of small model systems of biological importance (nucleobases complexes, drugs, isolated complexes of aminoacids, stacked or hydrogen bonded complexes,...). The study of these simple systems can provide clues for a better understanding of the behaviour of much more complex biological molecules. Almost a decade ago, the group realized that such studies were simple in the gas phase but very difficult in aqueous solution, hampering the real application of the information obtained to the biological scenario. This led to the development of methods to describe solvent, some of which are considered the current "state of the art" in the field and to the development of approaches for accurate representation of molecular interactions. During 2007 the group explored small models for ionic interactions considering calyx-[4]-pyrroles, a system studied previously due to its biotechnological importance and modified nucleobases. In the methodological side, the team adapted the MST methodology within the framework of the RM1 semiempirical Hamiltonian. This allowed us to treat with accuracy and computational efficiency solvation terms for biologically important molecules, and in particular

pharmaceutical drugs. The team also presented during 2007 a new method to derive better force-fields by explicit inclusion of polarization effects. In this approach atomic polarizabilities are fitted to second order perturbational approaches of the polarization energy computed with our GMIPp method, which allowed us to derive polarizability consistent with atomic charge distributions. The team is now exploring the possibility of developing a new force-field for nucleic acids based on such polarization models.

Analysis of stressed or unusual nucleic acids

Major breakthroughs in the field of nucleic acids simulations emerged from the work of this group in 2007. Probably the two most influential ones were: i) the development of a new force-field for nucleic acids simulations (parmbsc0) and ii) the derivation of the first microsecond-long trajectory for duplex DNA. The development of parmbsc0 provides the community with one of the most accurate force-field for simulation of nucleic acids. The force-field is now used as the default for nucleic acids simulations by the AMBER community and the Ascona-B-DNA consortium is using it in massive simulations to describe the sequence-dependent properties of DNA. Preliminary calculations in the group reveal that parmbsc0 is accurate enough to decipher the secondary physical code that helps the cell to label especially relevant regions of DNA (like promoters; see below).

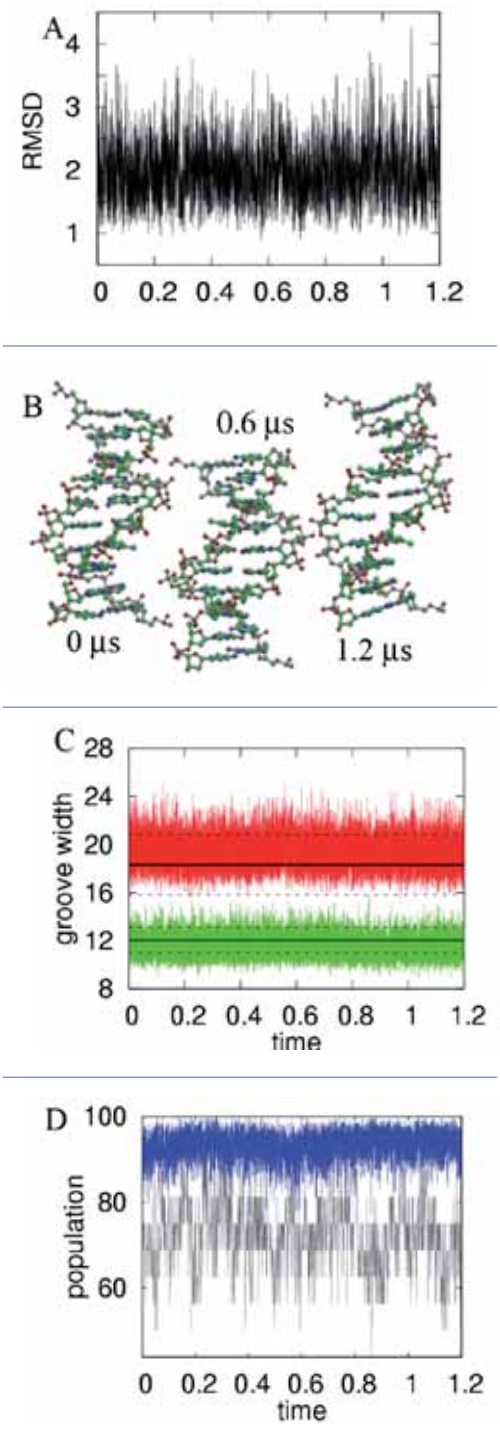
The availability of parmbsc0 and the massive compute power of MareNostrum allowed us to run for the first time in history a microsecond-long simulation of DNA duplex. This calculation, which represents a 10 fold increase in the length of the longest published trajectory at the time, was previously impossible due to the fragility of DNA to long simulations with older force-fields. Our massive analysis provided very accurate information on the rare events that control DNA flexibility (α/γ N/S, B_I/B_{II} transitions, base openings, local bendings, ion insertions,...) and on the pattern of intrinsic DNA deformability which dominates transitions between DNA conformations and the binding of control proteins.

The availability of parmbsc0 also provided us with a key tool to analyze conformational changes in nucleic acids, such as the A←→B transition of DNA which was found to follow the intrinsic deformation pattern of B-DNA, and the transition in ONA·RNA hybrids, which are needed for RNase H recognition and cleavage.

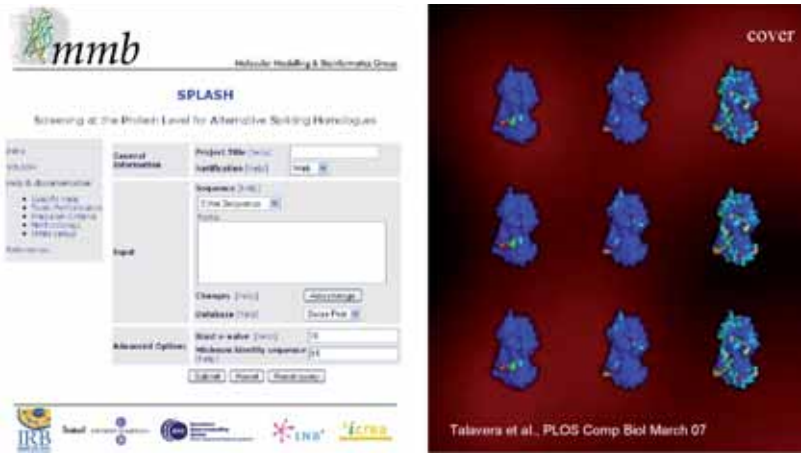
The team is exploring the limits of parmbsc0 and using it to describe highly stressed DNA, which might behave outside the harmonic limit and to explore unusual structures like triplexes and tetraplexes both in mild and aggressive environments.

Genome mining

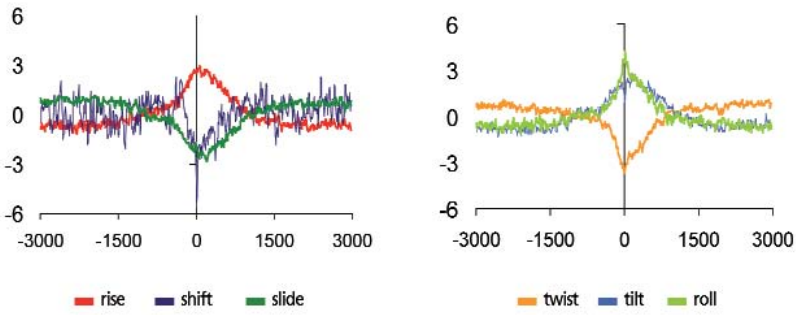
As with many bioinformatics groups obtaining information on key biological processes by analysis of available biological databases is of great interest. Efforts in the last few years have been focussed on two directions: i) analysis of the structural and genetic consequences of alternative splicing and ii) analysis of genomes to determine a pattern of DNAs with unusual structures or properties.



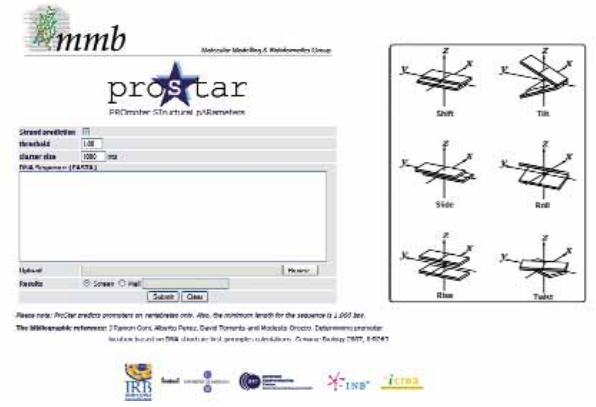
Examples of the use of parmbsc0 to obtain 1.2 microsecond trajectory of B-DNA. A: RMSd with experimental structure, B: detail of the structures at different time frames, C: distribution of groove widths and D, population of canonical α/γ and B_I/B_{II} conformers



Detail of the web application Splash for annotation of AS events and of examples of AS mapped on protein structure



Representation of average helical stiffness parameters in human DNA as a function of the distance to transcription start site (TTS)



Main page of the ProStar web application with a graphical indication of the six stiffness parameters used to predict promoter location

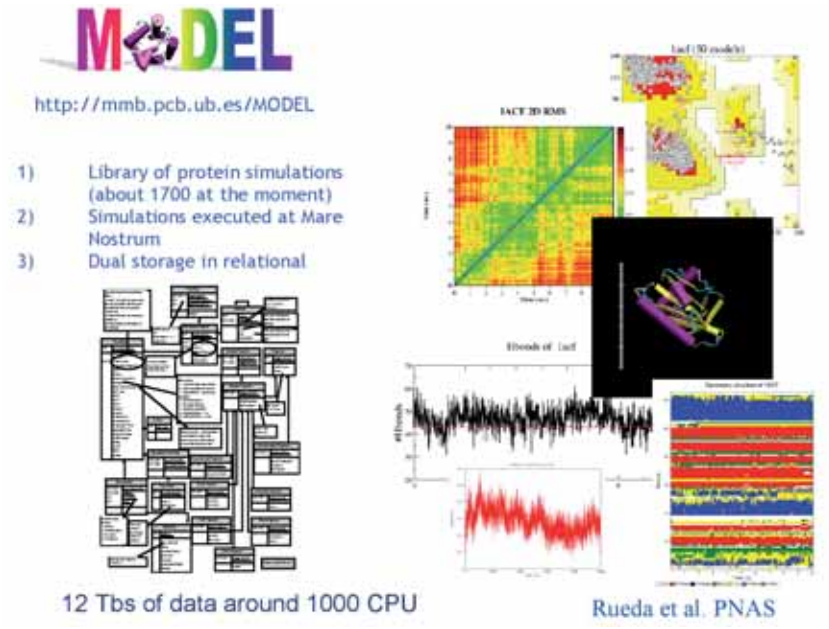
The analysis of alternative splicing yielded important scientific outputs during 2007 such as the characterization of the degree of genetic variability induced by AS in mammals and how similar is this variability to that induced by gene duplication. Also remarkable in this area is the development of tools for correct annotation of alternative splicing events, which helps in the correct annotation of protein isoforms in different tissues or development stages, the resulting web application (SPLASH) was implemented as the default procedure for the annotation of splicing events in the National Institute of Bioinformatics.

The development of tools for the description of DNA physical properties based on atomistic simulations during 2007 opened the door to genome-wide analysis of the physical properties of DNA. By doing this analysis we realized that promoter regions displayed unusual physical properties (see figure). Using this finding the team trained a simple method (named ProStar), which despite its simplicity, showed excellent performance to find human promoters even in cases where promoters are located in unusual positions such as exons, introns or 3'UTRs. The method is especially powerful for the location of unusual promoters, where it performs better than methods based on orthology and gene structure conservation. ProStar is now available as a web application of the National Institute of Bioinformatics.

Following the same lines the team is now completing the physical atlas of human DNA and providing the community with Dnalive, a very powerful tool that plots all the known 3-D structural information on long DNA fibbers including protein complexes. The algorithms implemented in DNalive allow, for example, the determination of putative protein-protein complexes mediated by the chromatin fibber.

Dynamics of proteins

The creation of the MODEL (Molecular Dynamics Extended Library) data base was the focus of a large amount of effort in the group. During 2007 we completed 90% of the library, and reported the first meta-analysis of a small subset of proteins covering all protein metafolds which were analysed with the four most popular force-fields (AMBER, CHARMM, OPLS and GROMOS). The studies on this subset of MODEL (named μMODEL) helped to validate force-field calculations by extensive comparison with all available experimental data and helped to determine some interesting properties of protein flexibility, such as the mixed liquid-solid character of proteins or the role of hydrogen bonds as the major determinants of protein flexibility. The team is in the process of finishing Cluster-90 calculations for MODEL. The group is also completing two parallel studies using μMODEL to determine the role of environmental changes in proteins. These two large studies will be finished during 2008.



MODEL server and database, with some details on the amount of data collected

The availability of several Terabytes of trajectories created many interesting possibilities for analysis of protein properties at the genome-wide scale. For example, the team used a new technique developed in the group and based on MD simulations of force-grids, to analyze and characterize all protein channels. Similarly, MODEL infrastructure was used to improve the resolution of NMR-derived protein structures within the COCO approach developed in collaboration with groups at EBI and Nottingham University.

During 2007 the group explored the possibility of using MODEL as a benchmark for the development of coarse-grained models of protein flexibility. Particularly, the team analyzed the suitability of NMA methods based on quasi-GO models, finding that after a careful calibration they can provide quite reasonable representation of protein dynamics. More recently the team demonstrated that these simple potentials can be incorporated into Brownian dynamics protocols to analyze flexibility in protein clusters and that ultra-simplified discrete molecular dynamics simulations can satisfactorily reproduce complete MD trajectories. These results open the possibility of performing massive analysis (at the organelle or cellular level) of multi-protein dynamics.

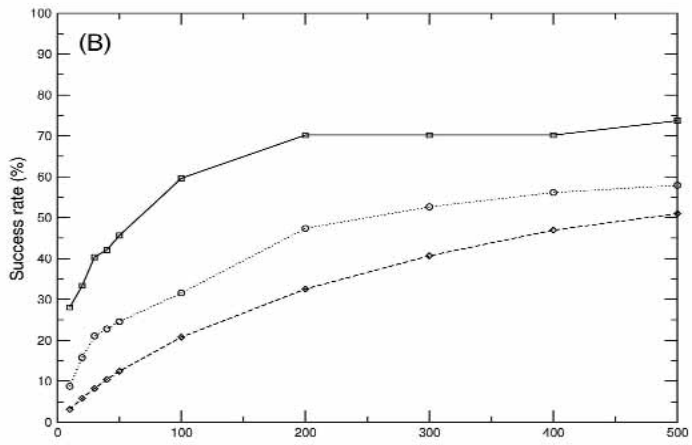
Finally, within this subarea of research, the team should note its contributions to computer assisted therapy design, both in the determination of possible targets and in the development of new drugs for the treatment of inflammation.

Protein Interactions and Docking

The focus of the Protein Interactions and Docking (PID) group is the study of molecular recognition between proteins in living organisms. Protein-protein interactions are fundamental for the majority of cellular processes and their study is of enormous biotechnological and therapeutical interest besides being one of the most important challenges in current Structural Biology. Thus, the PID group is developing computational tools for the structural prediction of protein interactions, on the basis of physico-chemical principles. The group not only wants to contribute to the basic understanding of the mechanism of protein-protein association, but also aims to design molecules capable of targeting protein interactions of biomedical interest. The use of massive computing enables the development and benchmarking of cutting-edge docking tools at large scale.

Computational Tools for Protein-Protein Docking

In 2007, the PID Group continued developing and optimizing computational tools for protein-protein docking, such as the pyDock computer algorithm for the structural prediction of protein-protein interactions. The method relies on FFT (Fast Fourier Transform) generation of rigid-body docking orientations, which are then ranked according to a previously optimized scoring function based on Coulombic electrostatics and ASA-based desolvation energy. When necessary, a soft van Der Waals energy and/or knowledge-based restraints can be added. The scoring function developed by the group, in spite of its simplicity, has arguably the best predictive rates amongst all current rigid-body docking methods. Rigorous internal tests show that, whenever an acceptable solution is present in the docking set, pyDock is able to rank it within the top 50 in around 50% of the cases (see figure). The method was parallelized in MareNostrum and extensively benchmarked against the most up-to-date docking methods. The inclusion of pairwise residue potentials derived from a large database of complex structures drastically reduces the computational time without affecting the predictive results. The new method SIPPER is currently being benchmarked in a large dataset of protein complexes of known structure.



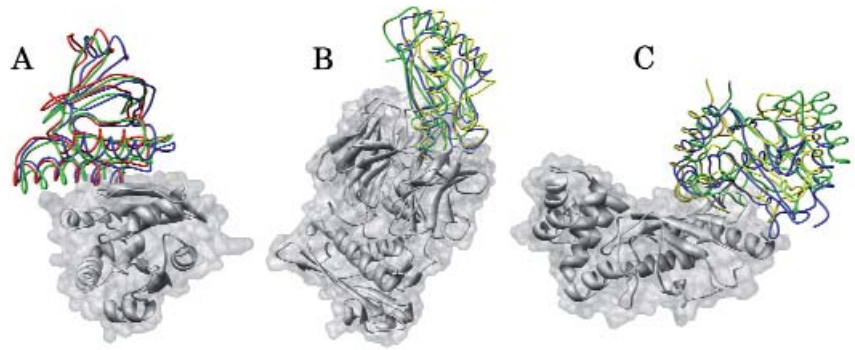
Scoring by pyDock of rigid-body docking sets generated by ZDOCK (black line and squares). Dotted line (circles) is the success rate of the default ranks obtained by ZDOCK. Dashed line (diamonds) is the expected success rate by random

During 2007, the group also adapted the above mentioned docking scoring function for its use in FFT-based sampling. This new *ProtDock* algorithm, faster and more efficient than previous comparable docking tools, is currently being benchmarked on a large set of protein complexes. The group is collaborating with other laboratories within the BSC for the optimization of these tools in a variety of architectures, including the new Cell processor. The group also worked on the development of new methods for the generation of docking poses, like Rotation-Based Uniform Sampling (RBUS), and new measures for evaluating the docking results, like Docking Angular Distance (DAD) which is much faster and accurate than current approaches.

In 2007, the group successfully explored the use of its docking tools for the assembly of multi-domain proteins without needing to exploit structural data from homologues. The use of restraints based on inter-domain linker end-to-end distances consistently improved the results of unrestricted docking in terms of predicting pair-wise domain assemblies.

Success in CAPRI International Competition

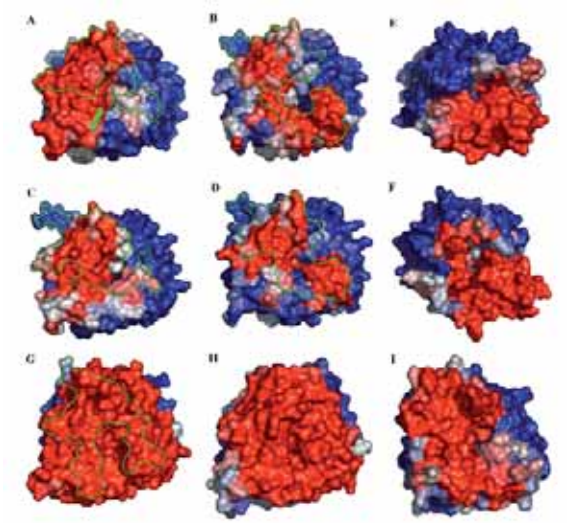
In 2007, the group continued its successful participation in CAPRI (Critical Assessment of PRedicted Interactions; http://capri.ebi.ac.uk), which is an international evaluation of protein-protein docking algorithms developed upon the CASP model, and in which all expert groups in protein docking from around the world are participating. In the 3rd CAPRI edition the PID group submitted acceptable models for one of the targets and more interestingly was one of only three groups that were able to identify a correct structure for all targets (see figure). The 4th CAPRI edition is still on-going, but the group has already obtained excellent results for the first target, being the only group that detected a high quality docking model.



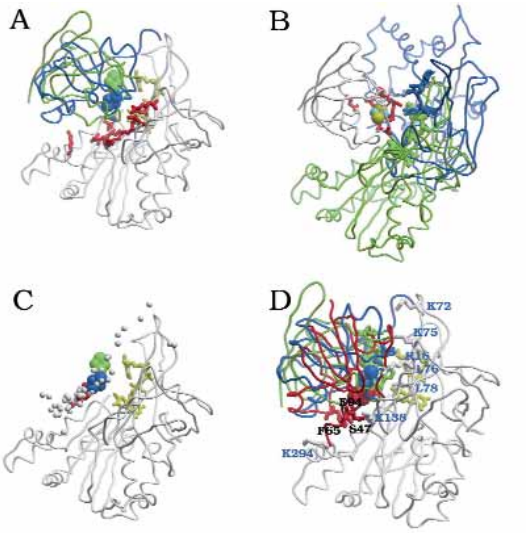
Representation of the group's best submissions in CAPRI. Best submitted model ("predictors") is represented in red, and best detected model ("scorers") is represented in blue. The real position of the ligand in the complex X-ray structure is represented in green. In yellow is represented the model generated with experimental restraints

Predicition of Protein Interaction Sites and Hot-spots

In 2007, the group applied its previously developed Normalized Interface Propensity (NIP) method to the identification of hot-spot residues at binding interfaces. The NIP values were able to predict experimental hot spots with 79% accuracy. This has a high potential interest for drug design targeting protein-protein interactions, since these hot-spots are believed to be the most promising binding sites for small-molecule inhibitors. In addition the fast interaction site method ODA, previously developed by the group, was also applied at proteomic scale to the study of large protein families, such as the carboxypeptidases. The figure shows how the computational analysis of the protein surfaces gives additional information for the classification of protein families. This work has been extended to other protein families.



Representation of the surfaces of the ODA patches for the MCPs. In panel A, the zinc ion is shown in green at the bottom of the active site cleft, which is indicated by a green arrow. The structures have similar orientation, and are grouped into four classes. Upper left side and center, mammalian M14A MCPs: A) bCPA1, bovine CPA1, B) pCPB, porcine CPB, C) hCPA4, human CPA4, D) hCPB, human CPB; upper right side, M14B MCPs: E) dCPD, domain II of duck CPD, F) hCPM, human CPM; lower left side, insect M14A MCPs: G) iCPA, CPA from *H. armigera*, H) iCPB, CPB from H. zea; lower right side, a bacterial M14A MCP: I) mCPT, CPT from *T. vulgaris*. The color ramp is from red (ODA energy value < -10.0 kcal/mol) to blue (ODA energy value = 0.0). The experimental interface is shown in green contour line for those cases where the structure of the complex is known (A-D,G)



Computational analysis of FNR:Fd binding. The crystallographic positions of Fd in *Anabaena* (green) and in maize (blue) are shown. (A) Predicted FNR binding residues in red. (B) Predicted Fd binding residues in red. (C) Lowest-energy FNR:Fd docking solutions after docking and refinement: center of coordinates of S_2Fe_2 in top 100 solutions is represented as balls (the ten lowest-energy conformations are represented in red). (D) Lowest-energy model for FNR:Fd docking. Position of the residues experimentally known to be critically important for the interaction (FNR in white, with residue labels in blue; Fd in red, with residue labels in black)

Computational Study of Transient Interactions

Computer docking simulations are not just aiming to predict the x-ray structure of a given complex, but are also providing information of the energy landscape and other species populated during association. This is expected to be particularly important in the highly transient interactions of electron transfer processes. In 2007, the group used ab initio docking to study the interactions between ferredoxin-NADP+ reductase (FNR) and its redox partners ferredoxin (Fd) and flavodoxin (Fld). The models generated by the group fit well to experimental mutational data (see figure), and they allow the proposal of alternative binding modes that could still contribute to electron transfer, in addition to the ones found in x-ray structures. This is a nice example of the use of computer simulations to provide new insights into a biological problem that were not foreseen from the experimental data. In addition, the group studied other transient interactions such as the complex between cythochrome c oxidase and the proteins plastocianin and cyt c6.

Modelling of Complexes of Biological and Therapeutical Interest

The computer tools developed by the group, and the theoretical knowledge that is being acquired in the field of protein-protein association, have the ultimate goal of helping to solve real problems of biological and therapeutical interest. During 2007, the group collaborated with different experimental laboratories to help in characterizing challenging multi-protein systems such as the bacteria multi-drug pump, the protein complexes of the plant immune system, the interaction between ATP-dependent helicase RhlB and ribonuclease RNAse E, the dimerization of the 4F2h ectodomain, and the interaction betwen HHa and HNS proteins.

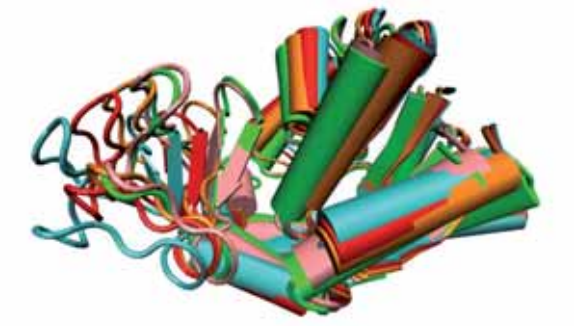
Electronic and Atomic Protein Modeling

The overall objective of the lab is to explore the chemical and physical responses to local and global configuration changes in proteins, with emphasis on substrate biochemistry and ligand docking and diffusion. Such a goal may be achieved by coupling a quantum-mechanical description of the reactive process with advanced sampling techniques. For this purpose, several simulation protocols and algorithms, which combine protein structure prediction algorithms with hybrid quantum mechanics/molecular mechanics methods, QM/MM, are being studied. During 2007 we focused on two main areas:

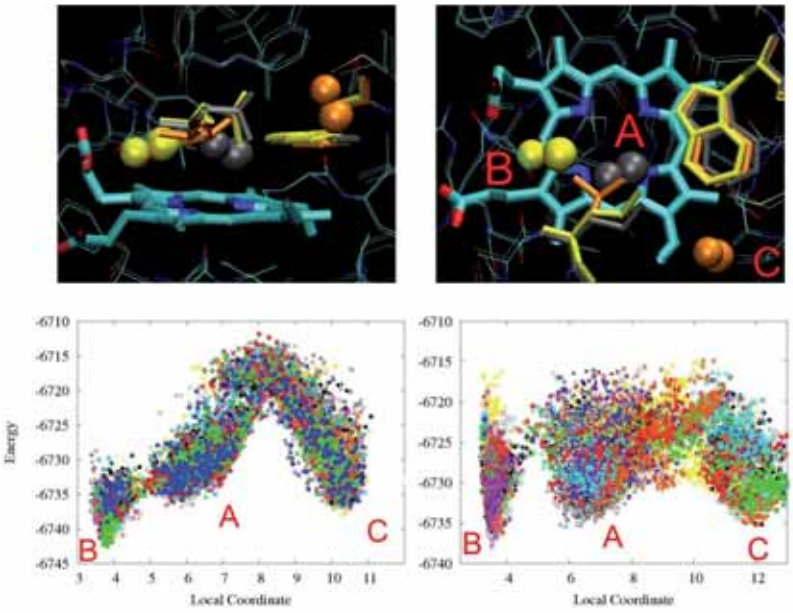
- The development of our protein energy landscape exploration (PELE) method by adding backbone sampling capabilities
- The study of the biochemical reactivity in heme proteins. This last area has centered on two main aspects:
  - Biochemical ligand reactivity on Hemoglobins
  - Electron transfer pathways in cytochromes

The team added a backbone perturbation to our methodology to improve the sampling of larger conformational changes. Previously the PELE method was based on three moves: a ligand perturbation, a side chain sampling and a minimization. Initially, the method was thought to explore ligand dynamics and to improve the all-atom ligand docking. The team soon realized that there was the need for a more robust protein conformational sampling. Many exit and entry pathways, as well as cross docking studies, required a larger backbone rearrangement than the one provided by the simpler side chain + minimization algorithm. Furthermore, the team wanted to expand the method to more general tasks, beyond the ligand dynamics studies.

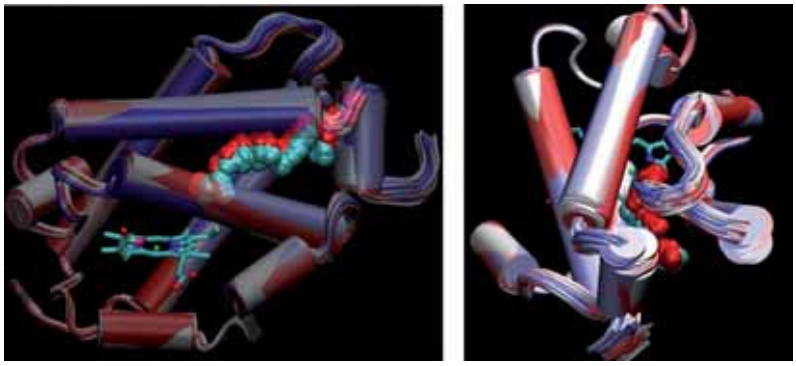
This year the team added an anisotropic network model (ANM) to PELE. The program computes the normal modes provided by the ANM coarse grained model and obtains an alpha carbon displacement vector. Thus, following the ligand perturbation



Adenylate kinase conformational search by using PELE with the new ANM approach



Top panels: Top and side view for two representative snapshots for the A, B and C binding sites. *Bottom panels*: Energy landscape for the CO migration between the A, B and C binding sites for the wild type (bottom left) and G8F mutant (bottom right). Energies are in kcal/mol. The local coordinate reflects the distance of the CO center of mass to one of the heme propionates



Two different views of the exit channel for the CO ligand. We observe the rearrangement of the different helices along the ligand migration

(which mostly involves a ligand translation and rotation) each alpha carbon has the option of being displaced by some amount along the displacement vector. The algorithm proceeds by performing a quick minimization with a gaussian bias potential towards the new alpha carbon coordinate. The last two steps are the same as in the original PELE algorithm, involving side chain prediction and unconstrained minimization. The user has control over vector magnitude, directions, normal mode mixing capabilities, how often the ANM vector is recomputed, number of side chains to be sampled (the ones more excited along the perturbation...) and so on.

The addition of ANM into PELE also allowed us to expand the method beyond the ligand dynamics. For this the ligand perturbation step is replaced by a random move in the ANM vectors. One obvious application is to obtain an all atom energy profile along large protein conformational changes. The team is currently testing the algorithms with the adenylate kinase test case, which has been well characterized by x-ray, and steered molecular dynamics. With a few hours of CPU time the group can obtain an all atom pathway for the opening and closing of the protein in very good agreement with the experimental (and other theoretical approaches) results. The figure shows a few snapshots of the overall motion. The team is now writing the methodology manuscript (also pending on running 2-3 more examples).

During 2007 the team also applied the new PELE code to ligand diffusion. In particular the group focused on the carbon monoxide migration in the truncated hemoglobin-II from M. tuberculosis, trHbO. This study was conducted in collaboration with the experimental laboratory of Syun-Ru Yeh, at the Albert Einstein school of Medicine in New York. The Yeh lab has produced kinetic data for the wild type and the G8F mutant. The team performed the ligand dynamics exploration obtaining a different mechanism for both species, in excellent agreement with the kinetic data. The figure shows two views for the three cavities of the CO ligand in the vicinity of the heme group (which we name A, B and C cavities or binding sites). The figure also shows the energy profile for the wild type (left panel) and the mutant (right panel).

As seen in the trajectories and as reflected in the figure energy profiles, for the wild type the ligand evolves quickly into the B cavity before rebinding into the active site (geminate rebinding). For the mutant the ligand stays in the main active site, A cavity, with a faster geminate rebinding rate.

The passage into the C cavity, bringing the ligand into the protein exit pathway into solution, is considerably faster in the mutant, as observed in the A to C barriers. The exit pathway is coupled with a large protein rearrangement associated with helices motion. The addition of the ANM capabilities into PELE was crucial for the characterization of this process. The segond figure shows the main exit pathway and the helices reorganization. The manuscript for this study is finished and will be submitted shortly.

The team also combined ligand dynamics and QM/MM reactivity in the study of the mechanism of product release in NO detoxification from Mycobacterium tuberculosis truncated hemoglobin N, trHbN. The PELE exit pathway for the nitrate product agreed with the steered molecular dynamics pathway, opening a novel mechanism for the product release. In the same study, the group also discovered the importance of the hydration level in the active site for the chemical bond breaking of the nitrate substrate. This work was published in *JACS* in collaboration with the Prof. Estrin (Buenos Aires University) and Prof. Luque (University of Barcelona) laboratories (the PI of the group is a corresponding author in the manuscript).

This methodological improvement in our code will be directed to the refinement of docking poses. The group reached a collaboration agreement with Schrodinger Inc., a software company based in New York, to develop new all-atom refinement techniques for docking poses. The main goal is to add backbone flexibility to the already existing flexible docking capabilities of the company (mostly side chain flexibility in the induced fit options in their Glide program).

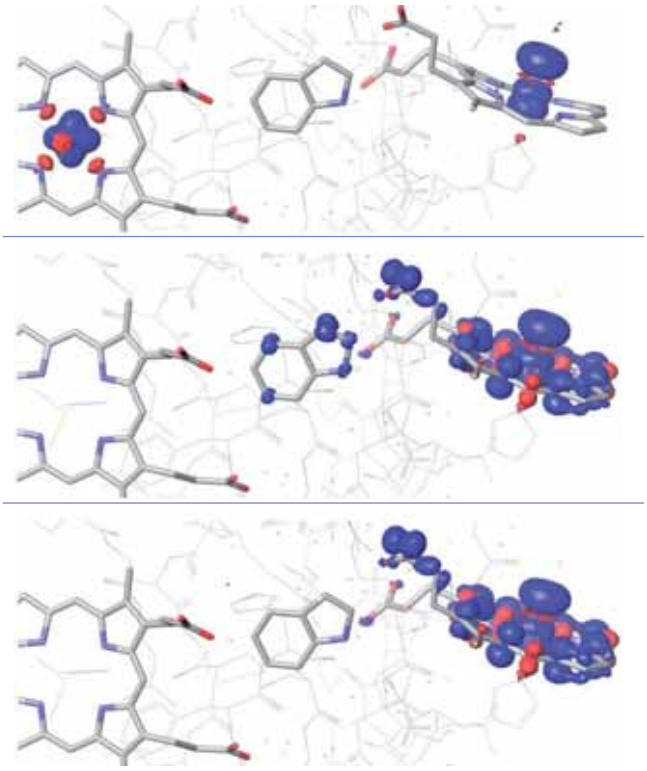
Biochemical reactivity in heme proteins

Hemoglobins

The study about the hydration importance for the nitrate release in trHbN, the JACS publication, has already been mentioned. This work was performed by coupling molecular dynamics sampling of the water molecules in the active site with QM/MM calculations of the energy profile for the substrate release.

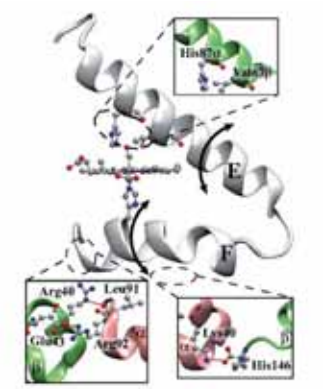
In the carbon monoxide migration study in the truncated hemoglobin-II from M. tuberculosis mentioned above, the team also performed the QM/MM energy profile for the CO deligation in both the wild type and the mutant. The results, in line with the ligand dynamics and the kinetic data, indicate again the larger stability of the A binding active site for the mutant species.

Probably the most important study with Hb, has been in human haemoglobin. For the first time in this important system the team showed that computational QM/MM methods can provide good values of ligand binding energies in Hb, and of their dependence on allostery. The team showed that 40% of the binding energy differences between the R and T quaternary structures resulted from strain induced in the heme and its ligands. The remaining energy difference resides in protein contacts, involving residues responsible for locking the quaternary changes. In the α-chains, the most important contacts involve the FG corner, at the 'hinge' region of the $\alpha 1\ \beta 2$ quaternary interface. The energy differences are spread more evenly among the β-chain residues, suggesting greater flexibility for the β - than the α-chains along the



Schematic showing the haemoglobin heme, proximal, and distal histidines, E- and F-helices. (Insets) Magnifications of those regions that were determined to be important for affinity modulation of CO. The arrows highlight the motions of the E- and F-helices, both are pushed downward in the deoxy state and upwards when ligation takes place

quaternary transition. Despite this chain differentiation, the chains contribute equally to the R-T energy difference. Thus nature has evolved a symmetric response to the quaternary structure change, which is a requirement for maximum cooperativity, via different mechanisms for the two kinds of chains. This study, in collaboration with the Spiro Lab (formerly at Princeton university now at University of Washington) resulted in the *PNAS* publication: "A quantum chemistry picture of hemoglobin affinity".



Cpd I spin density for three different quantum regions (see main text) in CcP. The spin density is shown for the quartet spin state

Cytochromes

One of the main subjects of study in the lab is the mechanism of electron transfer in heme proteins, and, in particular, in cytochromes. This line of studies is derived from early work in the lab showing the importance of the heme propionate side chains in adjusting the metal redox state. The group expanded our previous results with two more systems: ascorbate peroxidase and the bacterial cytochrome C peroxidase. For both systems, available crystal structures revealed an intriguing arrangement of the heme propionate side chains in heme-heme and heme-substrate complexes. By means of mixed quantum mechanical/molecular mechanics calculations, the team studied the involvement of these propionate groups into the substrate oxidation in ascorbate peroxidase and into the heme to heme electron transfer in bacterial cytochrome c peroxidase. By selectively turning on/off different quantum regions, we obtained the electron transfer pathway which directly involves the porphyrin ring and the heme propionates. The results might represent a general motif for electron transfer in/out of the heme group, and change our view for the propionate side chains as simple electrostatic binding anchors. This study is under second review round in Biochemistry.

Current efforts are directed towards electron transfer studies into protein-protein electron exchange. The team expects in 2008 to be able to characterize long range electron transfer pathway across the protein-protein interactions in cytochromes. For this goal the team is designing novel QM/MM protocols were the group iteratively activate and deactivate the quantum description of different residues in the protein binding interphase.

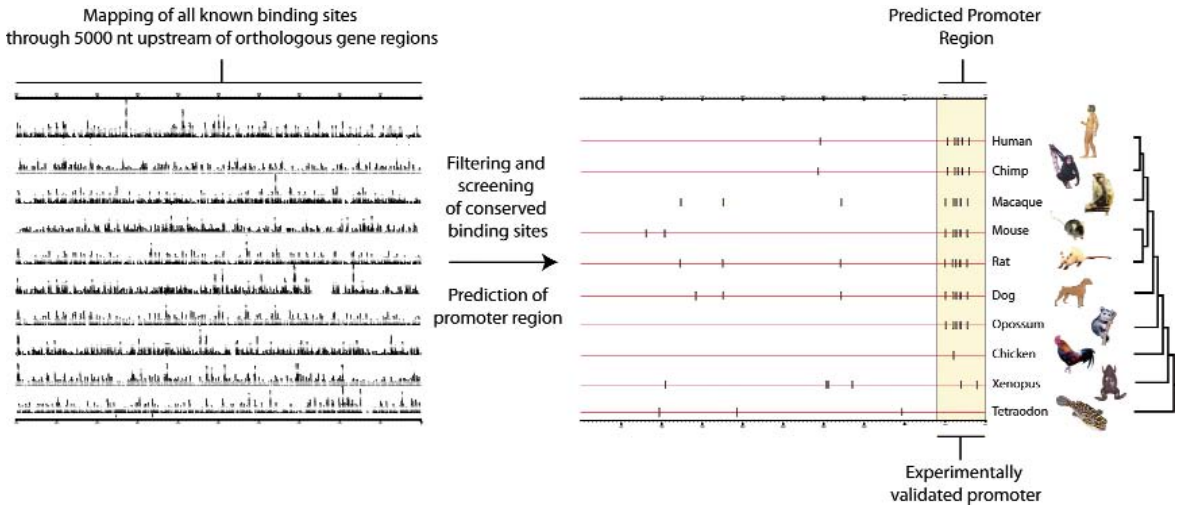
Computational Genomics

The goal of this research group is to contribute to the general knowledge and advance of biological sciences, particularly in the fields of evolution, molecular biology and biomedicine. The recent and ongoing increase in the massive range of biological data has created new possibilities in answering biological and biomedical questions, some of which have not been considered before. Based on

these datasets, and also on detailed experimental data, the team applies computational approaches to identify, classify and analyze functional genomic regions and regulatory associations between the components of defined biological systems. The combination and comparison of the results obtained from these approaches is allowing us to uncover and understand regulatory and metabolic scenarios and, therefore to identify the basis of complex diseases and biological diversity. Here, the group will explain the background, specific goals and current status of the different ongoing projects.

Analysis of gene regulation in Vertebrates

An important part of our time and energy was devoted to the identification and analysis of gene regulatory region of vertebrate genomes. This project is financed by the Spanish Ministry of Science and Education (BIO2006-15036) and is divided into several research lines that are carried out by different members of our group, and will converge to provide a wide picture of the sequence-function relationships of the regulation of gene expression. This will also allow for the identification and understanding of changes in regulatory regions that have contributed to the diversity of gene expression in different organisms.



Prediction of promoter region with the M3 program in available upstream region of the homeobox gene EVX1 in all vertebrates

Classification of Vertebrate Genes in Orthologous groups

During this year, the team completed and adapted to the computational environment (MareNostrum), a complicated pipeline that, starting from all known proteins sequences and the available genomic sequences of vertebrates, is capable of identifying all the genes that have been overlooked by current annotation pipelines (such as ENSEMBL, or NCBI), and also all non-functional copies of genes (pseudogenes) that provide information about the evolution of genes. For the development of this pipeline, the team had to unify and overcome all the limitations associated with the current annotation of genomes. After executing this pipeline on all available vertebrate genomes, we identified around 250.000 genes and pseudogenes that had to be classified in orthologous groups, i.e. according to their evolutionary origin and relationship. The identification of orthology is crucial to transfer the information regarding the function and regulation of genes from one organism to another and to find relationships between sequence and function. Current classification of orthologous groups are too simplistic and often misclassify a large number of genes that either arose independently in different lineages, or evolved at different speeds in the history of different organisms. To overcome these limitations, the team combined sequence comparison approaches (BLAST and HMMER searches) with the analysis of the location of genes in the different genomes, as well as with evaluation of sequence modification patterns in order to classify all 250.000

vertebrate genes into 18.000 orthologous groups. The results will be made freely available to all research groups of all fields through a web interface. This will constitute the largest and most accurate database of orthologous relationships available. The manual analysis of some of these groups revealed the existence of different gene variants in some species, which is relevant to understand the way by which genes and functions evolve. One of these new genes (named y+LAT-3) is likely to correspond to a new member of the LAT family of amino acid transporters and has been identified only in fish. The functional and cellular characterization of this novel amino acid transporter will soon be carried out experimentally by one of the members of this group in the laboratory of Manuel Palacín (IRB, Barcelona).

Identification of Vertebrate Promoters

The identification of orthologous groups among vertebrates is also crucial to develop the other central research line of our group, which pursues the identification of gene proximal regulatory regions (promoters) in all vertebrate genomes. The identification of promoters in eukaryotic genomes still remains a major challenge in different fields of research in biology, but particularly in Bioinformatics. Despite the recent increase in a variety of experimental and computational methodologies to identify the regions responsible for the control of gene expression, there is still no convincing solution for this problem. The variable nature of these regions and their low level of conservation among species makes it impossible to elaborate a collection of filters and rules that can be used for their computational prediction. This means that the vast majority of these methods fail and, by pursuing a large sensitivity, they end up with a high rate of false positives that make predictions difficult to trust and use to carry out studies of gene expression at any level. These limitations can be largely overcome by relaxing the search criteria and by using a large number of orthologous promoter sequences as compensation. This is precisely what the team has done. For our predictions of promoter regions, the team developed a search engine (called M3) that screens over different windows, a large number of orthologous regions searching for similar patterns of transcription factor (TF) binding sites (see figure). This search engine was optimized to consider and evaluate a large number of combinations of mapped TF binding sites with a considerable low computational cost. But, despite this advantage, the number of binding sites that map randomly over any DNA sequence remained too high to reduce the rate of false positive predictions. To solve this problem we developed, in collaboration with Enrique Blanco (Universitat de Barcelona) and Roderic Guigó (Center of Genomic Regulation, Barcelona), different criteria to pre-select a subset of informative binding sites by using real and randomized promoter regions. When applying the search engine with this selected set of binding sites over different known promoter regions used as control, the team was able to correctly identify 30% of them. Very surprising and promising is the very low rate of false positives (10%), the lowest associated to any promoter prediction method. This represents a promising starting point for tuning all possible variables to increase the sensitivity by maintaining this high specificity. Once this is achieved, the team will be able to identify in eukaryotes a large number of reliable promoter regions that will be provided through web interfaces, and will allow researchers to carry out molecular, evolutionary and biomedical studies related to the regulation of gene expression.

Besides the projects mentioned above, during the year 2007, this group maintained and started several lines of collaboration with different groups, not only from BSC, but from Europe:

(1) An internal collaboration with the group of Modesto Orozco permitted the development of a novel and efficient approach of promoter prediction based on first principles calculation of DNA, which has been recently published in Genome Biology. This method is also available through a web interface (http://mmb.pcb.ub.es/proStar/) and allows scientists from all kinds of fields to predict their promoters of interest using structural properties of DNA.

(2) Another collaboration that has been ongoing for the past years with the group of Manuel Palacín (IRB, Barcelona) culminated this year in another publication where the team reported the identification and first structural characterization of the first identified prokaryotic member of the LAT family of amino acid transporters. The contribution to this study comprised the initial

identification and phylogenic analysis of this transporter in the context of all prokaryotic amino acid carriers of the large APC superfamily. This study was also the starting point of a larger phylogenetic analysis of prokaryotic amino acid transporters that will allow us to set up the necessary methodology to cover more groups of organisms in the analysis of orthology.

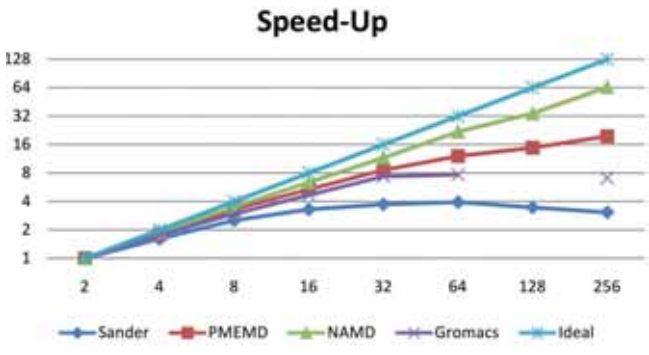
(3) A third ongoing collaborative effort in 2007 with the group of Peer Bork (EMBL, Heidelberg) required an extensive use of the MareNostrum computer (4000 CPUs during 5 days). The aim of this study is the identification of the phylogenic relationships and the classification of all known and predicted proteins on earth. For this the team compared all protein sequences derived from all possible genome-sequencing projects (from viral to environmental genomic initiatives) against themselves, which constitutes the larges sequence comparison done so far. The results of this study will have impact at different levels, from evolutionary to biomedical, and also ecological. This analysis has allowed the group to be part of an European grant that aims to identify microorganisms inside the human body through the shotgun sequencing of fluid samples.

(4) A collaboration with the group of Mikita Suyama, Kyoto University (Japan), and Miguel Manzanares (CSIC, Madrid) for the analysis of gene duplicates in vertebrates to evaluate the duplicability and the functional spectrum explored by different lineages through gene duplication.

INB - Computational node

The National Institute of Bioinformatics is a research facility created by Genoma España Foundation with the aim of giving support to Bioinformatics groups related to Spanish Genomic and Proteomics projects. The Institute has a nodal structure distributed among the most important bioinformatics research groups in Spain. Barcelona Supercomputing Centre's Life Sciences program hosts the Computational Bioinformatics node of INB (INB-GN6). The special purpose of the computational node, with the help of BSC computational resources and expertise, is to provide access to biological databases, both generic and related to supported projects, and to develop web services and applications covering a broad range of analysis software. INB web services are being developed following the BioMoby standard (http://www.biomoby.org).

The internal structure of the node consists of two teams, engineers from the external projects support team are assigned to the INB supported projects and help in the implementation and optimization of users' applications in the supercomputing environment. The Web Services and Database development team is in charge of building BioMoby web services and creating and managing biological databases.



Speed-up of several MD tools for systems ca. one million atoms

Projects Support

Molecular Dynamics Simulations

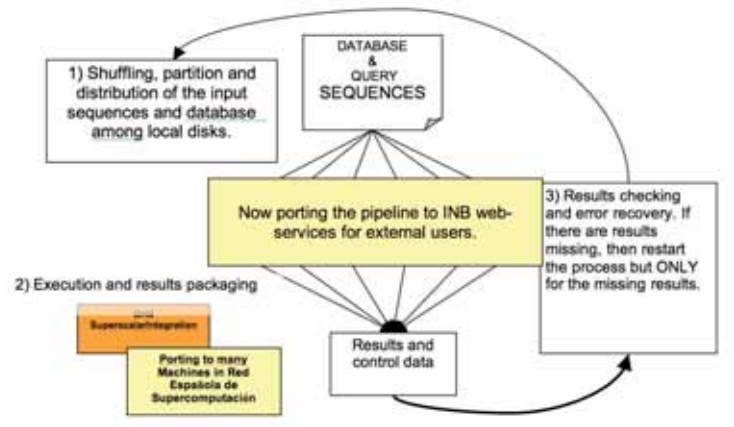
The main activity during 2007 in this area was to support MareNostrum users with projects using molecular dynamics, particularly in studies about protein flexibility. Some of the specific activities developed were:

- Force-field evaluation
- Evaluation and optimization of compiler settings for molecular dynamics software (see fig. 1 for a benchmarking example). Results of this activity were made available to any MareNostrum user.
- Development (in collaboration of M. Orozco's group) of an automatic interface to launch molecular dynamics simulations for non-experts. This activity was also part of the contribution of BSC to the DEISA consortium.
- Development of automatic tools for the analysis of molecular dynamics trajectories.

Protein-protein interactions

Main activities in this area centred in Docking and analysis of protein-protein interaction. The most relevant projects supported where:

- Prediction of specificity in protein interaction
- Prediction of interacting pairs based on co-evolutive patterns
- Extraction of functional pathways from protein interaction networks
- Study of interactions within Ras protein family
- Refinement of scoring function using PyDock
- Study of several filters of rht pre-scoring of docking solutions
- Development of a new protein-protein Docking (ProtDock)
- Introduction of low-resolution data to improve docking



Pipeline for massive BLAST analysis on whole-genome or metagenome data

Genomic Analysis

Despite the large number of tools available, massive genomic analysis is one of the most challenging activities for supercomputing environments, due to the lack of easy scalability of systems like MareNostrum. The most relevant activities in this area were:

I. Massive phylogenic analysis based on MrBayes, leading to determination of the evolutive origins of peroxysomal metabolome

II. Several projects based on BLAST and its variants (ENCODE, promoter evolution)

III. Massive metagenomic analysis. Due to the extraordinary amount of data, to develop this kind of analysis in MareNostrum it was necesaryto build a new computing pipeline.

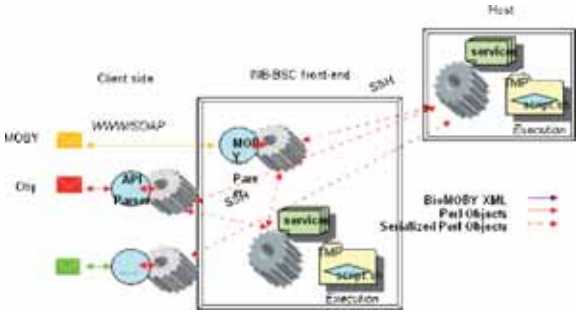
Web applications and Database Developments

Integration with BSC computational facilities

In 2007, the core of web-services and database offering was moved to BSC computer resources. However due to the nature of the web-services protocol, based on the BioMoby standards, they were still inaccessible for supercomputing users. A number of developments were carried out to integrate supercomputing facilities into the applications served to bioinformatics groups.

Work followed two basic lines:

1) Reorganisation of the internal structure of web-services. The existing web-services engine was split into a number of modules (see figure). Calculation modules for the most demanding applications were built using the most efficient architecture for the specific servers involved. In particular, modules for BLAST, FASTA, HMMER, and EMBOSS running on a SMP architecture (Altix 4700) were made available. This should be completed during the next period to include specific modules for MareNostrum. Traditional web services will be using BioMoby SOAP-based modules, running in the web front-end that communicate with calculation modules through ssh encrypted channels to maintain security standards within BSC. The new model allows the use of input modules based on different technologies (web applications, command line access).



Scheme of system architecture serving web-services

2) Building an applications programming interface (API) adapted to this architecture. The API, based on the existing MobyLite API, allows software integration with the calculation modules described above. The main difference from MobyLIte is the use of an encrypted communication channel (ssh) instead of SOAP/HTTP, making it compatible with the use of supercomputers such as MareNostrum or Altix, inaccessible from traditional web services. As with MobyLite, the main features of the CommLine API are:

   a. Use of Perl objects to represent BioMoby data types. Those objects are generated automatically from the information gathered from the catalogue.

   b. Use of Perl functions to represent web services.

   c. Communication among processes using serialized Perl objects, compatible with ssh protocol.

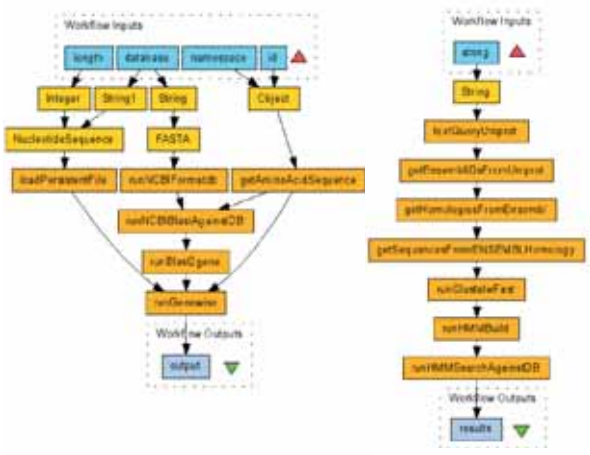
Developed Workflows

The combination of web services into pre-made workflows allows complex bioinformatics applications to be packaged into reusable modules. This is of key importance to allow non-expert users to take advantage of web-service architecture.

During 2007 two complex workflows (see figure) were developed and made available to general users. Both of them cover generic operations requested by supported groups involved in genomic analysis.

1) Search for bacterial origin of eucharyotic protein families. Direct support for the project "Characterization of peroxysomal metabolome and its evolutive origin" by A. Pujol (IRO)

Allows location of a set of proteins from bacterial origin showing a high homology (at the HMM level) with proteins from eucharyota. The workflow feeds data for a massive



Scheme of generated workflows. Left: Search for bacterial origin of eucharyotic protein families. Right: Gen identification from homology

phylogenetic analysis performed on MareNostrum based on the application MrBayes.
The workflow input data is a protein reference (Uniprot), and the steps are as follows:

- Search of homologues using Ensembl database (www.ensenbl.org)
- Generation of a multiple alignment using Clustal
- Generation of an HMM profile for the protein family
- Search in the appropriate proteomes using HMMsearch

Some of the required services (Uniprot search, multiple alignment and HMM related) where already available, however a full set of services based on Ensembl was built.

getEnsemblIdsFromUniprot
getHomologiesFromEnsembl
getSequencesFromEnsemblHomology

2) Gene Detection by Homology
A second workflow covers routine operations performed by bioinformatics groups working on genome annotation. The workflow allows the location of genes coding for homologues of a given protein. It uses tools specially adapted to genomic data as genewise. The steps are:

- Building of a Blast database with the desired genomic data
- Blast search using the desired protein as query and the built database
- Analysis of blast report using genewise

Building of the workflow required 4 new services:

runNCBIFormatDB
runNCBIBlastAgainstDB
runBlast2Gene
runGenewise

Data Persistence Model

A common issue in bioinformatics, especially when supercomputers are involved, is the need to handle large amounts of data. Areas such as genomic analysis of molecular dynamics simulations are good exemples of this problem. Web services do not provide a good solution as communication protocols (such as SOAP over HTTP) and communication channels do not support heavy traffic easily. Some BioMoby client software provides solutions including data persistence, but still requires expensive transmission of data through the communication channels. On the other hand, access to supercomputers through the BioMoby protocol requires command line based software. For this reasons a model to handle data persistence at the service level was outlined. The protocol was applied successfully to the above cases and has been submitted to BioMoby developers. The details of the protocol follows:

a. Data is stored by the service provider, and unique id/namespace pair is assigned to it. Therefore, data can be identified as a standard Biomoby object.
b. Services providing data persistence generate an output object with the required structure. However, the object should not contain data, instead they contain a "cross-reference" to the stored object. The amount of data transmitted is minimal.
c. Services accepting persistent data search for "cross-references" pointing to the appropriate namespace, and use them to retrieve real data from the local store.
d. A series of services, like loadPersistentFile, getPersistentFile, or existsPersistentFile allow the stored data to be accessed directly if necessary.

Web applications

A series of web applications oriented to non-expert users were developed. These applications are based on a Java applications server and provide a friendly user interface to the services offered.

1) Database search tools. Launches about 40 retrieval services based on the available databases (see table 1), including both keyword search and direct retrievals.

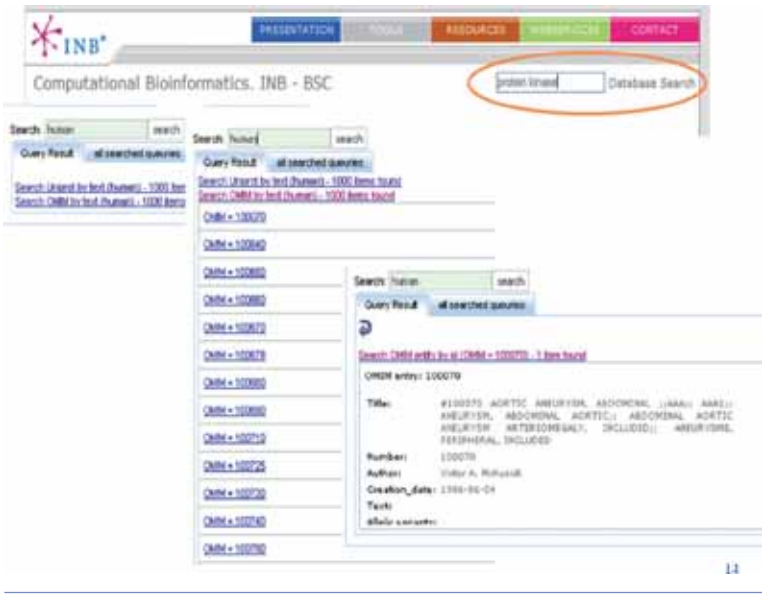
2) Sequence comparison portal. Offers sequences comparison based on Blast, and Fasta combined with the appropriate databases.

Epidemiology database. IMID-Kit project

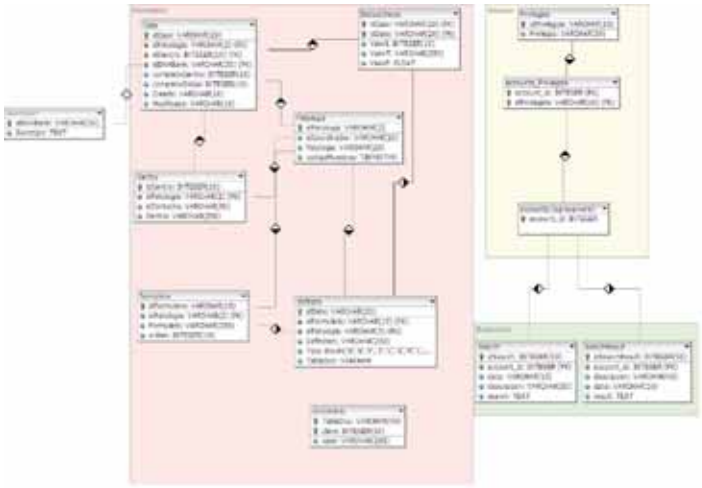
The so-called "Desarrollo de un kit diagnóstico para las enfermedades inlamatorias mediadas por mecanismos inmunes (IMID-Kit)" project seeks to establish a pattern of genetic markers to help the diagnosis of a number of auto-immune diseases.The project is funded by the Spanish Ministry of Science and has over 30 clinical centres and scientific groups from several institutions participating. The overall project involves genotyping of over 12000 rheumatoid arthritis, Crohn disease and Psoriasis cases, and controls.

During 2007, the team at BSC was involved in building the project web site (http://imid-kit.bsc.es), a central group work environment, and the epidemiology database and associated applications.

Due to the diversity of the clinical data required, the epidemiological database was constructed as an open model that allows incorporation of a variety of data definitions (see Fig. 6 for database structure). The data definitions, instead of being specified in the database, are built from reading the clinical questionnaires, and both the web interfaces for introduction of data (figure 7) and search are built automatically from these definitions.

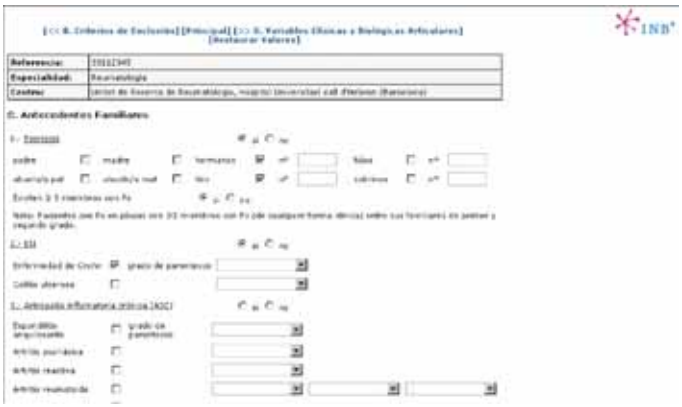


Screenshots of database search tool



Structure of IMID-Kit Epidemiological database

Screenshots of generated IMID-Kit web questionnaires



Screenshots of generated IMID-Kit web questionnaires

DB-NAME	TEXT	BLAST	MYSQL	BLAT	FASTA
Bacteria		+			
blocks	+				
cath	+		+		
cdd	+	+			
dbSNP			+		
embl	+				
emblnew	+				
fasta	+				
fssp	+				
genbank	+	+			+
GO			+		
Homo Sapiens				+	
interpro	+				
nr	+	+			+
omim	+		+		
pdb	+	+	+		
pdbaa		+			
pfam	+				
prodom	+				
prosite	+		+		
rebase	+				
refseq	+	+			+
refseq_aa		+			+
scop	+		+		
swissprot		+			+
tfscan	+				
transfac	+				
trembl		+			+
uniprot	+	+	+		+
UCSF		+			

Table 1: Available databases and formats

José María Cela
Computer Applications
Director

The Computer Applications in Science and Engineering (CASE) department was created in January 2007. It is devoted to enhancing the links between two players.

On the one hand the scientific community and high-tech industry, with strong needs for high performance simulation codes requiring high computational power. On the other hand the high performance computational science experts of the department, who have both the expertise and resources to get the best out of supercomputers.

The mission of the department is therefore to transfer their know-how and technology to both the scientific community and to high-tech industry and to create the necessary synergy brought by the new generation of supercomputers.

In order to achieve these objectives, the department researchers develop computational tools capable of simulating highly complex problems seamlessly adapted to run on high-end parallel supercomputers with the best possible efficiency.

The team covers all levels of "computational tools": physical models, numerical methods and parallel programming techniques and post-processing analysis. The work undertaken by the department depends on the research problems faced. For third-party applications, the group works on code performance optimization that follows a detailed diagnostic stage, helping the researchers that developed the original application to port it to supercomputers. Moreover the team can improve the numerical schemes used by those applications applying our experience in computational mechanics. On the other hand, an in-house application, Alya, is used as the simulation tool for many multi-physics problems. It is a high performance computational mechanics and design code written to the highest standards in accuracy, efficiency and scalability.This interdisciplinary strategy makes the CASE Department a highly interactive one, with a large list of successful collaboration projects, which grows by the day.

The CASE department has two main research themes:

- Physical and Numerical Modelling (PNM)
- High Performance Computational Mechanics (HPCM)

PNM research lines are horizontal and HPCM lines are vertical, in the sense that PNM is in charge of all the developments of the applications applied in HPCM.

PNM includes basic themes, like numerical modelling of physical phenomena, stabilization techniques, algorithms and solution strategies, parallelization strategies, coupled problems with domain decomposition methods, optimization algorithms and error estimation techniques. In addition, PNM researchers investigate pre-process, post-process, data management and visualization topics.

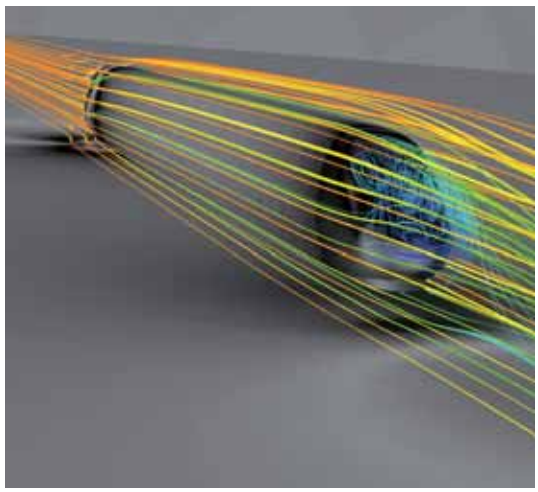
HPCM comprises application research in different science and technology domains where simulations are needed: aerospace, bio-mechanics, solid state physics, high energy physics, geophysics, environment, meteorology, etc.

Physical and Numerical Modelling (PNM)

In order to solve so-called Grand Challenge Problems, where a massive amount of computer power is essential, this group establishes collaboration agreements with leading research groups in Spain. Some of these collaborations result in an improvement in performance of pre-existent codes and algorithms to run on supercomputers. Other collaborations are based in an in-house tool, Alya, which is a simulation code for High Performance Computational Mechanics.

The research themes cover a full range of techniques required to simulate a physical problem, usually governed by partial or ordinary differential equations. This objective can be achieved thanks to the multi-disciplinary background of the CASE department researchers. The research areas include:

- Mathematical modelling of a given physical process;
- Numerical modelling of the mathematical equations, that is space and time discretization: high order time integration schemes; variational multi-scale; Finite element; domain decomposition (Chimera, non-overlapping meshes); turbulence models;
- Numerical algorithms to solve the discrete equation efficiently, or to couple a set of algorithms to solve complex physical problems: explicit and implicit schemes, monolithic and fractional algorithms, preconditioners and multigrid;
- Efficient implementation in a computational mechanics code: distributed/shared memory parallelization with MPI/OpenMP, code optimization; architecture dependent implementation (VMX, Cell);
- Code performance analysis and optimization.

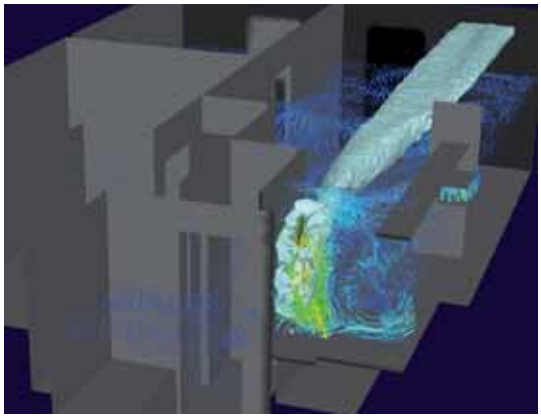


ALVIA High Velocity Train CAF. Series S120

High Performance Computational Mechanics (HPCM)

A wide variety of technological projects were carried out in the Department, mainly driven by industry needs. In most of the projects, the Alya in-house code had a primary role. The projects included:

- Geophysics for seismic imaging: reverse time migration and wave equation modelling.
- External aerodynamics: aerospace and automotive industry flows.



Airflow in a room

- Building, Energy and Environment: ventilation flows for energetically efficient buildings; semi-transparent photovoltaic façades.
- Bio-mechanics: electro-mechanical model of the heart and computational hemodynamics.
- Aero-acoustics: sound produced by turbulent flow around high speed trains.
- Ab-initio molecular dynamics: A DFT molecular dynamics simulation using sparse matrices that allows the ab-initio analysis of molecules with very large number of atoms.
- Spectroscopy: computational quantum mechanics for time dependent DFT used to simulate large molecules energy emission.
- Meteorology: computational atmospheric physics for mesoscale simulations.

Research projects

OPTIDIS: Optimum Design in Building using Computational Fluid Dynamics Method, funded by Ministry of Science and Technology. From 31/12/2005 until 31/12/2008.

KALEIDOSCOPE: Design state of the art seismic imaging tools for oil prospecting. Funded by REPSOL. From 1/1/2007 until 31/12/2010

SUPPORTING RESEARCH ACTIVITIES: In order to increase our relation with international research groups, The CASE department received during the year 2007 5 European researchers through the HPC-Europa program of the EU FP6 (RII3-CT-2003-506079):

- Anne-Cecile Lesage, INRIA (France), HPC for Computational Fluid Dynamics, 08/01/2007 - 05/03/2007.
- Robert Kloefkorn, University Freiburg (Germany), Efficient use of Local Grid Adaptivity Including Dynamic Load Balancing in Parallel Computations, 01/09/2007 - 01/12/2007.
- Florian Lorenzen, Free University Berlin (Germany), Spectra computations of martensitic phase transformations in linear and nonlinear elasticity, 03/09/2007 - 30/09/2007.
- Benson Muite, University of Oxford (UK), Towards Direct-Gap Nanotransistor: massive parallel CRYSTAL06 code for Wurzite Silicon assessment, 01/11/2007 - 15/12/2007.
- Marek Prymon, Krakow University of Technology (Poland), Simulation of air conditioning system based on thermal energy storage in building structure, 10/09/2007 - 10/12/2007.

In addition, the department received the visit of Tayeb Trari through the TEMPUS scheme JEP-31131-2003, MEDA. The topic of his stay was Large Eddy Simulation of Turbulent Channel Flow on Nonconforming Mesh Following Taylor microscales.

Sergi Girona
Operations Director

The Operations group has two major missions: systems management and user support. The systems management area includes system administration, security, resource management, networking and helpdesk.

This group of people makes the BSC systems available 7 days a week, 24 hours a day. The service is guaranteed via an automatic mechanism which notifies events at any time and reacts automatically to retrieve most technical problems. The user support group includes direct user support with knowledge in programming models, libraries, tools, applications, etc. The BSC webmaster is also included in this team.

During 2007, the Operations group focused on four major areas:

- Deployment to full production of several systems:
  - Backup and Hierarchical storage system
  - DB and data storage for BSC researchers
  - Secure gateway access to BSC resources
  - New batch scheduler for MareNostrum: Slurm/Moab
  - Shared memory multiprocessor system
  - Upgrade of external link to 10 Gbit/s
- MareNostrum physical environmental optimization
- Spanish Supercomputing Network (RES, Red Española de Supercomputación)
- User support

Among these activities, the complete group participated in European projects such as DEISA, e-DEISA and HPC-Europa. In DEISA, the team is responsible for integrating BSC resources into the DEISA infrastructure including networking, file system, resource management, user support, system administration and security. E-DEISA is focused on infrastructure operations, application hyperscaling, benchmarking and middleware. In HPC-Europa, the team provided support for different visitors including knowledge and support in parallelizing codes.

Systems Management

MareNostrum

BSC-CNS hosts MareNostrum, one of the most powerful supercomputers in Europe. MareNostrum is managed by the Operations Department which takes care of its availability, security and performance. MareNostrum is a Linux system based on the BladeCenter architecture with PowerPC processors and a Myrinet interconnection. MareNostrum is installed inside a chappel properly prepared to host a Supercomputer of this magnitude. Using 180 sqm, in a glass box of 5 meters high, with 1meter false floor, it has a very effective computing room enviroment, with a global consumption of more than a 1.2 Mwatts, including not only MareNostrum, but also all required components to run the system. The current PUE, Power Usage Effectiveness, is 1.4; a value that operations group maintains and improves with best practices.

The current system counts with:

- Peak performance of 94.21 Teraflops
- 10240 IBM 970MP Power PC 2.3GHz processors (2560 dual 64-bit processor blade nodes)
- 20TB of main memory
- 370TB of disk storage
- Interconnection networks: Myrinet, Gigabit Ethernet, 10/100 Ethernet

The overall utilization of the system is maintained in the average of 85%, considering utilization as the accounted hours on top of the total hours for 10240 processors in one year. This good figure is obtained not only by the proper planning of each individual job, but also on how the access is granted at MareNostrum and all the Supercomputers of the Spanish Supercomputing Network.

Robot Storagetek SL8500

Backup and hierarchical storage system

Due to the high demand for storage at BSC, coming from MareNostrum and other storage systems an SL8500 library was installed. During 2007 tape technology was migrated from LTO3 to LTO4 increasing the total storage capacity to 6 PB (6000 Terabytes) without compression. A total of 23 tape drives and 7500 tapes, each with 800 GB capacity, were installed to provide this storage.

Histogram GB of data backed-up daily

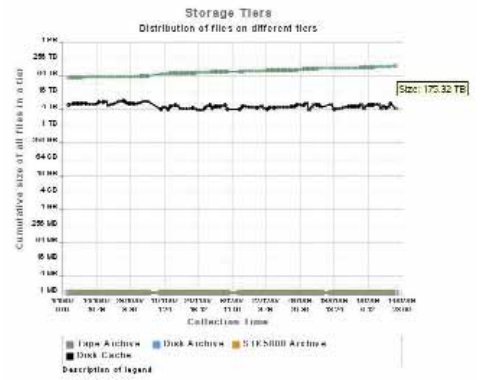
The SL8500 library in conjunction with 5 servers and 31.4 TB of disk space were configured and installed to perform two main services: backup of all compute systems at BSC and Hierarchical Storage Management (HSM).

A backup service using Tivoli technology was deployed permitting a daily backup of all data from MareNostrum and other systems. Three dedicated servers were installed and configured with the following backup roles:

TSM1: MareNostrum Home directories

TSM2: Tape management, MareNostrum project and applications directories

TSM3: BSC Servers



HSM usage histogram

Hierarchical Storage Management system, using SAMFS technology, permitted us to increase the storage capacity of MareNostrum up to Petabytes. HSM is a storage technology that provides automatic data migration from a costly device to one with lower cost. A storage of 9 TB of FiberChannel disks serves as costly or first level of storage and the SL8500 tape library serves as the second level of storage.

Tools were provided to MareNostrum users for the movement of data between HSM and MareNostrum local filesystems.

Storage Control air and disks

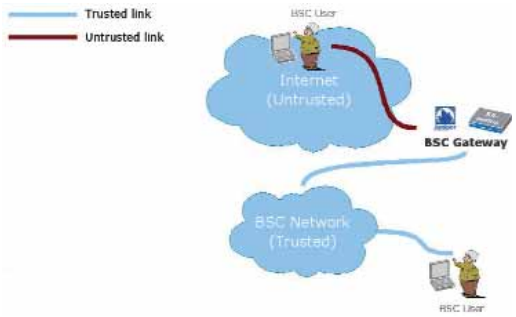
DB and data storage for BSC researchers

A system for database storage was installed at BSC in order to provide a service to the Life Science and Earth Science departments. This equipment is composed of a StorageTek 6540 disk controller system with an upgraded capacity in 2007 from 32 TBytes to 54 TBytes, in 200 disks (300 GB FC 10krpm), two Brocade 4100 switches (32 ports and 4Gb each), and 2 Sun Fire X4200 servers.

This storage was offered to a heterogeneous group of workstations and servers inside BSC via several technologies, such as NFS version 3 and 4 and direct mounting through Fiberchannel and Samba.

Secure gateway access to BSC resources

A new network & security infrastructure was installed at BSC that provides a unique technology to access BSC resources from internal and external networks. During 2007 deployment of this infrastructure started with the installation of secure gateway access to enable access to BSC internal resources from the Internet.



Gateway architecture

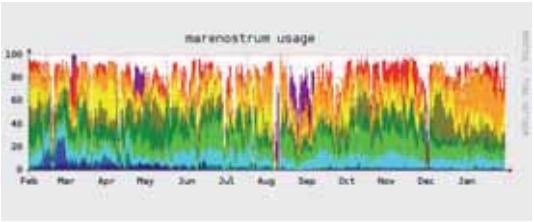
The technology used is SSL VPN, which first performs a user authentication followed by host checking to determine the level of reliability that the connecting client machine has. Depending on this level one of 2 roles will be offered to the user:

1) BSC basic external access: Only internal resources via web access will be provided, such as webmail, web document management, intranet, etc.

2) BSC VPN external access: Apart from web services the possibility of establishing a VPN connection to BSC is offered, so the user is able to work from any location as if she was at the office.

New batch scheduler for MareNostrum

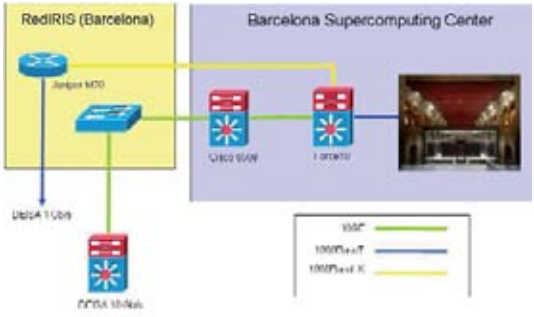
A new batch job scheduler was installed in MareNostrum which enabled us to improve flexibility when executing jobs with a high number of resources, to increase reliability and to simplify configuration. Some other advanced scheduling mechanisms can now be offered and exploited such as, fair-sharing, quality of service, pre-emption and migration of jobs.



MareNostrum usage histogram divided by research groups

Another main characteristic of the new scheduling system consists of the interoperation with other clusters and schedulers in Grid environments or in a multi-cluster architecture, which is a strong requirement for some BSC projects such as the Red Española de Supercomputación, DEISA, eDEISA, DEISA2.

In addition the monitoring system was improved and expanded with new metrics available to understand and optimize MareNostrum's resource usage.



BSC Network architecture for DEISA

Shared memory multiprocessor system

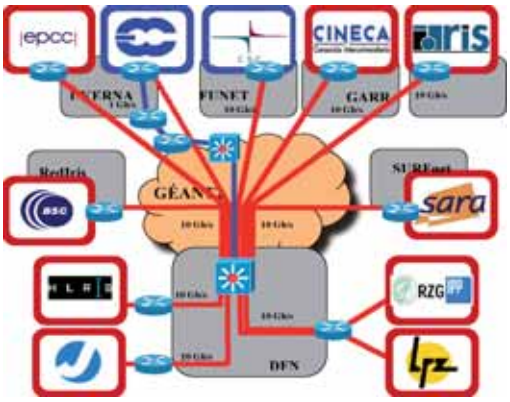
In 2007 BSC added a shared memory system to their facilities, allowing BSC researchers to perform specific pre-processing and post-processing analysis that requires large memory systems. In the first quarter of 2007 the Altix system with its 128 cores of Montecito processors and 0.5 Terabytes of main memory entered production to support these activities.

In the last quarter of 2007, the Altix system was adapted to be able to host job runs from external users coming from the MareNostrum access committee. This involved the installation of the Slurm/Moab scheduling system and user management unification.

Upgrade of external link to 10 Gbit/s

During 2007 connectivity to the European GEANT2 network was upgraded from a bandwidth of 1 Gbit/s to 10 Gbit/s. This improvement permited the deployment of collaborative DEISA services between MareNostrum and the other DEISA supercomputers throughout Europe.

The Operations group was responsible for the installation, configuration and deployment of 10 Gbit/s network hardware in MareNostrum and other BSC supercomputers, and the movement to production of the link in concordance with all other DEISA sites and infrastructure.



DEISA Network Architecture

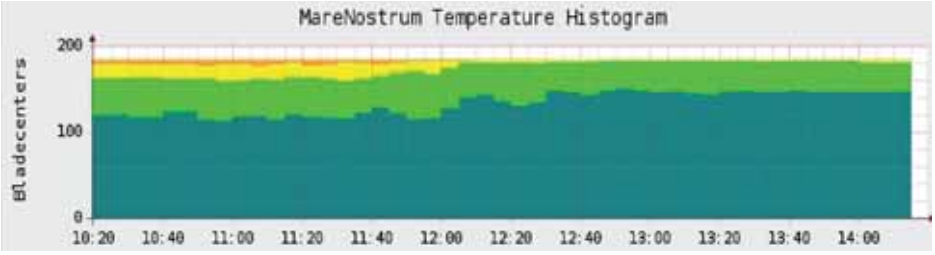
MareNostrum physical environmental optimization

The importance of the environmental impact of supercomputing centers increases every year in common with all areas of society. The term adopted for computing, known as green computing, consists of the study and improvement of the machines and facilities which operate them with respect to the environment. This is particularly important for high performance computing with a large operational environmental impact. One of the key metrics is the power consumption per square meter floor space and with several actions, the Operations team achieved a reduction of the power consumption of MareNostrum of 10%.

The first step was the inclusion of environmental metrics (temperature, humidity, fan speed, compressors online, etc.) from all the machines that form MareNostrum as well as the air conditioning system, into the BSC online monitoring system. Collecting all this information provided knowledge of the physical environment and indicated where improvements could be made.

These observations led to several modifications:

- Elimination of front doors and air baffles of all the MareNostrum racks & bladecenters
- New tiles were installed in front of each computation rack to improve air flow
- Changes in the balance of the air conditioning machines
- Methacrylate screens were designed and installed in front of each rack of machines to guide the cold air flow directly to the computers, instead of each rack having to take cooling air from the general environment at a higher ambient temperature.



MareNostrum temperature histogram

These environmental improvements produced consequential benefits to the reliability of MareNostrum, by reducing failures and increasing the time between failures on the air conditioning system and Mare-Nostrum hardware.

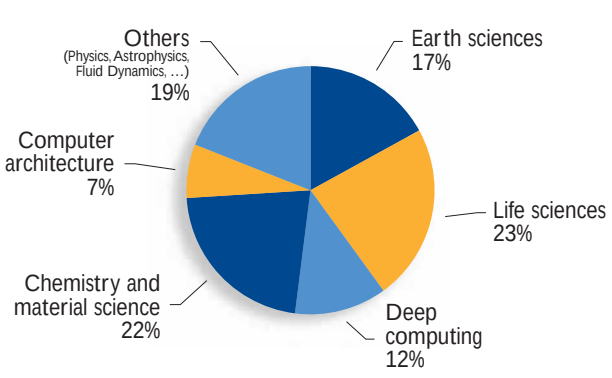
New methacrylate screens design for cooling improvement

User Support

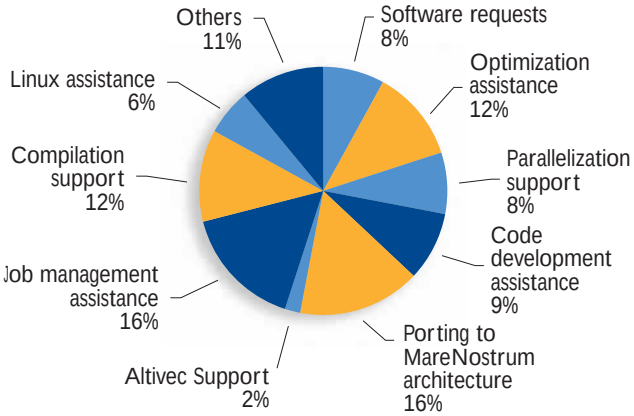
The User Support Group provides assistance with all aspects of scientific computing, including general user support, code optimization, parallel model building support and porting serial and parallel codes to supercomputers such MareNostrum. The group is also involved in the creation of scripts for ease of use as well as assistance with software packages and tutorials on specialized topics or programs.

The number of support requests received in 2007 was 8534 and these are presented in the figures below categorised into 10 different types of support activity and also split by support request area.

USER SUPPORT REQUEST PER AREA



USER SUPPORT REQUEST PER TOPIC



User Management interface

In 2007 the support group set up a user management web interface which improved the RES management from the group leaders point of view as well as for the administration staff. In the first case it is now much easier to apply for computational resources at MareNostrum and keep track of the whole process. For scientists it is a user friendly way to manage their activity: adding or removing researchers, consulting the CPU time consumed, posting reports, etc. For BSC support staff, it is an important feedback mechanism and, at the same time, the team can easily oversee all the activities accepted in the current period. For the Access Committee the environment is used for evaluation of activities, to keep track of the information of different periods, and to consult user reports. Of course this infrastructure is also open to improvements.

RES screenshot

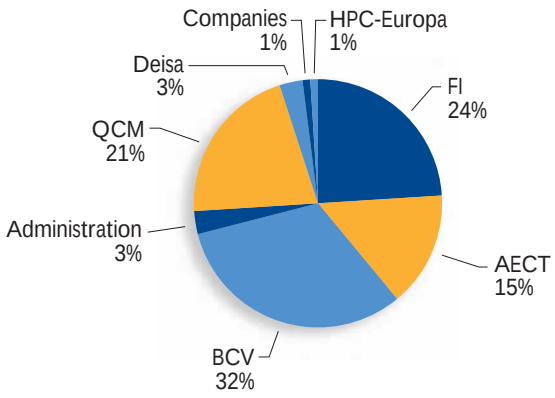
Accounting

The system use is defined as follows:

$$\left(\frac{total_{cpu_{hour_{used}}}}{total_{hours}} \right) \times 100$$

MareNostrum was in production for the whole year, except for maintenance periods. Using the remaining part of the year as the basis for calculations, the system utilization is approximately 80% with a total of 72 million computational hours consumed. In addition to BSC internal groups, approximately 150 external activities accessed the RES systems. These groups can be classified into the following scientific areas:

USE OF RES COMPUTATIONAL RESOURCES CLASSIFIED BY SCIENTIFIC AREA



Ernest Quingles
Management Director

The aim of the Management Department is to optimize coordination of the management areas and to consolidate a complete managing support to better face the new challenges of the centre.

During 2007 the new Management Department was re-organized into three management units: Business Finance and Administration; Project Management and Technology Transfer; and Institutional Communication and Promotion. In summary, the personnel increased from 137 at the end of 2006 to 200 at the end of 2007, including permanent, temporary and shared staff, resident students and permanent visiting researchers. BSC-CNS also increases its extraordinary budget thanks to the extraordinary contribution of private companies such as Repsol, IBM and Microsoft.
The center continued with its effort participating in European projects and disseminating the centre's activities, corporate image and events organization.

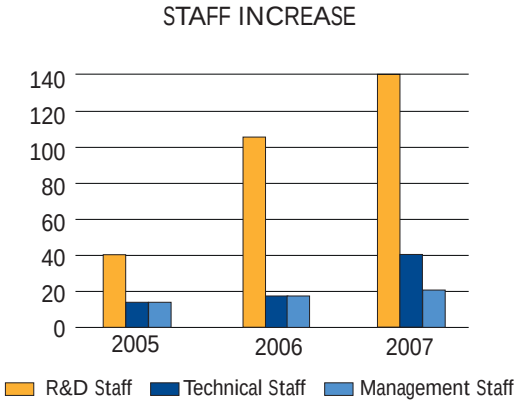
Human Resources, Finance and Administration Support

Administration & Finance Support includes the following groups: Human Resources, Finance & Accounting and Administration Support.

Human Resources

In 2007, both the Scientific and Support staff structures grew into consolidated personnel structure.

This led to the consolidation of the three scientific departments and the support department (Operations), with the constitution of two new support departments into a new organization consisting of 9 support groups and 17 research groups, with a total of 163 staff members. The research departments are made up of 9 new groups from The Computer Science department, 4 new groups from the Earth Science department and 4 from the Life Science department.



The new support departments created in 2007 are:

1. The Computer Applications in Science & Engineering (CASE) department, develops, adapts and optimizes numerical applications for scientific problems in supercomputer systems.
2. The Management Department includes the three major services groups previously created: Administration, Finance and Human resources, Projects Management and Technology Transfer and Marketing and Communication areas.

Since the creation of the center in 2005 there has been a high level of activity and continuous increase in staff as well as an increase in the complexity of the organizational structure.

In 2007 the total headcount of the organization included 88 permanent staff members and 75 dedicated to specific projects. BSC-CNS initiated 47 recruitment process based on the principles of ability, publicity and open competition.

BSC-CNS staff included shared staff from other public institutions such as the Technical University of Catalonia (UPC) and the Institute de Recerca de Barcelona - Parc Scientific de Barcelona -Universitat de Barcelona (IRB-PCB-UB) who must adhere to the established rules and agreements for each of the centers to which he or she is affiliated. BSC-CNS hopes to welcome staff from additional institutions in 2008.

BSC-CNS also welcomed high level scientific personnel from special mobility programs such as the Ramon y Cajal Program, the ICREA Program and other personnel training research programs sponsored by various Spanish Ministries. At the same time, the BSC-CNS Fellowship program welcomed applicants from relevant scientific disciplines to participate in several European research projects and collaborations with international industry such as IBM and Microsoft. These fellowships were offered for periods of one year, renewable for the duration of the project. At the end of 2007, BSC-CNS had 25 student researchers associated to various research projects.

The following is a breakdown of BSC-CNS staff:

DEPARTMENT	2005	2006	2007
Director, Associate Director	2	2	2
Management	9	13	18
Operations	11	16	21
Computational Applications	0	0	20
Computer Sciences	28	70	89
Earth Sciences	4	12	16
Life Sciences	9	24	34
TOTAL	63	137	200

Finance & Accounting

The following is a detailed description of the financial accounts for 2007. The annual accounts were drawn up following the accounting principles laid out in the General Spanish Public Accounting Plan.

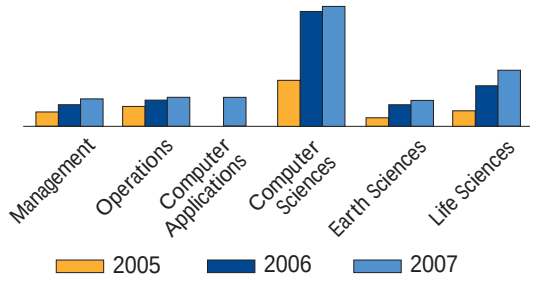
The operating budget of the BSC-CNS Consortium for fiscal year 2007, included expenses incurred from the fulfillment of its financial obligations, and income from contributions of the administration and organizations that compose it, as well as income derived from agreements reached with private organizations.

Income

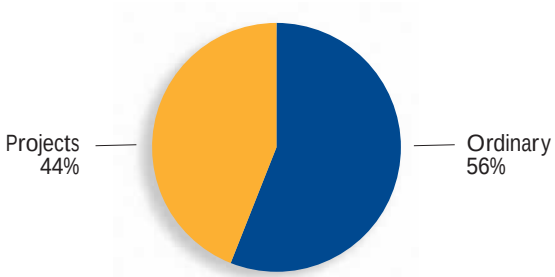
The Consortium income for fiscal year 2007 came from contributions from the Ministry of Education and Science (MEC), Generalitat de Catalunya (GdC) and European Commission (EC), as well as from agreements, contracts or other collaborative agreements with private organizations. Furthermore, the consolidated budget of BSC-CNS included the assignment of its own resources coming from the previous year's provisions and financial results obtained.

INCOME	€ AMOUNT		
	Ordinary Budget	Projects Budget	Total
Current Income	6.380.000	2.174.251	8.554.251
Ministerio de Educación y Ciencia	*4.049.000*	*883.173*	*4.932.173*
Generalitat de Catalunya	*2.331.000*	*360*	*2.331.360*
European Commission		*863.638*	*863.638*
Ministerio Medio Ambiente		*427.080*	*427.080*
Private Companies	3.000	3.125.282	3.128.282
Capital Transfers	295.653		295.653
TOTAL	6.678.653	5.299.533	11.978.186

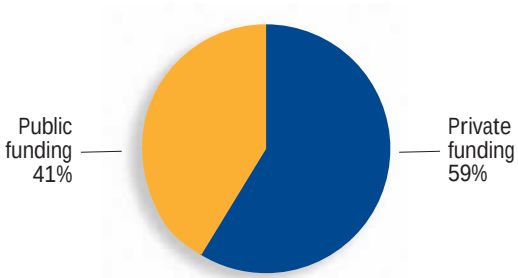
PERSONNEL EVOLUTION



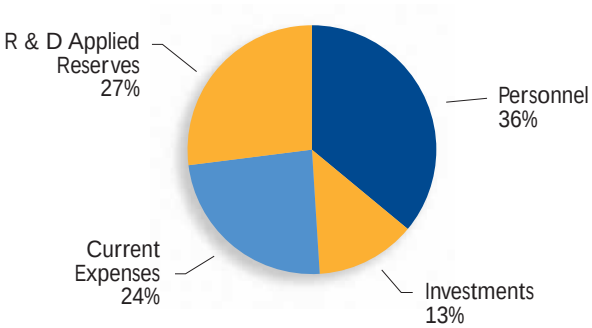
INCOME ORIGIN



PROJECTS FUNDING 2007



EXPENSES CATEGORIES



Expenses

The current expenses of the BSC-CNS Consortium in the fiscal year 2007 include the office space rental, security services, maintenance and cleaning services, telephones and networking, legal services, marketing, insurance and power. The expenses also include all investments which were financed with the extraordinary budget received from projects. In addition, BSC-CNS acquired the furniture, fixtures and fittings, and the necessary computer equipment. In 2007, BSC-CNS invited 21 public calls in order to accept 6 supply tenders and 15 services tenders. All of the acquisitions were made following the legal procedures established by the law regulating contracting in public administrations, and all contracts have been open to public tenders.

EXPENSE	€ AMOUNT		
	Ordinary Budget	Projects Budget	Total
Personnel	3.108.357	1.108.026	4.216.373
Investments	787.790	813.280	1.601.070
Current Expenses	2.357.798	528.026	2.885.824
R&D Applied Reserves	424.718	2.850.201	3.274.919
TOTAL	6.678.653	5.299.533	11.978.186

Administration Support

The Administration Support Group is responsible for activities including the organization of official meetings and events, travel planning, space allocation, supply orders and execution of the tender process as well as providing general administrative support and reception services.

In 2007, the group handled the logistics for all official meetings and including regular Access Committee meetings, Executive Commission meetings as well as the meetings of the Board of Trustees. This included arranging for meeting spaces, catering services and travel-related assistance. Moreover, the group was responsible for receiving visitors for national and international mobility programs, representatives of various institutions and companies in addition to invited speakers from all over the world.

Annual meeting 2007

The group also played a significant role in finding and adapting office space to accommodate the various research groups. They worked with the contractors to arrange the spaces, move equipment and furnish offices; they also provided facilities management services. At the end of 2007, the Administration Support Group organized the second general meeting of BSC-CNS employees that took place at Conventions Center of UAB (Hotel Serhs Campus) situated in Bellaterra (Barcelona). One hundred and seventy staff members participated in the event.

The Department and General Directors presented the activities and results obtained in 2007 and their objectives for 2008. The BSC-CNS staff was provided the opportunity to ask questions about the BSC-CNS organization as well as to propose ideas to improve the center.

Finally, many people joined the Team building session which consisted of a range of challenges which allowed the members of the different departments participate as a team in a different environment.

The activities strengthened links and team work through activities requiring coordination, communication, imagination and initiative skills.

Institutional communication and promotion

The communication and promotion area is in charge of disseminating information about research activities as well as promoting science in society.

In the course of 2007, BSC-CNS received a total of 4300 visitors from national and international centers, including universities, research centers, industry and non-profit organizations.

Conferences

BSC-CNS members participated in the following conferences and courses in order to disseminate BSC-CNS activities:

International

- ISC 2007, Dresden, Germany, June 2007.
- SC2007, Reno, USA, November 2007.

National

- Aules Empresa, Facultad d'Informàtica, Campus Nord UPC, Barcelona.

BSC-CNS in the Media

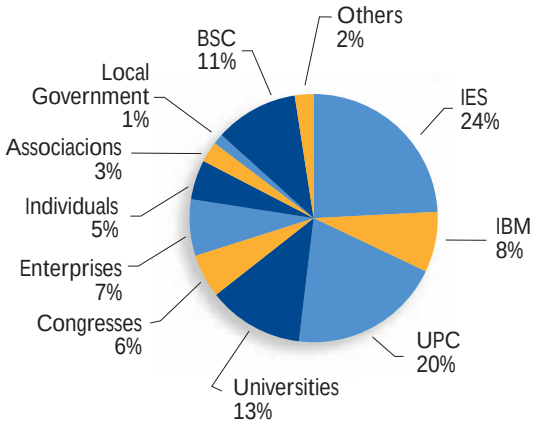
Media coverage of the BSC-CNS increased considerably in 2007. Including both in national and international newspapers and magazines, BSC was mentioned 136 times. In total, BSC issued 12 press releases in Spanish, Catalan and English that are included online http://www.bsc.es/plantillaA.php?cat_id=44. Print media has been the media where BSC has received most coverage.

Events Organized by BSC-CNS

In 2006, BSC-CNS organized and attended the following congresses, seminars and workshops:

- WMO/GEO Expert Meeting on an International Sand and Dust Storm Warning System, November 7-9, 2007.
- Official Opening of the Spanish Supercomputing Network (Red Española de Supercomputación), 13th March 2007.
- Bioinformatics Resource Days, November 26-28, 2007.
- BSC-IRB Barcelona Conference on Computational Biology, May 24-25, 2007.
- DEISA training session, 7-9 March, 2007.

MARENOSTRUM VISITS



Project Management and Technology Transfer

In 2007, the BSC-CNS team responsible for Project Management and Technology Transfer, worked on the management of proposals and projects funded by public calls as well as by sponsored research contracts.

A detailed description of the activities performed by this department during 2007 is structured into the following three sections: project management, technology transfer and private contracts.

Project Management

In 2007, BSC-CNS participated in an increasing number of funded projects and grants, with the consequent increase in project management activity.

International Activities

At international level, the Barcelona Supercomputing Center had already participated in an impressive number of activities. In 2006, BSC-CNS was active in the Sixth Framework Programme of the European Commission and participated in several activities to prepare for the transition to the Seventh Framework Programme, launched in December 2006.

2007 activity	Active Projects	Started Participation	Proposals Submitted
	DEISA	MERASA	ETSF
	eDEISA	ELIXIR	EUFORIA
	HPC-EUROPA		W2PLASTICS
	SARC		VAP
	BREIN		HiPEAC2
	BEinGRID		PRACE
	XTreemOS	VELOX	
	SORMA		OGF-EUROPE
18	8	2	8

2007 Activity Resume

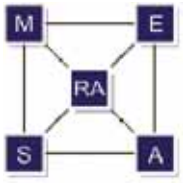
In 2006, BSC-CNS started to participate in eight FP6 projects: DEISA, eDEISA, HPC-EUROPA, SARC, BREIN, BEINGRID, XTREEMOS and SORMA. DEISA and eDEISA are infrastructure projects. HPC-EUROPA includes a transnational access activity as well as research and development. SARC, BREIN, BEINGRID, XTREEMOS and SORMA are primarily R&D projects.

In 2007, BSC-CNS joined two FP7 projects: MERASA and ELIXIR and continued its involvement in the ones named above.

In the second half of 2007, several proposals entered in the negotiation stage of the Information and Communication Technology priority of the Seventh Framework Program, due to begin in 2008.

A total of 18 projects were worked on as indicated in the chart above.

The following is a brief description of the projects and activities in which BSC-CNS participated in 2007. Some of the more technical aspects of projects SARC, BREIN, BEINGRID, SORMA, XTREEMOS and HPC-EUROPA are described in the section on Research Activities.



MERASA Project

The increasing demand for functionality in current and future real-time embedded systems is driving an increase in performance of processors.

The MERASA project aims to develop multi-core processor designs (from 2 to 16 cores) for hard real-time embedded systems hand in hand with timing analysis techniques and tools to guarantee the analysability and predictability regarding timing of every single feature provided by the processor.

Design exploration activities are performed in conjunction with the timing analysis tools.The project will address both static WCET analysis tools (the OTAWA toolset) as well as hybrid measurement-based tools (RapiTime) and their interoperability. It will also develop system-level software with predictable timing performance.
To constrain production costs and technology integration risks, hardware based real-time scheduling solutions are investigated that empower the same multi-core processor to handle hard, soft, and non real-time tasks on different cores. The developed hardware/software techniques are evaluated by application studies from aerospace, automotive, and construction-machinery areas performed by selected industrial partners.

ELIXIR Project

The mission of ELIXIR is to construct and operate a sustainable infrastructure for biological information in Europe to support life science research and its translation to medicine and the environment, the bio-industries and society. The objective of the ELIXIR preparatory phase is to produce a memorandum or memoranda of understanding between organisations (government

agencies, research councils, funding bodies and scientific organisations) within the member states, with the purpose of constructing a world class and globally positioned European infrastructure for the management and integration of information in the life sciences.

DEISA Project / eDEISA

DEISA is a consortium of leading national supercomputing centres in Europe that are coordinating their actions to jointly build and operate a distributed terascale supercomputing facility.

BSC-CNS joined the DEISA Project (http://www.deisa.org) in May 2005. The project has secured funds until May 2008 and has received funds for extended activities through eDEISA (extended DEISA).

In 2007, the BSC-CNS participated in the following activities related to the DEISA and eDEISA Projects: management through participation on the Executive Committee, dissemination, service activities and life science joint research activities.

In addition, four proposals were submitted to the DEISA Extreme Computing Initiative (DECI) from Spain (the total number of proposals submitted by the 11 partners was 63) of which one was selected for execution.

HPC-Europa Project

HPC-Europa is a consortium of six leading High Performance Computing (HPC) infrastructures, including BSC-CNS, and five centers of excellence. This consortium aims to provide advanced computational services in an integrated manner to the European research community. The culture of co-operation fostered by the consortium's joint research and networking activities generates critical mass for computational science. It enables researchers working in any eligible country in Europe to visit a participating research institute to carry out a collaborative visit of up to 3 months' duration and to gain access to some of the most powerful High Performance Computing (HPC) facilities in Europe.

In 2007 the BSC welcomed the following researchers:

Name	Affiliation
Jelena Tamuliene	Institute of Theorical Physics and Astronomy of Vilnius University (Lithuania)
Koray Sevim	Izmir Institute of Technology (Turkey)
Viktorya Aviyente	Bogaziçi (Turkey)
Marc Weber	EDFL, Swiss Federal Institute of Technology of Lausanne (Switzerland)
Francesco Aquilante	Lund University (Sweden)
Marcin Palusiak	University of Lodz (Poland)
F.Matthias Bickelhaupt	Vrije Universiteit (Netherlands)
Sébastien Fernandez	Université Pierre & Marie Curie Paris 6 (France)
Charles Laughton	University of Nottingham (United Kingdom)
Ricardo Grau-Crespo	University College London (United Kingdom)
Lucy Allen	University of Leeds (United Kingdom)
Anne-Cecile Lesage	INRIA, Institut National de Recherche en Informatique et en Automatique (France)
Luca Bergamaschi	University of Padova (Italy)

Gabriele Manca	University of Pisa (Italy)
Andreass Krapp	Philipps-Universität (Germany)
Angeles Martinez	University of Padova (Italy)
Brian Wylie	Forschungszentrum Juelich (Germany)
Gian Pietro Miscione	Universita' degli Studi di Bologna (Italy)
Petko Ivanov	Bulgarian Academy of Sciences (Bulgaria)
Carlo Ottaviani	Università di Camerino (Italy)
Dimitris Maganas	University of Athens (Greece)
Martinus Zwijnenburg	Royal Institution of Great Britain (United Kingdom)
Sandro Meloni	ENEA, Italian National Agency for New Technologies Energy and the Environment (Italy)
Anna Sadowska	University of Gdansk (Poland)
Caroline Clarke	University of Cambridge (United Kingdom)
Andrea Ciardi	Observatoire de Paris (France)
Robert Kloefkorn	University Freiburg (Germany)
David Michéa	University of Pau (France)
Ana Lucia Varbanescu	Delft University of Technology (Netherlands)
Sebastian Hanigk	Technische Univerität München (Germany)
Francesco Ancilotto	University of Padova (Italy)
Krzysztof Zborowski	Jagiellonian University (Poland)
Emanuele Di Palma	ENEA, Italian National Agency for New Technologies, Energy and the Environment (Italy)
Umberto Martinez Pozzoni	University of Milano - Bicocca (Italy)
Manuel López-Ibáñez	Napier University (United Kingdom)
Florian Lorenzen	Free University Berlin (Germany)
Matthew John Harvey	Imperial College London (United Kingdom)
Benson Muite	University of Oxford (United Kingdom)
Alfonso Jaramillo	Ecole Polytechnique (France)
Roberto Orlando	Università del Piemonte Orientale (Italy)
Prymon Marek	Krakow University of Technology (Poland)
Piotr Storoniak	University of Gdansk (Poland)
Fatima Lucas	Università della Calabria (Italy)
Michael Gerndt	Technische Universität München (Germany)
Mónica Calatayud	Universite P. et M. Curie (France)
Ozgur Gul	Sabanci University (Turkey)
Marco Pinna	University of Central Lancashire (United Kingdom)
Andrei Zvelindovsky	University of Central Lancashire (United Kingdom)

Please find below the list of the publications of all BSC visitors with the HPC-Europa grant:

- F. Aquilante and T. B. Pedersen, Quartic scaling evaluation of canonical scaled opposite spin second-order Møller-Plesset correlation energy using Cholesky decompositions, Chem. Phys. Lett. 449 (2007) 354
- F. Aquilante, R. Lindh and T. B. Pedersen, Unbiased auxiliary basis sets for accurate two-electron integral approximations, J. Chem. Phys. 127 (2007) 114107
- R. Mayol, F. Ancilotto, M. Barranco, E.S. Hernandez and M. Pi, "Novel aspects of wedge filling by liquid helium", J. Low Temp. Phys. 148, 851 (2007).
- F . Caupin, F. Ancilotto, M. Barranco, R. Mayol and M. Pi, "Freezing of He-4: comparison of different density functional approaches", J. Low Temp. Phys. 148, 731 (2007).
- F. Ancilotto, M. Pi, R. Mayol, M. Barranco, K.K. Lehmann, "Squeezing a helium nanodroplet with a Rydberg electron", J. Phys. Chem. A 111, 12695 (2007).
- A. Hernando, R. Mayol, M. Pi, M. Barranco, F. Ancilotto, O. Bunermann, and F. Stienkemeier, "The structure and energetics of He-3 and He-4 nanodroplets doped with alkaline earth atoms", J. Phys. Chem. A. 111, 7303 (2007).
- M. Pi, R. Mayol, A. Hernando, M. Barranco and F. Ancilotto "Explosion of electron bubbles attached to quantized vortices in liquid He-4", J. Chem. Phys. 126, 244502 (2007)
- Marcin Palusiak, Sílvia Simon, Miquel Sola; "The Proton Transfer Reaction in Malonaldehyde Derivatives. Substituent Effects and Quasi-Aromaticity of the Proton Bridge", Chemical Physics (2007), 342, 43-54.
- F. M. Bickelhaupt, M. Solà, C. Fonseca Guerra, Highly Polar Bonds and the Meaning of Covalency and Ionicity - Structure and Bonding of Alkalimetal Hydride Oligomers, Faraday Discuss. 2007, 135, 451-468.
- F. M. Bickelhaupt, M. Solà, C. Fonseca Guerra, Table Salt and other Alkalimetal Chloride Oligomers: Structure, Stability and Bonding, Inorg. Chem. 2007, 46, 5411-5418.
- Anna Sadowska, Janusz Rak, Lluis Blancafort, Alexander Voityuk, "Effect of DNA environment on electron transfer in stacked DNA nucleobases. A CASSCF/CAS-PT2 study", Central European School on Physical Organic Chemistry, 4-9 June 2007, Karpacz (Poland).
- P. Vignolo and G. Morigi, "Photonic properties of one-dimensional atomic lattices", at the ICREA Workshop "Disorder in cold atoms", Universitat Autònoma de Barcelona, 24th-26th January '07.
- A.G. Yiotis, J. Psihogios, M.E. Kainourgiakis, A. Papaioannou and A.K. Stubos, A lattice Boltzmann study of viscous coupling effects in immiscible two-phase flow in porous media, Colloids And Surfaces A, 2007. (In press)
- F. Lippold, "Fluid-Structure-Interaction in a tidal current turbine", Poster presentation and abstract for ICFD 2007, Reading, UK.
- A. Bertoldo, FEMS: An Adaptive Finite Element Solver. International Workshop on Parallel and Distributed Scientific and Engineering Computing (PDSEC) at the International Parallel and Distributed Processing Symposium (IPDPS), Long Beach, California USA, 2007. To be published
- A. Koseska, A. Zaikin, J. García-Ojalvo, and J. Kurths, "Stochastic suppression of gene expression oscillations under intercell coupling", Phys. Rev. E 75, 031917 (2007).
- A. Koseska, E. Volkov, A. Zaikin, and J. Kurths, "Inherent multistability in arrays of autoinducer coupled genetic oscillators", Phys. Rev E 75, 031916 (2007).
- E. Ullner, A. Zaikin, E.I. Volkov, and J. Garcia-Ojalvo, "Multistability and Clustering in a Population of Synthetic Genetic Oscillators via Phase-Repulsive Cell-to-Cell Communication", Phys. Rev. Lett. 99, 148103 (2007).

• A. Koseska, E. Volkov, A. Zaikin, and J. Kurths, "Quantized time production cycling time in artificial gene networks induced induced by noise and intercell communication", Phys. Rev E 76, 020901 (2007), also in the September 1, 2007 issue of Virtual Journal of Biological Physics Research.

• A. Koseska, A. Zaikin, J. Liepe, and J. Kurths, "Variety of dynamical regimes in a population of coupled synthetic genetic oscillators", Proceedings of the 3rd International conference "Physics and Control", IPACS electronic library, http://lib.physcon.ru/?item=1376, (2007).

PRACE (Partnership for Advanced Computing in Europe)

In 2007, BSC-CNS participated in the PRACE project proposal which was written and presented under the call INFRA-2007-2.2.2.1 - Preparatory phase for 'Computer and Data Treatment' research infrastructures in the 2006 ESFRI Roadmap. This call was issued under the Research Infrastructures section of the Capacities category of The European Community's Seventh Framework Programme on research and development. The proposal deadline was May 2, 2007 and the two-year project was approved for financing with a planned start date in January 2008.

The proposal built on work done during the HET (High Performance Computing in Europe Taskforce) project, and presented a comprehensive plan for bringing the European High Performance Computing service to technical, legal and financial maturity. The ambitious project aims to prepare the ground for the emergence of a new HPC research infrastructure at European level in 2010.

National Activities

In 2007 BSC-CNS also participated in a significant number of national and regional calls. It was actively involved in several R&D projects funded by the Spanish National plan, received grants from the Spanish Ministry of Science and Education (MEC), BSC-CNS also received from this Ministry matching funds to participate as a partner in European projects and grants from Spanish Ministry of Environment (MMA). The grants are distributed between the different departments as follow:

The Earth Science department also coordinates a Spanish Ministry of Environment (MMA) grant called CALIOPE whose main objective is the development of an operational air quality modeling system for Spain that provides a very high resolution air quality forecasting service for the Iberian Peninsula, Balearic and Canary Islands with nesting in urban areas.

The Earth Science Department is involved in two R&D projects funded by the Spanish National Plan called:

1) Improvement of the Dust Regional Atmospheric Model (DREAM) for prediction of Saharan dust events in the Mediterranean and the Canary Islands.

2) High-resolution modeling of air pollution by anthropogenic and natural particulate matter in the Iberian Peninsula.

The Computer Science Department received grants from the Spanish Ministry of Science and Education (MEC) to improve its infrastructure with respect to: 1) increased storage capacity, 2) fire protection and 3) expansion of the Spanish Supercomputing Network plan.

Since October 2007 BSC-CNS is coordinating a Consolider project called “Supercomputación y eCiencia” which will consolidate the research know-how of 21 Spanish research groups. The project offers a national framework for research groups in supercomputing applications to collaborate together with expert hardware/software machine designers in order to design and use these machines efficiently in the near future. All BSC-CNS departments are involved in this project which aims to exploit synergies between different scientific areas.

2007 National Activity

Spanish Ministry of Science and Education	Active projects	Proposals submitted
Coordination of the Spanish eSciences groups (CONSOLIDER)	1	-
ICTS investments and mobility	1	1
FI FELLOWSHIPS	2	-
PI FELLOWSHIPS	1	-
FIE FELLOWSHIPS	3	-
RAMON Y CAJAL FELLOWSHIPS	1	-
Spanish Ministry of Environment	Amount of projects	
CALIOPE	1	1
Total	10	2

Since the start of 2007, BSC-CNS also participates to an indicative of the Spanish Ministry of Education and Science (MEC), in a national access program called ICTS, whose objective is to leverage the knowledge in supercomputing and eScience from BSC-CNS. This program allowed 25 researchers to access the BSC-CNS facilities in 2007; their expenses were covered by the Spanish Ministry of Science and Education. Selection meetings are held every four months.

The following researchers obtained fellowships in 2007:

Fellowship type	Name
PI Fellowship	Marco Paolieri
FIE Fellowship	Vladimir Gajinov, Margaride Maragues, Antonio Quesada
FPI Fellowship	Karsten Haustern, Maria Teresa
Ramón y Cajal Fellowship	Arnau Folch
CICYT Fellowship	Carlos Pérez, Pedro Jiménez

The following researchers joined the ICTS program in 2007:

Researcher	University	Total Researcher per University
Ismael Marín Carrión Francisco J. Tapiador	Universidad de Castilla-La Mancha	2
Gustavo Yepes Alonso Luis Alberto Martínez Vaquero Matthias Hoeft Raúl Sevilla González Arman Khalatyan	Universidad Autónoma de Madrid	5
Romain Teyssier	CEA Saclay (France)	1
Horacio Emilio Pérez Sánchez	Forschungszentrum Karlsruhe (Germany)	1
Santiago Cuesta Lopez	Universidad de Zaragoza	1
Juan Salvador Ardid Ramírez David Gómez-Cabrero López		
Nicolau Sunyer Ferrer	Universitat de Girona	1
Ricardo Perez Tudela Estela Carmona Novillo		
Antonio Gordillo Guerrero Sergio Perez Gaviro	Universidad Complutense de Madrid	2
Reyes Malavé Osuna	Universidad de Málaga	1
Amaia Saracibar Ruiz de Ocenda	Universidad del País Vasco	1
Joan Salvador Ardid Ramírez	Universitat de Barcelona	1
Andreas Giotis	National Center for Scientific Research	1
Hugo Gutiérrez de Terán	Universidad de Santiago de Compostela	1
	TOTAL	21

Technology Transfer

In 2007, BSC-CNS continued collaborating in many of the technology transfer projects that had started in 2005 and 2006. It also began work on new projects with industry partners such as IBM, Microsoft, and Repsol.

In 2007, I3@BSC conducted basic research in the areas of high performance computing and associated computer architectures, including proof of concept testing for system level and applications software on a large scale cluster system such as MareNostrum.

BSC-CNS also started a project with Gas Natural to study the impact on the air quality of the cities of Barcelona and Madrid that the introduction of natural gas-powered vehicles has.

BSC-CNS started working with Airbus to improve its eLSA code (fluid dynamics) which was initially developed by ONERA in France and is currently used worldwide by Airbus.

The design of the next generation chip multiprocessor will clearly affect how computers work ten years from now and beyond. BSC-CNS continues to work with Microsoft to explore potential chip designs for general purpose and the personal mass computer market. At this time, the project focuses primarily on architectural ideas, with an understanding of the importance of total system integration with software.

The BSC-CNS started work on the Kaleidoscope Project with Repsol YPF. The focus of this project is to optimize and execute in MareNostrum, as well as in cell processors, the Reverse Time Migration (RTM) codes used in next generation seismic imaging technology. These codes are expected to accelerate and streamline oil and gas exploration by several orders of magnitude compared to current industry standards.

BSC-CNS continued its collaboration with Desafío Español Copa América 2007 to develop advanced software algorithms that improve the design of competition sailboats. In addition, the BSC-CNS will help to obtain a meteorological model based in a neuronal network that will allow a real-time forecasting.

SGS TECNOS S.L. The aim of this agreement was to perform an impact assessment on the air quality study of the from combined cycle power stations.

PB Power. The aim of this agreement was to perform the air quality modelling together with the collaboration of Siemens.

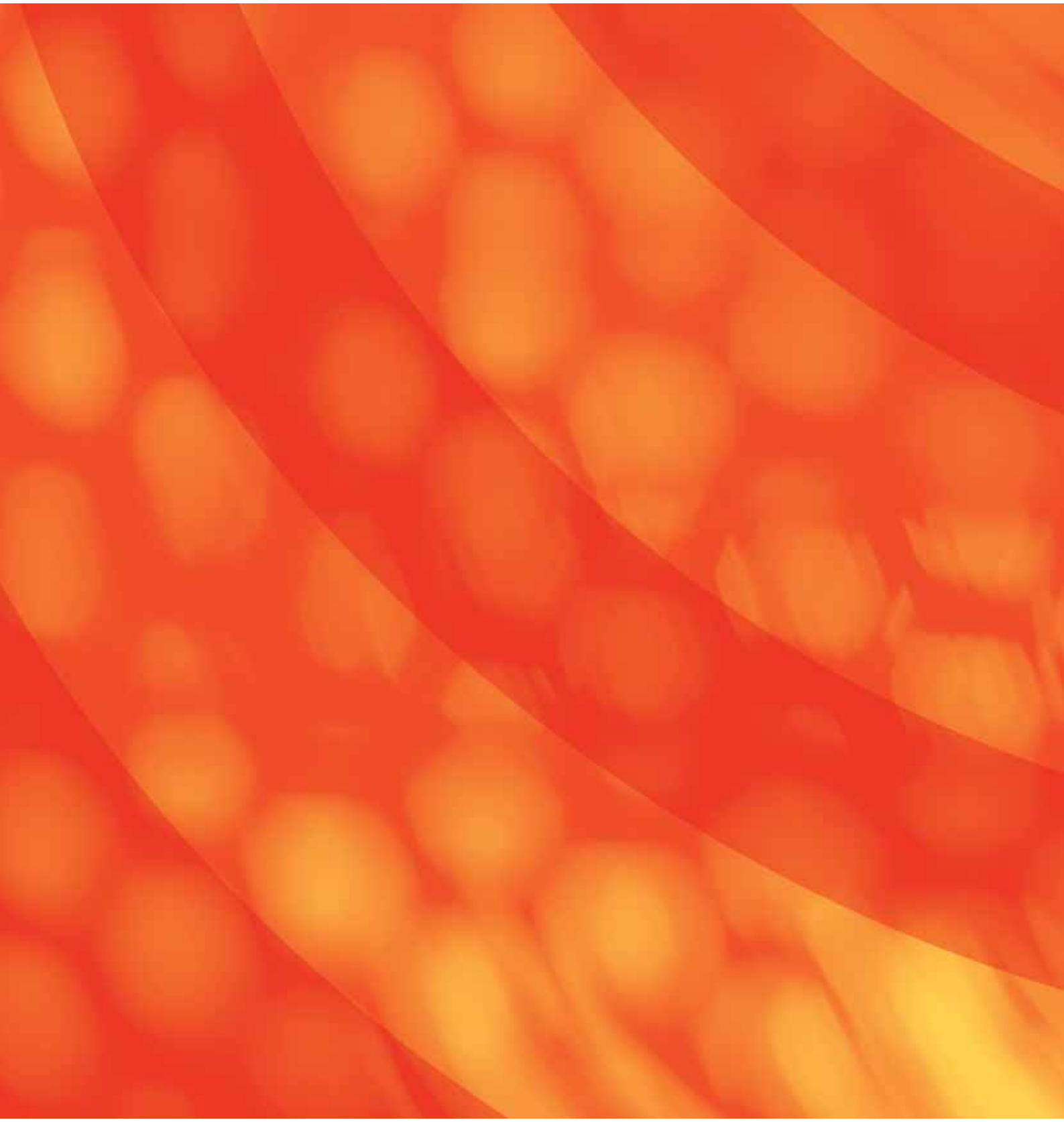
The aim of this agreement was to perform the air quality modelling together with the collaboration with Gas Natural.

BCNEcologia The aim of this agreement was to perform a simulation for the Air Quality Plan of Catalonia.

Memorandums of Understanding

During 2007 the BSC-CNS signed the following Memorandum of Understanding:

INM (Spanish National Meteorology Institute). The objective of this agreement was to implement, disseminate and validate the operational prediction of the North African dust transport in the Iberian Peninsula as well as to perform modeling, detection, follow-up and characterization studies of atmospheric material.



4 Research Results

Publications and communications

Journals and Book Chapters

- J. Piernas, T. Cortes, J. M. García. The Design of New Journaling File Systems: The DualFS Case. IEEE Transaction on Computers, Vol. 52, num. 2, February 2007.
- Miquel Moreto, Francisco J. Cazorla, Alex Ramirez, and Mateo Valero. Explaining Dynamic Cache Partitioning Speed Ups. In IEEE Computer Architecture Letters. Volume 6, Issue 1, March 2007.
- S. Reyes, C. Muñoz-Caro, A. Niño, R. M. Badia and J. M. Cela, "Performance of computation-intensive, parameter sweep applications on Internet-based Grids of computers. The mapping of molecular potential energy hypersurfaces", Concurrency and Computation: Practice and Experience, Vol. 19, No. 4, March 2007
- Ariel Goyeneche, Francesc Guim, Ivan Rodero, Gabor Terstyanszky and Julita Corbalan. Extracting performance hints for Grid Users using data mining techniques: a case study in the NGS. Mediterranean Journal of Computers and Networks. Special issue on on Data Mining Applications on Supercomputing and Grid Environment, vol. 3, no. 2, p. 52-61, April 2007.
- F. Guim, I. Rodero, J. Corbalán, J. Labarta. Portal de Acceso a Recursos HPC en Entornos Grid. Boletín RedIRIS, no. 80, April 2007.
- Raül Sirvent, Rosa M. Badia, Pieter Bellens, Vasilis Dialinos, Jesús Labarta and Josep M. Pérez. Demostración de uso de GRID superscalar. Boletín RedIRIS, no. 80, April 2007.
- Tim Harris, Adrian Cristal, Osman S. Unsal, Eduard Ayguade, Simon P. Jones, Fabrizio Gagliardi, Burton Smith and Mateo Valero. Transactional Memory: An Overview. IEEE Micro. Hot Tutorials Special Issue. Vol. 27, Issue 3. pp. 8-29. May/June 2007.
- Raül Sirvent, Josep M. Pérez, Rosa M. Badia, Jesus Labarta. Programación en el Grid: una aproximación basada en lenguajes imperativos. Computación Grid: del Middleware a las Aplicaciones, pp. 33-52, June 2007.
- Eduard Ayguade and Matthias Mueller. Guest Editors' Introduction to Special Issue on OpenMP (vol. 1). International Journal of Parallel Programming, Vol. 35, No. 4, pp. 331-333. August 2007.
- F. Guim, I. Rodero, J. Corbalan, J. Labarta, A. Oleksiak, J. Nabrzyski. Uniform Job Monitoring in the HPC-Europa Project: Data Model, API and Services. International Journal of Web and Grid Services, vol 3, n.3, August 2007.
- Josep M. Perez, Pieter Bellens, Rosa M. Badia and Jesus Labarta, "CellSs: Programming the Cell/B.E. made easier", IBM Journal of R&D, Volume 51, Number 5, August 2007.
- Eduard Ayguade and Matthias Mueller. Guest Editors' Introduction to Special Issue on OpenMP (vol. 2). International Journal of Parallel Programming, Vol. 35, No. 5, October 2007.
- K. Kurowski, A. Oleksiak, J. Nabrzyski, A. Kwiecien, M. Wojtkiewicz, M. Dyvzkowski, F. Guim, J. Corbalan, J. Labarta. Multi-criteria Grid Resource Management using Performance Prediction Techniques. Integrated Research in GRID Computing, Pages 215-225, November 2007.
- Raül Sirvent, Josep M. Pérez, Rosa M. Badia, Róbert Lovas, Gergely Sipos and Péter Kacsuk. GRID superscalar enabled P-GRADE portal. Integrated Research in GRID Computing, pages 241-254 , November 2007.
- Alberto Sánchez, María S. Pérez, Pierre Gueant, Jesús Montes, Pilar Herrero and Toni Cortes. Improving GridFTP transfers by means of a multiagent parallel file system. Multiagent and Grid Systems - An International Journal, Vol 3, No. 4. December 2007.
- D. Carrera, V. Beltran, J. Torres and E. Ayguadé. "A Hybrid Connector for Efficient Web Servers", Special Issue on High Performance Computing in Parallel and Distributed Systems of International Journal of High Performance Computing and Networking (IJHPCN). Issue 5/6 of 2007, Vol. 5. ISSN (Print): 1740-0562.

- J. Guitart, D. Carrera, V. Beltran, J. Torres, E. Ayguadé. "Designing an Overload Control Strategy for Secure e-Commerce Applications", Journal Computer Networks, Elsevier. 2007;51(15):4492-510.
- Nehir Sonmez, Christian Perfumo, Srdjan Stipic, Adrian Cristal, Osman S. Unsal, Mateo Valero, "Increasing the Performance of Haskell Software Transactional Memory", Trends in Functional Programming, Volume 8.
- Koen de Bosschere, Wayne Luk, Xavier Martorell, Nacho Navarro, Mike O'Boyle, Dionisios Pnevmatikatos, Alex Ramirez, Pascal Saintrat, Andre Seznec, Per Stenstrom, Olivier Temam. High Performance Embedded Architectures and Compilation Roadmap. Transactions on HiPEAC Vol 1, Lecture Notes in Computer Science 4050, pg. 5-29. Jan 2007.
- Oliverio J. Santana, Alex Ramirez and Mateo Valero. Enlarging Instruction Streams. IEEE Transactions on Computers, vol. 56(10), pg. 1342-1357. Oct 2007.

International Conferences and Symposiums

- J. Alonso, J. Guitart and J. Torres. "Differentiated Quality of Service for e-Commerce Applications through Connection Scheduling based on System-Level Thread Priorities". 15th Euromicro Conference on Parallel, Distributed and Network-based Processing (PDP'07) Naples, Italy, February 7-9, 2007.
- R. Nou, F. Julià, D. Carrera, K. Hogan, J. Labarta, J. Torres. "Monitoring and Analysis Framework for Grid Middlewares". 15th Euromicro Conference on Parallel, Distributed and Network-based Processing (PDP'07) Naples , Italy , February 7-9, 2007, February 2007.
- R. Nou, F. Julià and J. Torres. "Should the grid middleware look to self-managing capabilities?". The 8th International Symposium on Autonomous Decentralized Systems (ISADS 2007). IEEE and IFIP. Sedona, Arizona, USA. March 2007.
- Mauricio Alvarez, Esther Salami, Alex Ramirez and Mateo Valero. "Performance Impact of Unaligned Memory Operations in SIMD Extensions for Video CODEC Applications". IEEE International Symposium on Performance Analysis of Systems and Software (ISPASS 2007), San Jose, California, pp. 62-71, April 2007.
- Daniel Jimenez Gonzalez, Xavier Martorell and Alex Ramirez. "Performance Analysis of Cell Broadband Engine for High Memory Bandwidth Applications". IEEE International Symposium on Performance Analysis of Systems and Software (ISPASS 2007), San Jose, California, pp. 210-219, April 2007.
- Cristian Perfumo, Nehir Sonmez, Srdjan Stipic, Osman S. Unsal, Adrian Cristal, Mateo Valero, "UnreadTVar: Extending Haskell Software Transactional Memory for Performance", The Eighth Symposium on Trends in Functional Programming, April 2007.
- Eugenio Cesario, Toni Cortes, Erich Focht, Matthias Hess, Felix Hupfeld, Björn Kolbeck, Jesús Malo, Jonathan Martí and Jan Stender. XtreemFS - an object-based file system for large-scale federated IT infrastructures. LinuxTAG 2007, Berlin, Germany, , May 2007.
- M. Steinder, I. Whalley, D. Carrera, I. Gaweda and D. Chess. "Server virtualization in autonomic management of heterogeneous workloads". In 10th IFIP/IEEE International Symposium on Integrated Management (IM 2007), May 21-25, 2007
- N.Poggi, T. Moreno, J. Berral, R. Gavalda, J. Torres. "Web Customer Modeling for Automated Session Prioritization on High Traffic Sites". Proceedings of the 11th International Conference on User Modeling. Corfu, Greece, June 25-29, 2007.
- Francisco J. Cazorla, Peter M.W. Knijnenburg, Rizos Sakellariou, Enrique Fernandez, Alex Ramirez and Mateo Valero. On the Problem of Minimizing Workload Execution Time in SMT Processors. In IEEE International Conference on Embedded Computer Systems: Architectures, Modeling, and Simulation (IC-SAMOS), Samos, Greece. July 16-19, 2007.

- Seyed Masoud Sadjadi, J. Martínez, T. Soldo, L. Atencio, Rosa M. Badia, J. Ejarque. Improving Separation of Concerns in the Development of Scientific Applications. International Conference on Software Engineering and Knowledge Engineering, July 2007.
- Miquel Moreto, Francisco J. Cazorla, Alex Ramirez, and Mateo Valero. Online Prediction of Applications Cache Utility. In IEEE International Conference on Embedded Computer Systems: Architectures, Modeling, and Simulation (IC-SAMOS), Samos, Greece. July 16-19, 2007.
- R. Nou, F. Julià, J. Guitart, J. Torres. "Dynamic Resource Provisioning for Self-Adaptive Heterogeneous Workloads in SMP Hosting Platforms". ICE-B 2007, the International Conference on E-business. (IEEE Systems and ACM SIGMIS) Barcelona, Spain. July 2007.
- L. Silva, J. Alonso, P. Silva, J. Torres and A. Andrzejak. "Using Virtualization to Improve Software Rejuvenation". The 6th IEEE International Symposium on Network Computing and ApplicationS (NCA 2007). Boston. July, 12- 14, 2007. Best Paper award on Applications.
- Paul Carpenter, David Rodenas, Xavier Martorell, Alex Ramirez and Eduard Ayguade, "A Streaming Machine Description and Programming Model", SAMOS VII: International Symposium on Systems, Architectures, Modeling and Simulation, Embedded Computer Systems: Architectures, Modeling, and Simulation. Lecture Notes in Computer Science, Volume 4599/2007, pp. 107-116, ISBN 978-3-540-73622-6, Springer Berlin / Heidelberg, August 2007.
- Marc Casas-Guix, Rosa M. Badia, Jesus Labarta, "Automatic structure extraction from MPI applications tracefiles", in proc. of Euro-Par 2007, August 2007.
- J. Martí, J. Malo, T. Cortes. Increasing Parallelism for Workflows in the Grid. Europar 2007, Rennes, France, August 2007.
- J. Alonso, L. Silva, A. Andrzejak, P. Silva and J. Torres "High-Availability Grid Services through the use of Virtualized Clustering". The 8th IEEE/ACM International Conference on Grid Computing (GRID 2007), Austin, Texas, USA. (63-13), September 19-21, 2007
- Marc Casas-Guix, Rosa M. Badia, Jesus Labarta, "Automatic phase detection of MPI applications", Parallel Computing 2007, September 2007.
- Pilar González-Férez, Juan Piernas, and Toni Cortes. The RAM Enhanced Disk Cache Project (REDCAP). 24th IEEE Conference on Mass Storage Systems and Technologies (MSST07), San Diego, California, USA, September 2007.
- Miquel Moreto, Francisco J. Cazorla, Alex Ramirez,nd Mateo Valero. MLP-aware dynamic cache partitioning. In Parallel Architectures and Compilation Techniques (PACT). Brasov, Romania. September 15-19, 2007.
- Miquel Pericas, Ruben Gonzalez, Adrian Cristal, Francisco J. Cazorla, Daniel A. Jimenez and Mateo Valero. A Flexible Heterogeneous Multi-Core Architecture. In Parallel Architectures and Compilation Techniques (PACT). Brasov, Romania. September 15-19, 2007.
- Ivan Rodero, Francesc Guim, Julita Corbalan, Jesus Labarta. Design and Implementation of a General-Purpose API of Progress and Performance Indicators. Parallel Computing 2007, September 2007.
- Alberto Sánchez, Toni Cortes, Jesús Montes, Pierre Gueant and María S. Pérez. Lessons learnt from cluster computing: How they can be applied to grid environments. The 8th Hellenic European Research on Computer Mathematics & its Applications Conference, Athens Greece, September 2007.
- Javier Vera, Francisco J. Cazorla, Alex Pajuelo, Oliveiro J. Santana, Enrique Fernandez and Mateo Valero. FAME: FAirly MEasuring Multithreaded Architectures. In Parallel Architectures and Compilation Techniques (PACT). Brasov, Romania. September 15-19, 2007.
- Eduard Ayguade, Alejandro Duran, Jay Hoeflinger, Federico Massaioli, Xavier Teruel. "An Experimental Evaluation of the New OpenMP Tasking Model". In Proceedings of the 20th International Workshop on Languages and Compilers for Parallel Computing (LCPC2007), Urbana (IL), USA, October 2007.

- Jairo Balart, Marc Gonzalez, Xavier Martorell, Eduard Ayguade, Zehra Sura, Tong Chen, Tao Zhang, Kevin O'Brien and Kathryn O'Brien. "A Novel Asynchronous Software Cache Implementation for the Cell-BE Processor". In Proceedings of the 20th International Workshop on Languages and Compilers for Parallel Computing (LCPC2007). Urbana (IL), USA. October 2007.
- F. Guim, Julita Corbalan, Jesus Labarta. Modeling the impact of resource sharing in Backfilling Policies using the Alvio Simulator. 5th Annual Meeting of the IEEE International Symposium on Modeling, Analysis, and Simulation of Computer and Telecommunication System, October 2007.
- S. Kounev, R. Nou and J. Torres. "Autonomic QoS-Aware Resource Management in Grid Computing using Online Performance Models" 2nd International Conference on Performance Evaluation Methodologies and Tools (VALUETOOLS 2007) Nantes, France, October 23th-25th, 2007. ISBN: 978-1-59593-819-0
- T. Püschel, N. Borissov, D. Neumann, M. Macías, J. Guitart, J. Torres, J. Stößer "Extended Resource management using client classification and economic enhancements". eChallenges e-2007 Conference & Exhibition. October 2007, The Hague, The Netherlands. 2007.
- J.L. Gonzalez and Toni Cortes. An Adaptive Data Block Placement based on Deterministic Zones (AdaptiveZ). International Conference on Grid computing, high-performAnce and Distributed Applications (GADA'07), Vilamoura, Algarve, Portugal, November 2007.
- F. Guim, J. Corbalan, J. Labarta. Prediction of based Models for Evaluating Backfilling Scheduling Policies. 8th International Conference on Parallel and Distributed Computing, Applications and Technologies, December 2007.
- T. Puschel, N. Borissov, M. Macias, D. Neumann, J. Guitart, J. Torres "Economically Enhanced Resource Management for Internet Service Utilities", The 8th International Conference on Web Information Systems Engineering, WISE2007, Nancy, France. 3-7th December, 2007.
- Mauricio Alvarez, Esther Salami, Alex Ramirez, Mateo Valero. HD-VideoBench. A Benchmark for Evaluating High Definition Digital Video Applications. 2007 IEEE International Symposium on Workload Characterization (IISWC-2007). Boston, MA. Sep 2007.

Workshops

- A. Ramírez, O. Prat, J. Labarta and M. Valero. Performance Impact of the Interconnection Network on MareNostrum Applications. HiPEAC Workshop on Interconnection Network Architectures: On-Chip, Multi-Chip, Ghent, Belgium, in conjunction with the HiPEAC'07 Conference, January 2007.
- Javier Vera, Francisco J. Cazorla, Alex Pajuelo, Oliverio J. Santana, Enrique Fernandez, and Mateo Valero. Measuring the Performance of Multithreaded Processors. In SPEC Benchmark Workshop (in conjunction with the Annual Meeting of the Standard Performance Evaluation Corporation (SPEC)), Austin, USA. January 2007. Schaeffer Award to the technical quality of the paper.
- Carmelo Acosta, Francisco J. Cazorla, Alex Ramirez, and Mateo Valero. Core to Memory Interconexion Implications for Forthcomming On-Chip Multiprocessors. In Workshop on Chip Multiprocessor Memory Systems and Interconnects (in conjunction with the 13th Annual International Conference on High-Performance Architecture Phoenix, USA. February 2007.
- Milos Milovanovic, Osman S. Unsal, Adrian Cristal, Srdan Stipic, Ferad Zyulkyarov, Mateo Valero, "Compile Time Support for Using Transactional Memory in C/C++ Applications," 11th Annual Workshop on the Interaction between Compilers and Computer Architecture INTERACT, February 2007
- R. Nou, F. Julià and J. Torres. "The need for self-managed access nodes in grid environments". 4th Annual IEEE International workshop on Engineering of Autonomic and Autonomous Systems (EASe 2007). Tucson, Arizona, USA. March 26th-29th, 2007.

- Alejandro Rico, Felipe Cabarcas, David Rodenas, Xavier Martorell, Alex Ramirez, Eduard Ayguade, Implementation and validation of a Cell Simulator using UNISIM. 3rd HiPEAC Industrial Workshop. Haifa, Israel, April 2007.
- Toni Moreno, Nicolas Poggi, Josep Lluis Berral, Ricard Gavaldà, Jordi Torres. Policy-based autonomous bidding for overload management in eCommerce websites. Group Decision and Negotiation Meeting - GDN Section of INFORMS. Montreal, Canada, May 14-17, 2007.
- Ani Anciaux-Sedrakian, Rosa M. Badia, Raul Sirvent, Josep M. Perez, Thilo Kielmann, Andre Merzk. Grid Superscalar and Job Mapping on the Reliable Grid Resources. CoreGRID Workshop on Grid Programming Model Grid and P2P Systems Architecture Grid Systems, Tools and Environments, June 2007.
- J. Alonso, J. Torres and L. Silva. "Carrying the Crash-only software concept to the legacy application servers". CoreGRID Workshop on Grid Programming Model Grid and P2P Systems Architecture Grid Systems, Tools and Environments. June 12-13, 2007. Heraklion, Crete, Greece.
- Eduard Ayguade, Nawal Copty, Alejandro Duran, Jay Hoeflinger, Yuan Lin, Federico Massaioli, Ernesto Su, Priya Unnikrishnan, Guansong Zhang. "A Proposal for Task Parallelism in OpenMP". In Proceedings of the 3rd International Workshop on OpenMP (IWOMP). Beijing, China, June 2007.
- Francesc Guim, Julita Corbalan. A Job Self-Scheduling Policy for HPC Infrastructures. 13th Workshop on Job Scheduling Strategies for Parallel Processing (In Conjunction with ICS 2007), June 2007.
- Francesc Guim, Ivan Rodero, Julita Corbalan, A.Goyeneche. The Grid Backfilling: a Multi-Site Scheduling Architecture with Data Mining Prediction Techniques. CoreGRID Workshop in Grid Middleware 2007, June 2007.
- Francesc Guim, Ivan Rodero, Julita Corbalan, Jesus Labarta. Towards Uniform and Transparent Access to the Grid Universe Information Using the Palantir. CoreGRID Workshop in Grid Middleware 2007, June 2007.
- Milos Milovanovic, Roger Ferrer, Osman S. Unsal, Adrian Cristal, Eduard Ayguade, Jesus Labarta, Mateo Valero, "Transactional Memory and OpenMP," International Workshop on OpenMP, June 2007
- I. Rodero, F. Guim, J. Corbalan, L.L. Fong, Y.G. Liu, S.M. Sadjadi. Looking for an Evolution of Grid Scheduling: Meta-brokering. CoreGRID Workshop in Grid Middleware 2007, June 2007.
- Enric Tejedor, Rosa M. Badia, Thilo Kielmann, Vladimir Getov. A Component-Based Integrated Toolkit. CoreGRID Workshop on Grid Programming Model, Grid and P2P Systems Architecture, Grid Systems, Tools and Environments, June 2007.
- Javier Bueno, Jordi Vaquero, Juan Jose Costa, Toni Cortes, Xavier Martorell, Eduard Ayguade, "NanosDSM: a Software Distributed Shared Memory System for OpenMP", ACACES 2007 poster session. L´Aquila, Italy, pp. 153-156, July 2007.
- Felipe Cabarcas, Alejandro Rico, David Rodenas, Xavier Martorell, Alex Ramirez, Eduard Ayguade, "CellSim: A Cell Processor Simulation Infrastructure". ACACES 2007 poster session. L´Aquila, Italy, pp. 279-282, July 2007.
- Roger Ferrer, Marc Gonzalez, Xavier Martorell, Eduard Ayguade, "Mercurium C and C++ source to source compiler". ACACES 2007 poster session. L´Aquila, Italy, pp. 239-242, July 2007.
- Xavier Teruel, Xavier Martorell, Alejandro Duran, Roger Ferrer, Eduard Ayguade, "Extending Nanos RTL for OpenMP Task Support", ACACES 2007 poster session. L´Aquila, Italy, pp. 157-160, July 2007.
- Jordi Vaquero, Marc Gonzalez, Juanjo Costa, Javier Bueno, Xavier Martorell, Toni Cortes, Eduard Ayguade, "Improving Data Locality in NAS BT Benchmark", ACACES 2007 poster session. L´Aquila, Italy, pp. 199-202, July 2007.
- J.Alonso, J. Torres, L.Silva and P.Silva. "Dependable Grid Services: A case study with OGSA-DAI". CoreGrid Symposium 2007. IRISA, Rennes, France. August 27-28, 2007.

- Tim Harris, Srdjan Stipic, "Abstract Nested Transactions", Second ACM SIGPLAN Workshop on Transactional Computing TRANSACT, August 2007
- Cristian Perfumo, Nehir Sonmez, Osman S. Unsal, Adrian Cristal, Mateo Valero, Tim Harris, "Dissecting Transactional Executions in Haskell", Second ACM SIGPLAN Workshop on Transactional Computing TRANSACT, August 2007
- Sasa Tomic, Adrian Cristal, Osman Unsal, Mateo Valero, "Hardware Transactional Memory with Operating System Support, HTMOS", Workshop on Highly Parallel Processing on a Chip in conjunction with Euro-Par, August 2007
- V. Beltran, J. Torres and E. Ayguade "Improving Disk Bandwidth-Bound Applications Through Main Memory Compression" MEDEA Workshop MEmory performance: DEaling with Applications, systems and architecture. Brasov, Romania. Held in conjunction with PACT 2007 Conference Sept. 15-19 2007
- Felix Hupfeld, Toni Cortes, Björn Kolbeck, Erich Focht, Matthias Hess, Jesus Malo, Jonathan Marti, Jan Stender, Eugenio Cesario. XtreemFS: a case for object-based storage in Grid data management. 3rd VLDB Workshop on Data Management in Grids, Vienna, Austria, Sept. 2007.
- M.Macías, G.Smith, O.F.Rana, J.Guitart, J.Torres "Enforcing Service Level Agreements using an Economically Enhanced Resource Manager", Workshop on Economic Models and Algorithms for Grid Systems 2007. Austin, Texas, USA. September 2007.
- Milos Milovanovic, Roger Ferrer, Vladimir Gajinov, Osman S. Unsal, Adrian Cristal, Eduard Ayguadé and Mateo Valero. Multithreaded Software Transactional Memory and OpenMP. MEDEA 2007: MEmory performance Workshop: DEaling with Applications, systems and architecture. In conjunction with Parallel Architectures and Compilation Techniques (PACT-2007). Brasov, Rumania. September 2007.
- R. Nou, S. Kounev, J. Torres. "Building Online Performance Models of Grid Middleware with Fine-Grained Load-Balancing: A Globus Toolkit Case Study" 4th European Engineering Performance Workshop. 27-28 September 2007, Berlin, Germany.
- Ferad Zyulkyarov, Osman S Unsal, Adrian Cristal, Milos Milovanovic, Eduard Ayguade and Mateo Valero. Memory Management for Transaction Processing Core in Heterogeneous Chip-Multiprocessors. OSHMA 2007: Workshop on Operating System support for Heterogeneous Multicore Architectures. In conjunction with Parallel Architectures and Compilation Techniques (PACT-2007). Brasov, Rumania. September 2007.
- Xavier Teruel, Xavier Martorell, Alejandro Duran, Roger Ferrer, Eduard Ayguade, "Support for OpenMP Tasks in Nanos v4", In Proceedings of CASCON 2007, Toronto, Canada, October 2007 (short paper).
- N. Poggi, J.L. Berral, T. Moreno, R. Gavaldà, J. Torres. "Automatic Detection and Banning of Content Stealing Bots for E-commerce". NIPS 2007 Workshop on Machine Learning in Adversarial Environments for Computer Security. British Columbia, Canada. December 8, 2007.
- Rosa M. Badia, Raul Sirvent, Marian Bubak, Wlodzimierz Funika, Piotr Machner, " Performance Monitoring of Grid Superscalar with OCM-G/G-PM: Tuning and Improvements", CoreGRID Workshop on Grid Programming Model Grid and P2P Systems Architecture Grid Systems, Tools and Environments, 2007
- Milo_ Milovanovic, Roger Ferrer, Osman Unsal, Adrian Cristal, Eduard Ayguade, Jesus Labarta, Mateo Valero. "Transactional Memory and OpenMP". In Third International Summer School on Advanced Computer Architecture and Compilation for Embedded Systems (Hipeac - Acaces 2007)
- Christian Perfumo, Nehir Sonmez, Adrian Cristal, Osman S. Unsal and Mateo Valero. "Development and Analysis of a Haskell Transactional Benchmark Suite". In Third International Summer School on Advanced Computer Architecture and Compilation for Embedded Systems (Hipeac - Acaces 2007)

- Sutirtha Sanyal, Sasa Tomic, Adrian Cristal, Osman S. Unsal, Mateo Valero. "Challenges of implementing a TCC like Hardware Transactional Memory in a Full System Simulator". In Third International Summer School on Advanced Computer Architecture and Compilation for Embedded Systems (Hipeac - Acaces 2007)
- Ferad Zyulkyarov, Osman S. Unsal, Adrian Cristal, Mateo Valero. "Synthetic Workload for Transactional Memory". In Third International Summer School on Advanced Computer Architecture and Compilation for Embedded Systems (Hipeac - Acaces 2007)

National Conferences

- Rosa M. Badia, Pieter Bellens, Marc de Palol, Jorge Ejarque, Jesús Labarta, Josep M. Pérez, Raül Sirvent and Enric Tejedor. GRID superscalar: from the Grid to the Cell processor. Spanish Conference on e-Science Grid Computing. Madrid (Spain), , March 2007.
- R. M. Badia, P. Bellens, J. Ejarque, J. Labarta, M. de Palol, J. M. Pérez, R. Sirvent and E. Tejedor. SSH GRID superscalar: a Tailored Version for Cluster. 1st Iberian Grid Infrastructure Conference (IBERGRID). Santiago de Compostela (Spain), May 2007.
- S. Reyes, A. Niño, C. Muñoz-Caro, R. Sirvent and R. M. Badia. Monitoring Large Sets of Jobs in Internet-Based Grids of Computers. 1st Iberian Grid Infrastructure Conference (IBERGRID). Santiago de Compostela (Spain), , May 2007.
- Jesús Malo, Jonathan Martí, Toni Cortes. Replica management in GRID superscalar. Jornas Paralelismo, Zaragoza, September 2007.
- Milos Milovanovic, Osman Unsal, Adrian Cristal, Ferad Zyulkyarov, Srdjan Stipic, Mateo Valero, "Extending the C/C++ Language with Atomic Construct". XVI Jornadas de Paralelismo Conference, September 2007.
- Nehir Sonmez, Christian Perfumo, Srdjan Stipic, Adrian Cristal, Osman S. Unsal, Mateo Valero, "Increasing the Performance of Haskell Software Transactional Memory", XVI Jornadas de Paralelismo Conference, September 2007.
- Jesus Alastruey, Teresa Monreal, Francisco J. Cazorla, Victor Viñals y Mateo Valero, "Seleccción del Banco de Registros y de la Política de Asignación de Registros en Procesadores SMT", II Congreso Español de Informática, XVIII Jornadas de Paralelismo, Proceeding, Zaragoza, Septiembre 2007.
- Javier Vera, Francisco J. Cazorla, Alex Pajuelo, Oliveiro J. Santana, Enrique Fernandez y Mateo Valero. "A New Proposal to Evaluate Multithreaded Processors", Congreso: II Congreso Español de Informática, XVIII Jornadas de Paralelismo, Zaragoza, Septiembre 2007.
- Miquel Moreto, Francisco J. Cazorla, Alex Ramirez y Mateo Valero. "Online Prediction Throughput for Different Caches Sizes", II Congreso Español de Informática, XVIII Jornadas de Paralelismo, Zaragoza, Septiembre 2007.

Communications

- Osman Unsal, Adrian Cristal, Eduard Ayguade, Mateo Valero. "Top-Down Chip Multiprocessor Design". Microsoft Technical Computing Multi-Core Institute Internal Presentation, March 2007
- Rosa M. Badia. Platform Unaware Programing Models. DPA Workshop, Edinburgh, May 2007.
- Raül Sirvent. GRID superscalar y sus nuevas características de tolerancia a fallos. Escuela de Verano en Computación Grid: del Middleware a las Aplicaciones. Albacete, June 2007.
- A. Brinkmann and T. Cortes. Handling Heterogeneous Storage Devices in Clusters. IEEE Conference on Cluster Computing (Cluster 2007), Austin, Texas (Tutorial), September 2007.

- Felipe Cabarcas, Alejandro Rico, David Rodenas, Alex Ramirez. CellSim: a Modular Simulator for Heterogeneous Chip Multiprocessors. Tutorial at PACT (Parallel Architectures and Compilation Techniques), Brasov, Romania, September 15, 2007.
- Josep M. Perez, Modelos de Progamacion para Cell BE. I Olimpiada Informática Universitaria CELL + Linux, Universidad Internacional Menendez Pelayo, Santander, September 2007.
- Raul Sirvent. GRID superscalar. Curso de Postgrado CSIC de Grids y e-Ciencia. Santander, September 2007.
- Xavier Martorell. "Easying Program Transformations with the Nanos Mercurium C/C++ Compiler". Workshop on Challenges for Parallel Computing, in the context of the CASCON conference, organized by IBM Canada in Toronto, October 2007.
- D. Carrera. "Utility-based management of heterogeneous workloads with fairness goals". Invited talk in Adaptive systems Workshop. CASCON 2007.

Journals, books and book chapters

- J.M. Baldasano, J. Plana, M. Gonçalves, P. Jiménez, O. Jorba y E. López, Mejora de la Calidad del aire por cambio de combustible a gas natural en automoción. Aplicación a Madrid y Barcelona, Editor: Fundación Gas Natural (9/2007) ISBN 978-84-611-8540-5
- Baldasano J.M. El protocolo de Kioto, deu anys després. Theknos. Revista del Col.legi d'Enginyers Tècnics Industrials de Barcelona. Novembre 2007, 114: 24-30 [ISBN 1137-0017]
- Baldasano J.M., Evidencias del Cambio Climático (Cap. nº 3). Cambio Climático y sus Consecuencias. Editor Generalitat Valenciana: 43-56 [ISBN 978-84-482-4771-3] (2007)
- Baldasano J.M., Una visión sistemica global del futuro del mundo en que vivimos. ¿Deterioros irreversibles?. La difícil supervivencia de la especie humana. Ecología y Globalización. Editor Ramón Tamames. Ediciones 2010: 69-81. [ISBN 978-84-95058-67-7] (2007)
- Frontoso, M.G; Spinelli, N.; Pérez, C.; Sicard, M.; Comeron, A.; Baldasano, J.M. The vertical distribution of Saharan dust over the western and central Mediterranean through dust modelling and lidar observations. Geoscience and Remote Sensing Symposium, 2007. IGARSS 2007. IEEE International (1059-1062) ISBN: 978-1-4244-1212-9. Digital Object Identifier: 10.1109/IGARSS.2007.4422983 (2007)
- Güereca L.P., Agell N., Gassó S., Baldasano J.M., Fuzzy Approach to Life Cycle Impact Assessment: An Application for Biowaste Management Systems. International Journal of Life Cycle Assessment, DOI: http://dx.doi.org/10.1065/lca2006.10.276: 488-496 (2007)
- Jiménez P., O. Jorba and J.M. Baldasano (2007) Modeling the dynamics of air pollutants over the Iberian peninsula under typical meteorological situations. Air Pollution Modeling and its Application XVII. Editors: C. Borrego and E. Renner. Elsevier: 425-436.
- Jiménez P., Jorba, O., Parra, R., Pérez, C., Baldasano, J.M., Modeling Photochemical Pollution in the Northeastern Iberian Peninsula. Air Pollution Modeling and its Application XVII. Editors: C. Borrego and A-L. Norman. Springer, ISBN: 978-0-387-28255-8, 167-176 pp. (2007)
- Jiménez P., R. Parra and J.M. Baldasano, Influence of inicial and boundary conditions for ozone modeling in very complex terrains: a case study in the northeastern Iberian Peninsula. Environmental Modeling & Software 22: 1294-1306 (2007)
- Jiménez P., Parra, R., Gassó, S., Baldasano, J.M. Modeling the Weekend Effect in the Northeastern Iberian Peninsula. Air Pollution Modeling and its Application XVII. Editors: C. Borrego and A-L. Norman. Springer, ISBN: 978-0-387-28255-8, 177-186 pp. (2007)
- Kishcha P., P. Alpert, A. Shtivelman, S.O. Krichak, J.H. Joseph, G. Kallos, P. Katsafados, C. Spyrou, G.P. Gobbi, F. Barnaba, S. Nickovic, C. Perez, and J.M. Baldasano, Forecast errors in dust vertical distributions over Rome (Italy): multiple particle size representation and cloud contributions. Journal of Geophysical Research - Atmospheres, 112, D15205, doi: 10.1029/2006JD007427 (2007)
- Kishcha, P., Alpert, P., Shtivelman, A., Krichak, S.O., Joseph, J.H., Kallos, G., Katsafados, P., Spyrou, C., Gobbi, G.P., Barnaba, F., Nickovic, S., C. Pérez and J.M. Baldasano Forecast errors in dust vertical distributions over Rome. Air Pollution Modeling and its Application XVII. Editors: C. Borrego and E. Renner. Elsevier: 44-54. (2007)
- Papayannis A., H. Q. Zhang, V. Amiridis, H. B. Ju, G. Chourdakis, G. Georgoussis, C. Pérez, H. B. Chen, P. Goloub, R. E. Mamouri, S. Kazadzis, D. Paronis, G. Tsaknakis, and J. M. Baldasano, Extra-ordinary dust event over Beijing, China, during April 2006: lidar, sun photometric, satellite observations and model validation. Geophysical Research Letters (GRL), 34, L07806, doi:10.1029/2006GL029125 (2007)
- J.M. Baldasano, La Calidad del aire en la Comunitat Valenciana, Edición para la Comunitat Valenciana, Editor: Fundación GasNatural-Domenech e-learning multimedia S.A. (1/2007) - ISBN B-45261-2006

- Mattis I. et al., EARLINET correlative measurements for CALIPSO. Proc. of SPIE, vol. 6750, Lidar Technologies, Techniques and Measurements for Atmospheric Remote Sensing III, edited by U.N. Singh and G. Pappalardo: 67500Z-1-67500Z-12, doi: 10.1117/12.738090. (2007)
- Varios Autores, Calidad del aire en las ciudades. Clave de sostenibilidad urbana,. Ed. Observatorio de la Sostenibilidad en España, ISBN: 978-84-8476-323-9, 379 pp.

International Conferences and Symposiums

- Frontoso M., N. Spinelli, M. Sichard, A. Comerón, C. Pérez and J.M. Baldasano, Integrating regional model and lidar observations to derive a 2-years climatology of the vertical distribution of Saharan dust over the western and central Mediterranean. Earlinet-ASOS Workshop, Bilthoven (Netherlands), 28 February-2 March (2007)
- Gonçalves M., P. Jiménez-Guerrero and J.M. Baldasano, Assessing the effects of introducing natural gas vehicles on urban air quality. Case of Barcelona and Madrid cities (Spain). Models-3 Workshop: Recent Developments and Applications, Swindon (UK), 13th March (2007)
- Jiménez P., O. Jorba, C. Pérez, J. González and J.M. Baldasano, Sistema de pronóstico de la calidad del aire en el BSC-CNS. I Congreso Colombiano de Calidad del Aire y Salud Pública. Manizales (Colombia) 14-16 March (2007)
- Arevalo G., J.M. Baldasano y P. Jiménez, Inventario de Emisiones Atmosféricas en la Comunidad Valenciana (España) para uso en Modelos Fotoquímicos y de Material Particulado. I Congreso Colombiano de Calidad del Aire y Salud Pública. Manizales (Colombia) 14-16 March (2007)
- Baldasano et al, CALIOPE: An Operational Air Quality Forecasting System for the Iberian Peninsula, Balearic Islands and Canary Islands. WMO International Conference on: Secure and Sustainable Living: Social and Economic Benefits of Weather, Climate and Water Services, Madrid, 19-22 March (2007)
- Cuevas et al, WMO Sand and Dust Storm Warning System (SDS-WS) for Europe, Africa and Middle East: a GEO-oriented System. WMO International Conference on: Secure and Sustainable Living: Social and Economic Benefits of Weather, Climate and Water Services, Madrid, 19-22 March (2007)
- Jiménez-Guerrero, C. Pérez, O. Jorba y J.M. Baldasano, Influence of Saharan dust contribution on the particulate matter forecast in southern Europe. 6th International Conference on Urban Air Quality, Cyprus, 27-29 March (2007)
- Pérez, C., P. Jiménez, O. Jorba, J.M. Baldasano, E. Cuevas. S. Nickovic, and Querol, X., Long-term trends (1987-2006) of Saharan dust over the Mediterranean and the Canary Islands with the DREAM regional dust model. European Geosciences Union Conference, Viena, 18 April. (2007) Vol. 9, EGU2007-A-08525
- Jorba O., C. Marrero, E. Cuevas and J.M. Baldasano, Impact oh the Extratropical Store Delta over the Canary Islands on 28-30 November 2005: Severe Windstorm Event. European Geosciences Union Conference, Viena, 16-20 April (2007). Vol. 9, EGU2007-A-07608
- Jiménez P., C. Pérez O. Jorba and J.M. Baldasano, Annual Assessment of Levels and Composition of Anthropogenic and Natural Particulate Matter in Southern Europe. European Geosciences Union Conference, Viena, 16-20 April (2007) Vol. 9, EGU2007-A-06384
- Baldasano J.M., et al., CALIOPE: An Operational Air Quality Forecasting System for the Iberian Peninsula, Balearic Islands and Canary Islands. 15th World Meteorological Congress, Geneva (Switzerland), 7-25 May (2007)
- Cuevas, E. et al., WMO Sand and Dust Storm Warning System (SDS-WS) for Europe, Africa and Middle East: a GEO-oriented System. 15th World Meteorological Congress, Geneva (Switzerland), 7-25 May (2007)

- Jiménez P., O. Jorba, C. Pérez, S. Gassó and J. M. Baldasano, Enhancing High-Resolution Air Quality Forecasting in Marenostrum Supercomputer. 11th International Conference on Harmonisation within Atmospheric Dispersion Modelling for Regulatory Purposes, Cambridge (United Kingdom), 2-5 July (2007)
- Marrero C, O. Jorba, E. Cuevas and J. M. Baldasano, Extreme Wind Event Over the Canary Islands Related o The Extratropical Storm Delta: Sensitivity Study with a Limited Area Model. IUGG 2007 Perugia, Session: MS013 Topographic Effects on Weather and Climate (ICDM), Perugia (Italia), July (2007)
- Jiménez P., O. Jorba, C. Pérez, J. M. Baldasano, Isolating the Effects of Climate on Air Pollutants Concentrations during Summertime in the Mediterranean. IUGG 2007 Perugia, Session: MS016 Downscaling to Local and Regional Scales (ICCL), Perugia (Italia), July (2007)
- Pérez C., P. Jiménez, O. Jorba, J. M. Baldasano, E. Cuevas, S. Nickovic, X. Querol, Long-term simulations (1958-2006) of Saharan dust over the Mediterranean and the Eastern North Atlantic with the DREAM regional dust model. IUGG 2007 Perugia, Session: MS004 Mineral Dust Cycle and its Impact on Clouds and Radiation (ICCP), Perugia (Italia), July (2007)
- Papayannis A., C.Y. Fu, Z. Huaiqing,V. Amiridis, G. Chourdakis, G., Georgoussis, C. Pérez, H. B. Chen, P. Goloub, R. E. Mamouri, S. Kazadzis, D. Paronis, G. Tsaknakis, J.M. Baldasano, Extra-ordinary dust event over beijing, china during april 2006: lidar, sun photometric, satellite observations and model validation. In: XXIV International Union of Geodesy and Geophysics (IUGG) General Assembly, Perugia, Italy, 2-13 July (2007).
- Papayannis A., V. Amiridis, G. Tsaknakis, D. Balis, J. Bösenberg, A. Chaikovski, F. De Tomasi, V. Freudenthaler, I. Grigorov, I. Mattis, V. Mitev, D. Müller, L. Mona, S. Nickovic, J.M. Baldasano, A. Pietruczuk, G. Pisani, F. Ravetta,V. Rizi, M. Sicard, and T.Trickl, First systematic observations of Saharan dust over Europe during EARLINET (2000-2002): Statistical analysis and results. In: XXIV International Union of Geodesy and Geophysics (IUGG) General Assembly, Perugia, Italy, 2-13 July (2007).
- Frontoso, M.G., Perez, C., Sicard, M., Comeron, A., Spinelli, N., Baldasano, J.M., Integrating regional model and lidar observations to derive a 2-year climatology of the vertical distribution of saharan dust over the western and central Mediterranean. In: International Geoscience and Remote Sensing symposium (IGARSS), Barcelona, Spain, 23-27 July (2007).
- Jiménez-Guerrero P., M. García-Vivanco, O. Jorba, I. Palomino, C. Pérez, F. Martín and José M. Baldasano, Characterization and Origin of Ozone and Particulate Matter in the Iberian Peninsula by the Application of Air Quality Modelling and Trajectory Clustering Correlation Methodologies. 2nd ACCENT Symposium, Urbino (Italy), 23-27 July (2007).
- Jiménez-Guerrero P., M. García-Vivanco, O. Jorba, I. Palomino, C. Pérez, F. Martín and José M. Baldasano, An Intercomparison and Evaluation Study of Two Chemistry Transport Models in Southwestern Europe for an Annual Cycle. 2nd ACCENT Symposium, Urbino (Italy), 23-27 July (2007)
- Cachorro V.E., A. De Frutos, A. Berjón, M. Sorribas, B. De la Morena, E. Cuevas, A. Labajo, L. Alados-Arboledas, J.A. Martínez-Lozano, J.P. Díaz, J. Lorente, M. Cancillo, M. Pujadas, J. M. Baldasano, A.M. Silva, RIMA: Red Ibérica de Medida Fotométrica de Aerosoles Iberian network for photometric aerosol measurements. 34th Annual European Meeting on Atmospheric Studies by Optical Methods, Andenes (Noruega), 25-30 August (2007)
- Güereca, S. Gassó, J.M: Baldasano, P. Jiménez, Life Cycle Assessment of Five Municipal Waste Management Systems for Catalonia (Spain). 3rd International Conference on Life Cycle Management-LCM2007, Zurich(Switzerland) 27-29 August (2007)
- Mattis I. et al., EARLINET correlative measurements for CALIPSO. SPIE-2007, Lidar Technologies, Techniques and Measurements for Atmospheric Remote Sensing III, ---(2007)

- Gonçalves M., P. Jiménez and J.M. Baldasano, Air Quality Management Strategies in Large Cities: Effects of Changing the Vehicle Fleet composition in Barcelona and Madrid Greater Areas (Spain) by introduciing NGV. 29th NATO/CCMS International Technical Meeting on Air Pollution Modelling and its Application. Aveiro (Portugal) 24-28 September (2007)
- Pérez C., J.M. Baldasano, E. Cuevas, S. Nickovic, L.Barrie, X. Querol, Present and future capabilities of the Sand and Dust Storm Warning System for North Africa to provide knowledge on environmental risk indicators of meningitis epidemics. GEO Meningitis Environmental Risk Consultative Meeting, Geneva, 26-27 September (2007).
- Baldasano J.M, P. Jiménez-Guerrero, O. Jorba, C. Pérez, E. López, P. Güereca, F. Martin, M. García-Vivanco, I. Palomino, X. Querol, M. Pandolfi, M.J. Sanz and J.J. Diéguez, CALIOPE: An operational air quality forecasting sustem for the Iberian Peninsula, Balearic Islands and Canary Islands. 7th EMS Annual Meeting-8th European Conference on Applications of Meteorology, El Escorial (Madrid, España) 1-5 October (2007).
- Baldasano J.M., E. Cuevas, C. Pérez, O. Jorba, P. Jiménez-Guerrero, S. Basart, S. Alonso-Pérez, M.A. Martínez, X. Querol, J. Pey, L. Barrie and S. Nickovic, WMO Sand and Dust Storm Warning System (SDS-WS) for Europe, Africa and Middle East: a GEO-oriented System . 7th EMS Annual Meeting-8th European Conference on Applications of Meteorology, El Escorial (Madrid, España) 1-5 October (2007)
- Jorba, O., C. Marrero, E. Cuevas and J.M. Baldasano, Impact of the extratropical storm Delta over Canary Islands on 28-30 November 2005: severe windstorm event. 7th EMS Annual Meeting-8th European Conference on Applications of Meteorology, El Escorial (Madrid, España) 1-5 October (2007)
- Marrero C., O. Jorba, E. Cuevas and J.M. Baldasano, Sensitivy Study with a Limited Area Model Extratropical Storm Delta over the Canary Islands. 7th EMS Annual Meeting-8th European Conference on Applications of Meteorology, El Escorial (Madrid, España) 1-5 October (2007)
- Cachorro V.E., A. De Frutos, A. Berjón, M. Sorribas, B. De la Morena, E. Cuevas, A. Labajo, L. Alados-Arboledas, J.A. Martínez-Lozano, J.P. Díaz, J. Lorente, M. Cancillo, M. Pujadas, J. M. Baldasano, A.M. Silva, RIMA: Red Ibérica de Medida Fotométrica de Aerosoles Iberian network for photometric aerosol measurements. Expert Meeting SDSWS, BSC-CNS/WMO/INM/CSIC, Barcelona (España), 7-9 November (2007)
- Pérez, C., Baldasano J.M., P. Jiménez-Guerrero, O. Jorba, K. Haustein, E. Cuevas, S. Basart, S. Nickovic, Dust modeling and forecasting at the Barcelona Supercomputing Center: activities and developments. Expert Meeting SDSWS, BSC-CNS/WMO/INM/CSIC, Barcelona (España), 7-9 November (2007).
- Ramos, A. G., Cuevas, E., Pérez, C., Baldasano, J.M., Coca, J., Redondo, A., Alonso-Pérez, S., Bustos, J.J, Saharan Dust and Blooms of Diazotrophic Cyanobacteria off the NW African Upwelled Waters. Sand and Dust Strom Warning System Expert Meeting SDSWS, BSC-CNS/WMO/INM/CSIC, Barcelona (España), 7-9 November (2007).
- Baldasano J.M, P. Jiménez-Guerrero, O. Jorba1*, C. Pérez, E. López, P. Güereca, F. Martin, M. García-Vivanco, I. Palomino, X. Querol, M. Pandolfi, M.J. Sanz and J.J. Diéguez, CALIOPE: An operational air quality forecasting system for the Iberian Peninsula, Balearic Islands and Canary Islands. ACCENT/GLOREAM Workshop, Berlin (Germany), 28-30 November (2007).
- Gonçalves M., P. Jiménez-Guerrero and J. M. Baldasano, Contribution of atmospheric processes to photochemical pollution by using a process analysis tool in the north-eastern and central Iberian Peninsula. ACCENT/GLOREAM Workshop, Berlin (Germany), 28-30 November (2007).
- Marras S.., P. Jiménez, O. Jorba, C. Pérez, J.M. Baldasano, Present-day climatic simulations run with two GCMs: a comparative evaluation against ERA-40 reanalysis data (first results). AGU Fall Meeting 2007, San Francisco (USA,) 10-14 December (2007).

- Gonçalves, M., P. Jiménez-Guerrero, J.M. Baldasano, Reduction of NOx emissions on urban areas by changing specific vehicle fleets: Effects on NO2 and O3 concentration. AGU Fall Meeting 2007, San Francisco (USA,) 10-14 December (2007).

National Conferences

- Sans R. y J.M. Baldasano, Estudio y tratamiento del rechazo de los residuos municipales embalados, teniendo en cuenta dos soluciones para la revalorización de estos residuos. Jornadas FYTEC de I+D+i, Barcelona, 1 March (2007)
- Baldasano J.M., P. Jiménez, O. Jorba, E. López y A. Soret, Metodología para la Evaluación del Impacto Ambiental de Centrales Térmicas de Ciclo Combinado. IV Congreso Nacional de Evaluación de Impacto Ambiental. Madrid, 25-27 April (2007)

Communications

- Baldasano J.M., ¿Qué es el Cambio Climático? Museo de Arte Contemporáneo Unión Fenosa (MACUF), La Coruña,14 March (2007)
- Baldasano J.M., Cambio Climático ¿Realidad o Ficción? Enginyeria Sense Fronteras. ETSEIB-UPC, Barcelona,15 March (2007)
- Baldasano J.M., Cambio Climático: nuevos resultados y retos pendientes. Comisión de Medio Ambiente del Alto Consejo Consultivo de la Generalitat Valenciana, Valencia, 30 March (2007)
- Baldasano J.M., Gestión y Tratamiento de Residuos Municipales. Jornada de Gestió de Residus Municipals, Ayuntamiento de Vila-seca (Tarragona) 4 May (2007)
- Baldasano J.M., The Need of High Performance Computing for Enhancing Climate Change and Air Quality Forecasting Systems. International Supercomputing Conference ISC'07, Dresden (Germany) 26-28 June (2007)
- Baldasano J.M., La Supercomputación en el Cambio Climático y en los Sistemas de Pronóstico de la Calidad del Aire. Cursos de Verano de la Universidad de Málaga, Ronda (Málaga) 5 July (2007)
- Baldasano J.M., Los Supercomputadores del Futuro. Aplicaciones. Campus de Excelencia 2007. Fuerteventura (España), 11 July (2007).
- Baldasano J.M., Retos actuales en materia de contaminación atmosférica. XXVIII Edición de los Cursos de Verano de la Universidad de Cádiz en San Roque, dtor. J.M. Quiroga, 21 July (2007).
- Baldasano J.M., El nuevo informe del IPCC: Constataciones e Incertidumbres. Curso de Verano, Universidad Complutense de Madrid (UCM): La Bioesfera amenazada: España en el planeta Tierra, dtor. R. Tamames. El Escorial 7 August (2007)
- Baldasano J.M., Evidencias del Cambio Climático. Cursos de "La Granda", Fundación Escuela Asturiana de Estudios Hispánicos: El Cambio Climático y sus Consecuencias, dtor. S. Grisolia. La Granda (Asturias) 20 August (2007).
- Baldasano J.M., La Gestión de los Residuos Municipales. Nuevas Perspectivas. Universidad Internacional de Andalucia, Sede Antonio Machado. Baeza 29 August (2007)
- Baldasano J.M., Millota de la qualitat de l¡aire per canvi de combustible al gas natural en automoció. Aplicació a Madrid i Barcelona. Fundación Gas Natural, Barcelona 14 November (2007).
- Baldasano J.M., Ciencias de la Terra i Canvi Climàtic. 1 Congrès Científic Internacional. Calldetenes (Osona, Barcelona) 17 November (2007)
- Baldasano J.M., Situación Medioambiental Global. Problemas y Soluciones. Seminario Internacional de Energías Renovables, Cuenca (Ecuador) 17 April (2007).

- Baldasano J.M., Situación Medioambiental Global. Problemas y Soluciones. Universidad de Azuay, Cuenca (Ecuador) 19 April (2007).
- Baldasano J.M., Cambio Climático, Evidencias e Impactos. CORPAIRE, Quito (Ecuador) 19 April (2007).
- Baldasano J.M., La Calidad del Aire y su Pronóstico. CORPAIRE, Quito (Ecuador) 19 Abril (2007).
- Jiménez-Guerrero, P., The Application of Climate Models within Supercomputing Frameworks. Jornada Catalana de Supercomputación: Investigación sobre cambio climático. Centro de Supercomputación de Cataluña (CESCA) y Parque Científico (Barcelona). Barcelona, 27 September (2007).
- Jiménez-Guerrero, P., Modelling of Global and Regional Climate and Current Developments in MareNostrum Supercomputer. Jornadas sobre el Cambio Climático en la Europa Mediterránea: el Litoral y las Áreas de Montaña. Grupo de Expertos en Cambio Climático de Cataluña (GECCC). Barcelona, 8 November (2007).
- Pérez, C., Present and future capabilities of the Sand and Dust Storm Warning System for North Africa to provide knowledge on environmental risk indicators of meningitis epidemics. GEO Meningitis Environmental Risk Consultative Meeting, Geneva, 26-27 September (2007).
- Pérez, C., Modelización del ciclo atmosférico del polvo mineral desértico. Universidad politécnica de Catalunya. 14 de November (2007).

- Raul Alcantara, Changliang Xu, Thomas G Spiro and Victor Guallar. A quantum chemistry picture of hemoglobin affinity. Proc. Natl. Acad. of Science, 104 18451-18455 (2007).
- J.R.Blas, J.M.López-Bes, M.Márquez, J.L.Sessler, F.J.Luque and M.Orozco "Exploring the dynamics of Calix[4]pyrrole:The effect of solvent and fluorine substitution". Chem.Eur.J. (2007) 13, 1108-1116.
- Bonivento, D., Pontiggia, D., Matteo, A.D., Fernandez-Recio, J., Salvi, G., Tsernoglou, D., Cervone, F., Lorenzo, G.D. and Federici, L. "Crystal structure of the endopolygalacturonase from the phytopathogenic fungus Colletotrichum lupini and its interaction with polygalacturonase-inhibiting proteins". Proteins (2007) 70, 294-299.
- O.Carrillo and M.Orozco. "GRID-based molecular dynamics. A Tool for genomic-scale simulations of channels in proteins". Proteins. In Press (2007).
- Chandran, V., Poljak, L., Núñez Miguel, R., Fernandez-Recio, J., Parkinson, J., Burns, C., Carpousis, A.J. and Luisi, B.F. "Recognition and cooperation between the ATP-dependent helicase RhlB and ribonuclease RNase E". J.Mol.Biol. (2007) 367, 113-132.
- Cheng, T.M.K., Blundell, T.L. and Fernández-Recio, J. "pyDock: electrostatics and desolvation for effective scoring of rigid-body protein-protein docking". Proteins (2007) 68, 503-515.
- A.Emperador, O.Carrillo, M.Rueda and M.Orozco. "Exploring the suitability of coarse-grained techniques fort he representation of protein dynamics". Biophysical Journal. (In Press). 2007
- Fernández, D., Vendrell, J., Avilés, F.X. and Fernández-Recio, J. "Structural and functional characterization of binding sites in metallopeptidases based on ODA analysis". Proteins (2007) 68, 131-144.
- F.Forti, X.Barril, M.Orozco and F.J.Luque. "Extension of the MST continuum solvation model to the RM1 semiempirical Hamiltonian". J.Comp.Chem (In Press) 2007.
- J.Fort, L.R. de la Ballina, H.E.Burghardt, C.Ferrer-Costa, J.Turnay, C-Ferrer-Orta, I.Usón, A.Zorzano, J.Fernández-Recio, P.L.Fernández, M.Orozco, M.A. Lizarbe, I.Fita and M.Palacín. "Structure of human 4F2hc ectodomain: crystallographic and in vivo evidence for homodimerization". J.Biol.Chem (2007), 43, 31444-31452 PAPER OF THE WEEK
- Fort, J., de la Ballina, L.R., Burghardt, H.E., Ferrer-Costa, C., Turnay, J., Ferrer-Orta, C., Usón, I., Zorzano, A., Fernández-Recio, J., Orozco, M., Lizarbe, M.A., Fita, I. and Palacín, M. "The structure of human 4F2hc ectodomain provides a model for homodimerization and electrostatic interaction with plasma membrane". J.Biol.Chem. (2007) 282, 31444-31452.
- J.R.Goñi, A.Pérez, D.Torrents and M.Orozco. "Studying the role of DNA physical properties on gene regulatory mechanisms in vertebrates". Genome Biology (In Press) 2007.
- Grosdidier, S., Pons, C., Solernou, A. and Fernandez-Recio, J. "Prediction and scoring of docking poses with pyDock". Proteins (2007) 69, 852-858.
- Victor Guallar. QMMM Methods for the Spin Density in Heme Compound I. Proceedings of ICCMSE (2007), In Press
- C.A.Laughton, M.Orozco and W.Vranken. "COCO: A simple tool to enrich the representation of conformational variability in NMR structures". Bioinformatics. (In Press) 2007.
- Marcelo A. Marti, Axel Bidon-Chanal, Alejandro Crespo, Suyn-Ru Yeh, Victor Guallar, F. Javier Luque, and Dario A. Estrin. Mechanism of product release in NO detoxification from Mycobacterium tuberculosis truncated hemoglobin N. Journal of the American Chemical Society, In press (2007).
- Marcelo A. Marti, Luciana Capece, Axel Bidon-Chanal, Alejandro Crespo, Victor Guallar, F. Javier Luque, and Dario A. Estrin. NO reactivity with globins as investigated through computer simulation, Methods in Enzymology, In Press, (2007).
- Medina, M., Abagyan, R, Gómez-Moreno, C. and Fernández-Recio, J. "Docking analysis of transient complexes: Interaction of ferredoxin.NADP+ reductase with ferredoxin and flavodoxin". Proteins (2007) In press.

- J.Muñoz-Muriedas, X.Barril, J.M.López, M.Orozco and F.J.Luque "A hydrophobic similarity analysis of solvation effects on nucleic acids" J.Mol.Mod., (2007) 13, 357-365.
- A.Noy, F.J.Luque and M.Orozco. "Theoretical Analysis of Antisense Duplexes: Determinants of the RNase H Susceptibility". J.Am.Chem.Soc. (In Press). 2007
- A.Noy, A.Pérez, C.Laughton and M.Orozco. "Theoretical study of large conformational transitions in DNA: The BêíA conformational change in water and ethanol/water". Nucleic Acid Res. (2007) 35, 3330-3338.
- M.Orozco, I.Marchán and I.Soteras. "Continuum analysis of conformational sampling in solution". In Continuum Solvation Models in Chemical Physics: Theory and Application". B.Mennucci and J.Tomasi (Eds). Elsevier. Amsterdam, 2007. In Press
- M.Orozco, A.Noy and A.Pérez "Recent advances in the study of nucleic acids flexibility by molecular dynamics". Curr. Op. Struct. Biol. (In Press) 2007.
- J.A.Ortega, J.R.Blas, M.Orozco, A.Grandas, E.Pedroso and J.Robles. "Binding affinities of oligonucleotides and PNAs containing phenoxazine and G-clamp cytosine analogs are unusually sequence-dependent". Organic Letters. (2007), 9, 4503-4506.
- A.Pérez, F.J.Luque and M.Orozco. "Entering molecular dynamics in the biological time scale. Microsecond simulation of DNA". J.Am.Chem.Soc. (2007), 129, 14739-14745.
- A.Pérez, I.Marchán, D.Svozil, J.Sponer, T.E.Cheatham, C.A.Laughton and M.Orozco. "Refinement of the AMBER force-field for nucleic acid simulations. Improving the representation of conformations". Biophysical J. (2007) 92, 3817-3829.
- N. Reig, C. del Rio, F. Casagrande, M. Ratera, J.L. Gelpi, D. Torrents, P.J. Henderson, S. A. Baldwin, A. Zorzano, D. Fotiadis, M. Palacín. "Functional and structural characterization of the first prokaryotic member of the LAT family: a model for APC transporters" J.Biol. Chem (2007) 282(18):13270-13281
- M.Rueda, P.Chacón and M.Orozco. "Thorough Validation of Protein Normal Mode Analysis- A Comparative Study with Essential Dynamics". Structure. (2007) 15, 565-575.
- M.Rueda, C.Ferrer, T.Meyer, A.Pérez, J.Camps, A.Hospital, J.L.Gelpí and M.Orozco. "A consensous view to Protein Dynamics". Proc. Natl. Acad. Sci. USA. (2007) 104, 796-801.
- R. Soliva, J.L.Gelpi, C.Almansa, M.Virgili and M.Orozco. "Dissection of the recognition properties of p38 MAP Kinase. Determination of the binding mode of a new pyridinyl-heterocycle inhibitor family". J.Med.Chem. (2007) 50, 283-293.
- I.Soteras, C.Curutchet, A.Bidon-Chanal, F.Dehez, J.Angyan, M.Orozco, C.Chipot and F.J.Luque. "Derivation of distributed models of atomic polarizability for molecular simulations". J.Chem.Theor.Comp (2007) 3, 1901-1913.
- Talavera, C.Vogel, M.Orozco, S.A.Teichmann and X de la Cruz. "The (In)dependence ofalternative splicing and gene duplication". PLOS Comp.Biol. (2007) 3, 375-388. (Front Cover Article)
- D.Talavera, A.Hospital, M.Orozco and X de la Cruz. "A Procedure for the identification of homologous alternative splicing events". BMC. Bioinformatics. (2007) 8, 260-271.
- A.Vázquez-Mayogoita, O.Huertas, M.Fuentes-Cabrera, B.G.Sumpter, M.Orozco and F.J.Luque. "Ab initio study of naptho-derivatives of DNA bases". J.Phys.Chem.A (In Press)
- The Biomoby consortium (including M.Orozco, J.L.Gelpí and others). "Interoperability with Biomoby 1.0- it's better than sharing your toothbrush". Brieffings in Bioinformatics (In Press) 2007.

4.4 Computer Applications in Science and Engineering

Journals and Book Chapters

- G. Houzeaux and R. Codina. "A Finite Element Method for the Solution of Rotary Pumps". Comp. & Fluids, 36, 667-679, 2007.
- S. Reyes, C. Muñoz-Caro, A. Niño, R. M. Badia, J.M. Cela, "Performance of computationally intensive parameter sweep applications on Internet-based Grids of computers: the mapping of molecular potential energy hypersurfaces", Concurrency and Computations: Practice and Experience, Vol. 19, 463-481, Wiley InterScience, 2007
- Carles Serrat, Yu Loiko, J.M. Cela, Raul de la Cruz, "Coherent Stark nonlinear spectroscopy with chirped pulses", Physical Review, Vol. 75, 363-367, American Physical Society , 2007

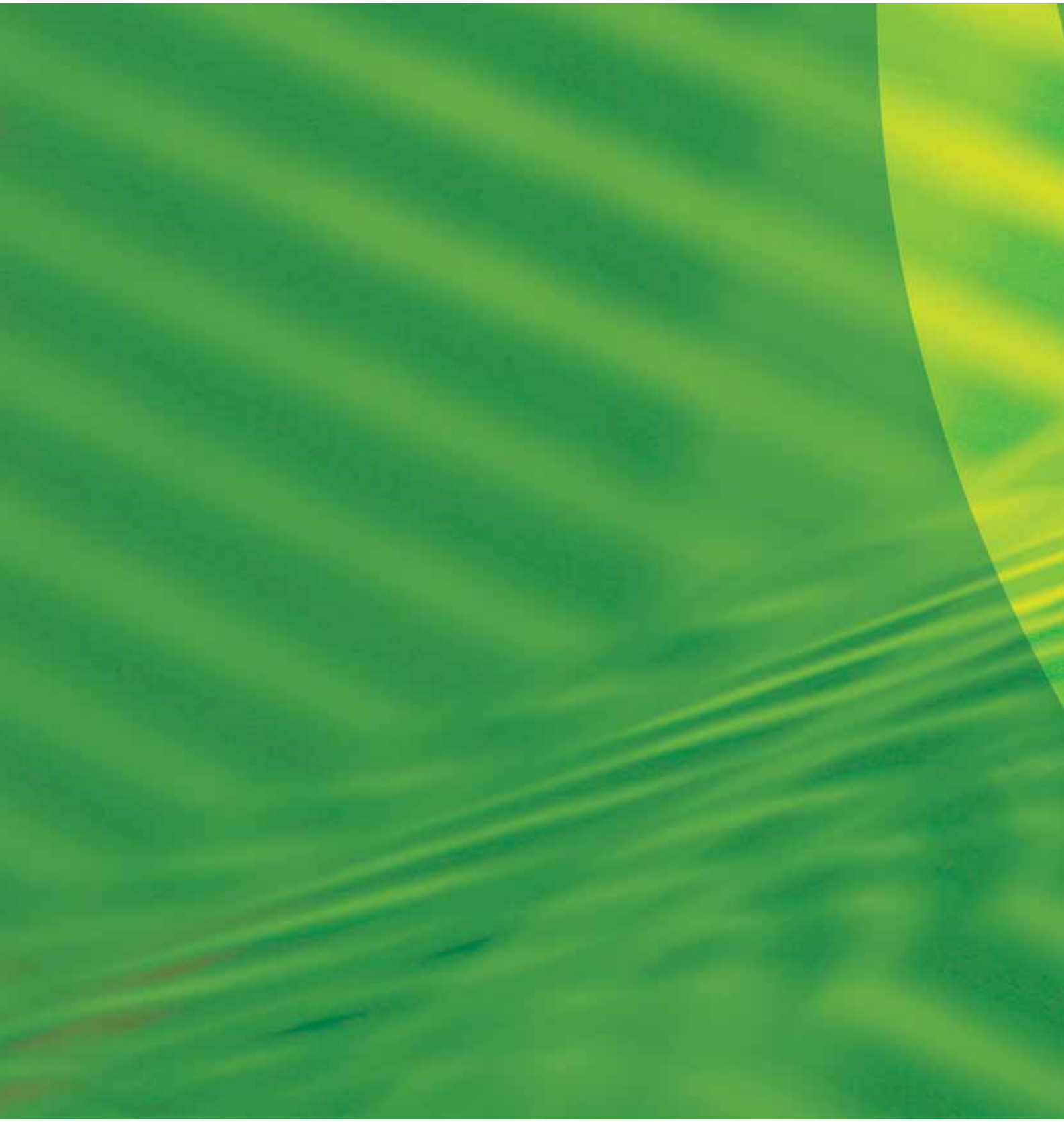
International Conferences and Symposiums

- G. Houzeaux and M. Vázquez. "High Performance Computational Mechanics at BSC-CNS", Computational Science - Understanding and Solving Multiphysics Problems for Industry and Society with Large Scale Simulation". Invited speaker, INRIA Rhône-Alpes, Grenoble (France), May 10-12, 2007.
- R. Codina, H. Coppola-Owen and G. Houzeaux. "The fixed mesh ALE approach: basic idea and two applications". Computational Models for Coupled Problems in Science and Engineering II, Eds. E. Oñate, M. Papadrakakis and B. Schrefler, Ibiza (Spain), 21-23 May, 2007.
- G. Houzeaux, M. Vázquez and R. Grima and H. Calmet and J.M. Cela. "Experience in Parallel Computational Mechanics on MareNostrum". PARCFD2007, Invited speaker, Antalya (Turkey), May 21-24, 2007.
- Vázquez, G. Houzeaux, R. Grima and J.M. Cela. "Applications of Parallel Computational Fluid Mechanics in MareNostrum Supercomputer: Low-Mach Compressible Flows". PARCFD2007, Antalya (Turkey), May 21-24, 2007.
- C. Lesage, M.Vázquez, G., Houzeaux. "Finite Element explicit numerical method to solve the Level Set advection equation on parallel computer". HPC-Europa Transnational Access Meeting, Bolonia (Italy), June 14-15, 2007.
- B. Eguzkitza, G. Houzeaux and M.Vázquez. "A Variational Multiscale Model Based on the Analytical Solution of the Approximate Subgrid Scale Equation". 9th US National Congress on Computational Mechanics, San Francisco (USA), 22-26 July, 2007.
- J. Cipriano and G. Houzeaux D. Pérez. "Development and characterization of semitransparent double skin PV facades with heat recovering". Building Low Energy Cooling and Advanced Ventilation Technologies in the 21th Century, 2nd PALENC Conference and 28th AIVC Conference, Crete Island (Greece), 27-29 September, 2007.

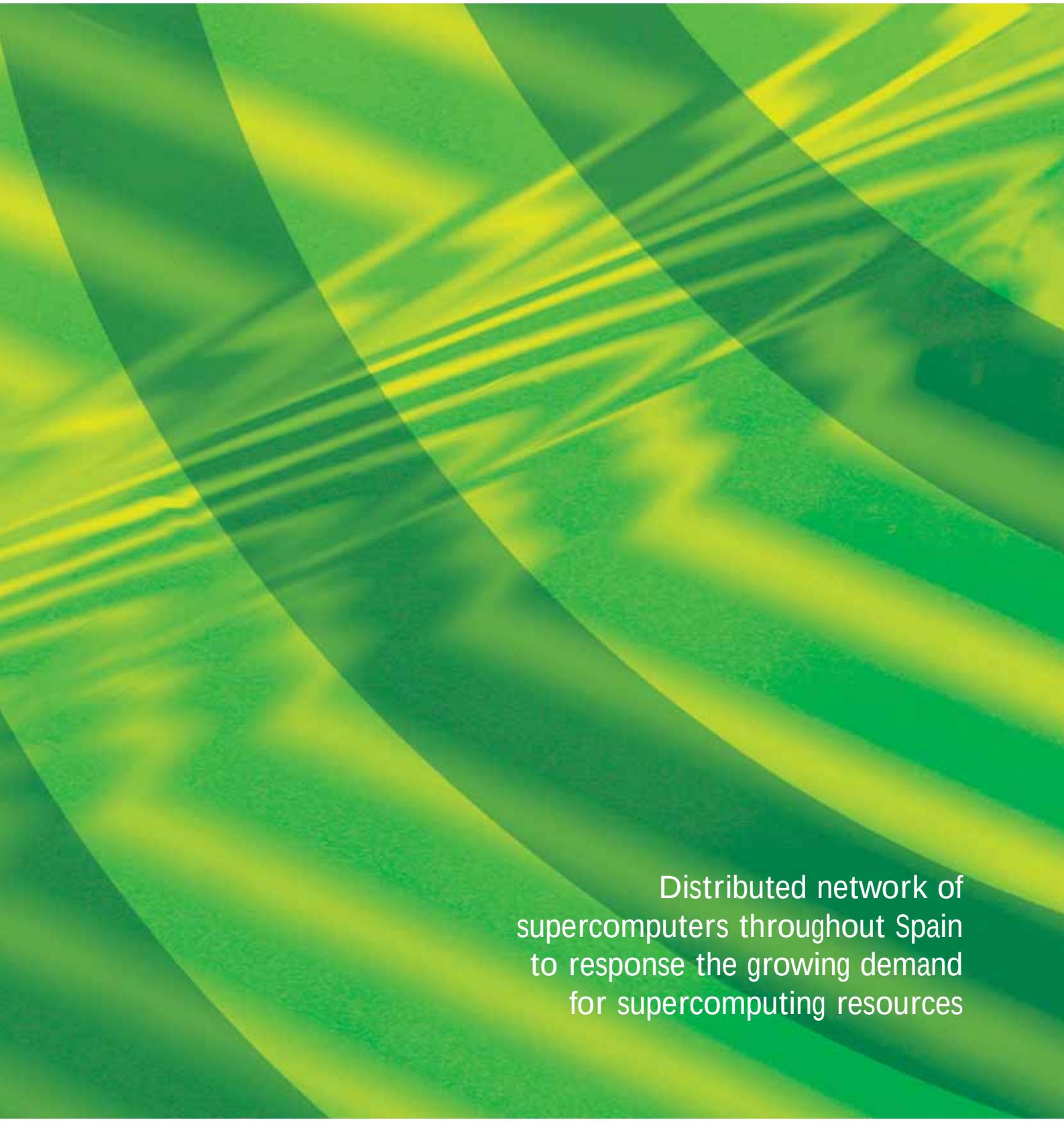
Internal reports

- J.M. Cela. "Kaleidoscope: Inital Finite Difference Code for wave equation". IR-07-001, January 2007.
- J.M. Cela. "Kaleidoscope: Stencil Transformation Code for wave equation". IR-07-002, February 2007.
- A.C. Lesage. "Kaleidoscope: Finite element explicit numerical method to solve the wave acoustic equation". IR-07-003, March 2007.
- M. Araya, M. Hanzich and J.M Cela. "Kaleidoscope: Improving Finite Difference Code by Blocking Algorithm". IR-07-005, April 2007.
- C. Lesage, M. Araya. "Kaleidoscope: Finite element explicit numerical method to solve the wave acoustic equation. Second order finite element and Parallelization tests". IR-07-004, April 2007.

- M. Araya, M. Hanzich, J.M. Cela. "Kaleidoscope: Improving Finite Difference Code by Blocking Algorithm and Thread Level Parallelism". IR-07-006, May 2007.
- M. Araya, M. Hanzich, JM Cela. "Kaleidoscope: Domain Decomposition and IO enhancements on Improving Finite Difference Code". IR-07-007, June 2007.
- M. Araya, M. Hanzich, JM Cela. "Kaleidoscope: Final enhancements to Finite Difference Code". IR-07-008, July 2007.
- C. Lesage, M. Araya Polo. "Kaleidoscope: Acoustic3D Finite Differences Code, Implementation of an improved Perfectly Matched layer". IR-07-009, July 2007.



5 Spanish Supercomputing Network



Distributed network of
supercomputers throughout Spain
to response the growing demand
for supercomputing resources

The Spanish Supercomputing Network (Red Española de Supercomputación RES) was inaugurated in March, 2007 responding to the scientific community's need for increased calculation capacity.

In November, 2006, BSC and IBM upgraded MareNostrum, substituting the JS20 bladecenters for JS21bladecenters and allowing us to double calculation capacity. Following this, the old MareNostrum hardware was used to create a distributed infrastructure of supercomputers in different sites in Spain. Half of the replaced technology was used to extend the capacity of the Polytechnic University of Madrid (UPM) Supercomputer. The other half was used to create the supercomputers in Cantabria University (UC), in Zaragoza University (UZ), in Valencia University (UV), in Málaga University (UMA) and in Astrophysics Institute of Canarias (IAC). RES is managed by the BSC.

All the nodes are accesible to users via a single Access Committee, with 44 scientits organized into four different panels, which distributes about 20 million hours every 4 months.

RES activity in 2007

On March 13th 2007, the Minister of Education and Science (Ministerio de Educación y Ciencia), Mercedes Cabrera, The Minister of University, Industry and Innovation of the Generalitat de Catalunya Josep Huguet, and The Rector of the Universitat Politècnica de Catalunya (UPC), Antoni Giró, visited the BSC installations for the official inauguration of the Supercomputing Spanish Network.

Official opening of RES

Agreements between BSC and the other sites were signed in 2007: On May 2 with the Astrophysics Institute of Canarias; on May 8 with Málaga University; on June 13 with Cantabria University and on August 8 with Valencia University. In a near future a new agreement will be signed with University of Zaragoza. The agreement with The Polytechnic University of Madrid had already been signed in December 2006.

Following this, the BSC and IBM engineers proceeded to install the RES nodes.

RES Finance

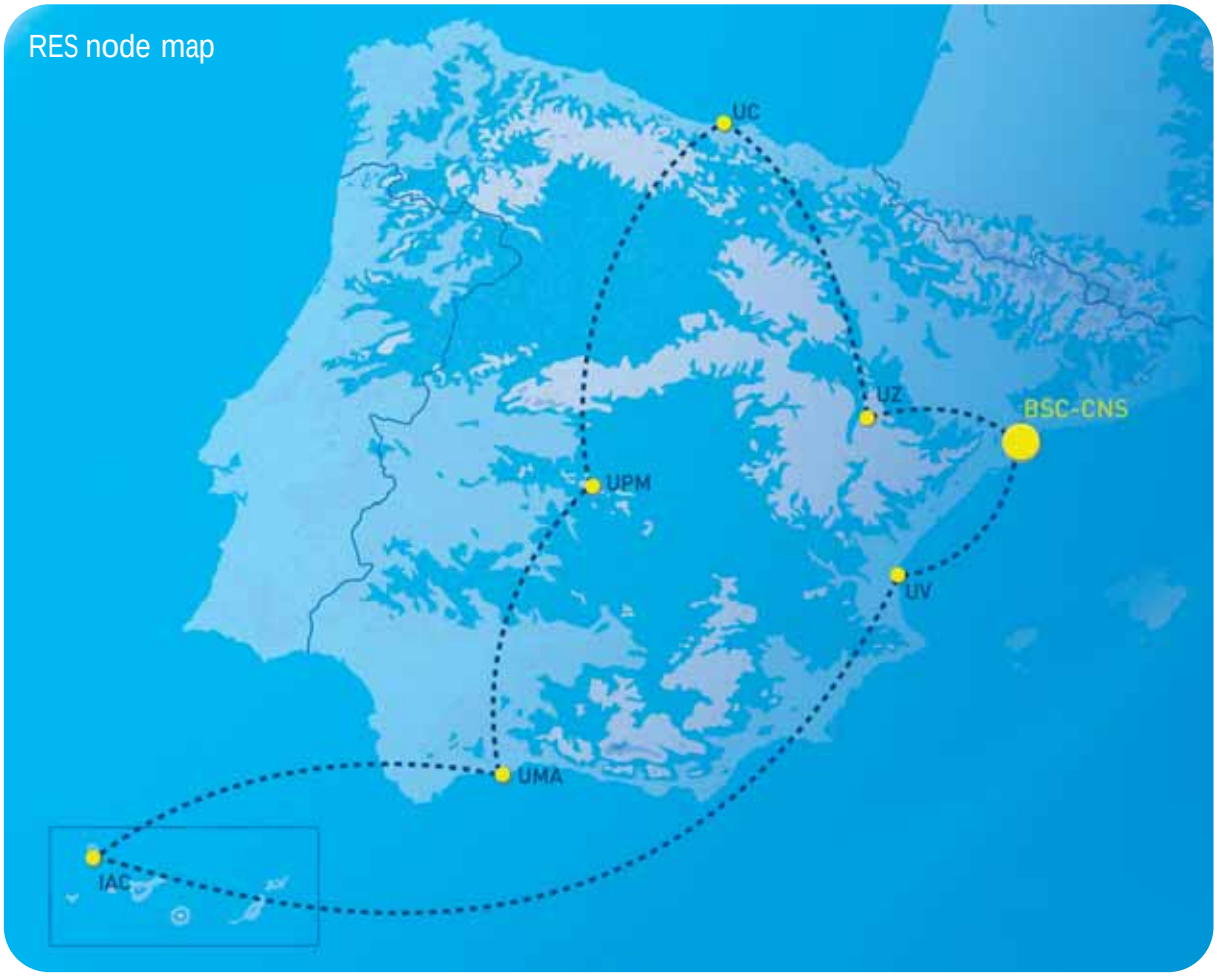
The RES helps with financing for travel-expenses, accommodations, material, etc. for seminars organization. The objective of these seminars is to improve the operation and administration of the network, systems and service.

Seminars

RES includes two kinds of seminars. On one hand, RES organizes Technical Seminars with the objective to get maximum participation of RES Engineers. With these seminars engineers share knowledge and experience. In this framework, RES also organizes Seminars with manufacturing companies to know better their products. In 2007, technical seminars took place during the installation of the facillities at Malaga and Santander.

On the other hand RES organizes Scientific Seminars with the objective to spread the advantages of supercomputing in studies and calculations for the scientific community. During 2007 one seminar took place, in Santader on the topic of Engineering Applications and Dynamic of Fluids.

RES node map



RES nodes

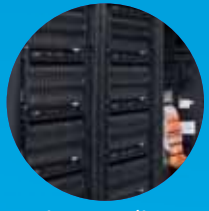
Magerit, Madrid
Universidad Politécnica de Madrid

Altamira, Santander
Universitat de Cantabria

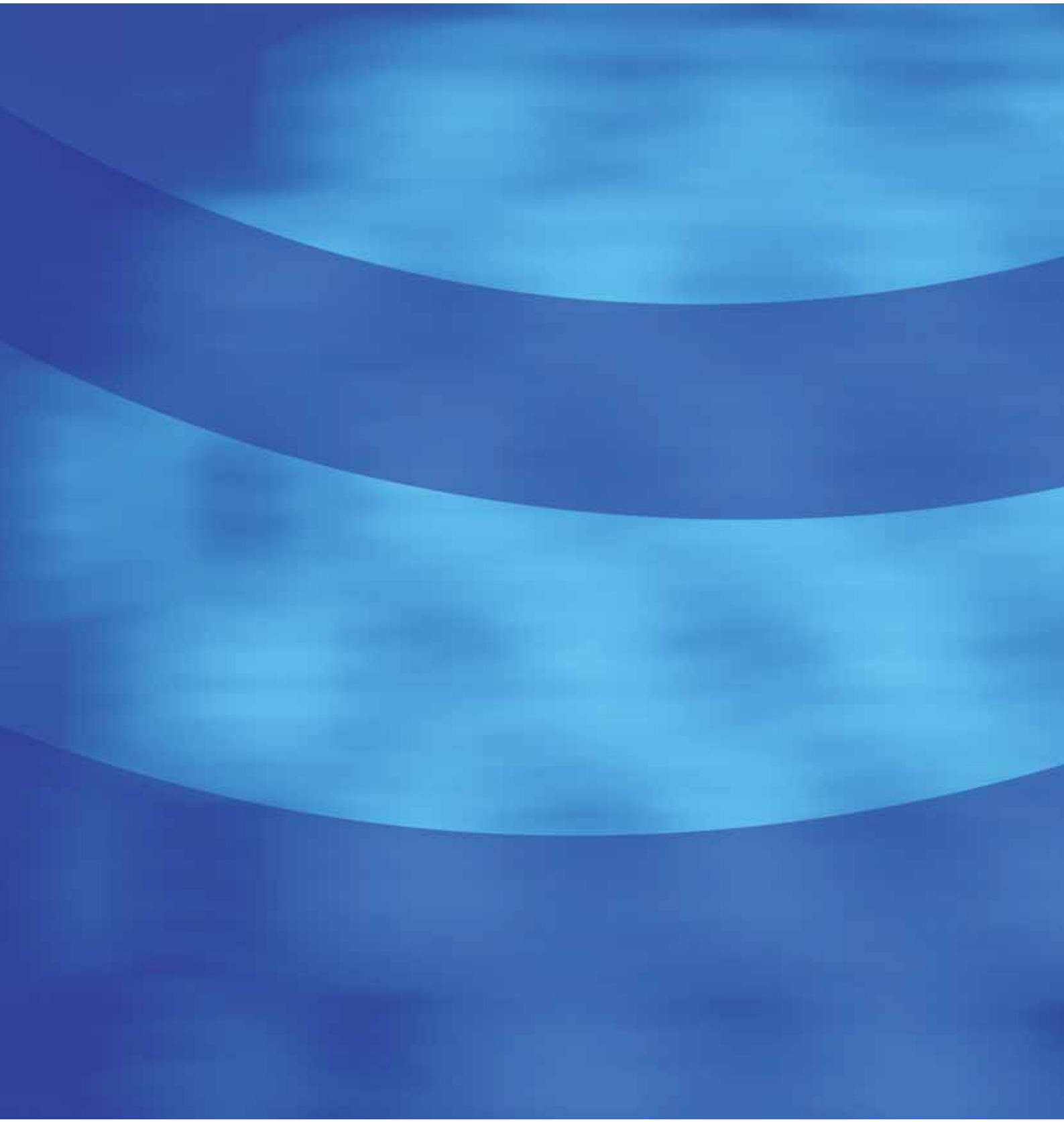
La Palma, La Palma
Instituto Astrofísico de Canarias

Tirant, Valencia
Universitat de València

CaesarAugusta, Zaragoza
Universidad de Zaragoza



Picasso, Málaga
Universidad de Málaga



6 RES Users

List of research results from all research areas for the year 2007

This section provides a summary of external research projects that used the RES nodes in 2007. It includes a list of the resulting papers that were published before the printing of this Annual Report. The researchers and their projects have been classified in terms of the knowledge areas of the Access Committee.

Biomedicine and Life Sciences

- Carlos Alemán - Universitat Politècnica de Catalunya, "Tubular Nanostructures Based on Protein Motifs"
- Jaume Bonet - Structural Bioinformatic's Lab. Biomedical Informatics Research Unit, Parc de Recerca Biomèdica de Barcelona, "Aligned profiles with multiples environments and methods: Selection of the best parameters"
- José María Carazo, Centro Nacional de Biotecnología - CSIC, "Maximum-likelihood classification of structurally heterogeneous electron microscopy data"
- Robert Castelo - Univ. Pompeu Fabra, Barcelona, "Simulation and learning of large biomolecular networks using graphical Markov models"
- Albert Compte - Institut d'Investigacions Biomèdiques August Pi i Sunyer (IDIBAPS), "Exploring the specificity of the relationship between cortical network function and biological simulation parameters with a particle swarm optimization algorithm"
- Xavier de la Cruz - Parc Científic de Barcelona, "Molecular Dynamics Simulation of the Folding/Unfolding Mechanism of Apoflavodoxin"
- Natalia Díaz - Universidad de Oviedo, "Computational Modelling of Matrix Metalloproteinases: Influence of the Hemopexin-like domain in the MMP-2 enzyme"
- Hernán J. Dopazo - Centro de Investigación Príncipe Felipe, "From Historical Gene Pattern to Darwinian Molecular Processes. Towards a complete catalogue of adaptative events ocurring after gene duplication in the human phylome"
- Gloria Fuentes - Centro Nacional de Investigaciones Oncológicas, "RAS superfamily and the interactions with their effectors: functional specificity"
- Ernest Giralt - Institut de Recerca Biomèdica (IRB Barcelona), "Evolutionary Algorithms and de Novo Peptide Design"
- Roderic Guigó - Parc de Recerca Biomèdica de Barcelona, "Use of TBLASTX to find regions of homology among multiple large-size full genomes"
- Francisco Javier Luque - Univ. Barcelona, "Unraveling the molecular mechanisms of ligand migration in Mycobacterium tuberculosis truncated haemoglobin N"
- Sara Marsal - Institut de Recerca Hospital Universitari Vall d'Hebron, "Whole genome epistatic modelling in Rheumatoid Arthritis and Chronic Inflammatory Arthritis"
- Feliu Maseras - Institut Català d'Investigació Química, "DFT modeling of reactivity in an ionic liquid"
- Milagros Medina - Universidad de Zaragoza, "Action mechanism of flavoenzymes: a MD Study"
- Arcadi Navarro i Cuartiellas - Universitat Pompeu Fabra, "Genomic Distribution of Ancestral and Recent Natural Selection in the Human Genome"
- Ángel R. Ortiz, Centro de Biología Molecular "Severo Ochoa", CSIC-UAM, "Including solvent effect and receptor flexibility in virtual screening via rescoring techniques"
- Manuel Palacín - Parc Científic de Barcelona, "Study of 4F2hc ectodomain-induced membrane curvature by means of MD"
- Florencio Pazos - Centro Nacional de Biotecnología (CSIC), "Prediction of Protein Interaction Specificity"

- Ruben Pérez - Universidad Autónoma de Madrid, "Interaction of Atoms and Molecules with metals and metallic oxides characterized by first-principles calculations and simulations of surface imaging techniques"
- Carme Rovira - Centre de Recerca en Química Teòrica, Parc Científic de Barcelona, "Unraveling the reaction and drug activation mechanisms in Mycobacterium tuberculosis catalase-peroxidase by means of Car-Parrinello QM/MM simulations"
- Carme Rovira - Centre de Recerca en Química Teòrica, Parc Científic de Barcelona, "Activation of glycoside hydrolases by specific carbohydrate-protein interactions"
- Sjors H.W. Scheres - Centro Nacional de Biotecnología, Campus Universidad Autónoma, "Analysis of large three-dimensional electron microscopy data sets by computationally intensive algorithms"
- Agatha Schlüter - Institut d'Investigació Biomèdica de Bellvitge, "Peroxisomal Metabolome Characterization and Evolutionary Origen"
- Wolfgang Wenzel - Research Center Karlsruhe, "De-novo protein folding and structure prediction with free-energy forcefields"

Astronomy, Space and Earth Sciences

- José Luis Álvarez Pérez - Universitat Politècnica de Catalunya, "Numerical Simulation of Emissivity of Soils and Ocean"
- Miguel Ángel Aloy - Universidad de Valencia, "Explaining blazars and gamma-ray bursts with numerical relativistic magnetohydrodynamics"
- Marc Balcells - Instituto Astrofísico de Canarias, "Galaxy transformations through interactions, mergers and accretion"
- Estel Cardellach - Institut d'Estudis Espacials de Catalunya (IEEC), "Scattering of navigation satellite signals on realizations of the sea surface"
- José Antonio Font - Departament of Astronomy and Astrophysics, Universitat de València, "Bar-mode Instability in rapidly Rotating Magnetized Polytropes"
- Pablo Fosalba - Institut de Ciències de l'Espai, IEEC/CSIC, "Large Numerical Simulations for Dark-Enery Surveys"
- Juan García Bellido - Universidad Autónoma de Madrid, "Gravitational waves from preheating after inflation"
- Dimitri Komatitsch - Institut Universitaire de France. University of Pau, "SPECFEM3D"
- Victor Martin-Mayor - Universidad Complutense de Madrid, "Heisenberg Spin Glasses: Large Lattices at Low Temperatures"
- Fernando Moreno Danvila - Daniel Guirado Rodríguez, Instituto de Astrofísica de Andalucía, "Polarimetry of Light Scattered by Irregular Particles"
- Fernando Moreno-Insertis - Instituto de Astrofísica de Canarias, "Eruptive phenomena in the atmosphere of the Sun and cool stars"
- Manuel Prieto Rubio - Universidad de Oviedo, "A Quantum Mechanical Approach to the Nucleation Process of Calcium Carbonate"
- Blai Sanahuja, - Facultat de Física. Universitat de Barcelona, "Modelling Interplanetary CME-driven shocks and solar energetic particle events"
- Jordi Torra i Roca - Universitat de Barcelona, "Gaia: preparation of the data reduction"
- Gustavo Yepes Alonso - Universidad Autónoma de Madrid, "The MareNostrum Numerical Cosmology Project: Grand Challenge simulations of structure formation in the Universe"

Physics and Engineering

- Juan A. Acebron - Departament d'Enginyeria Informàtica i Matemàtiques, Universitat Rovira i Virgili, "Probabilistic Domain Decomposition for Partial Differential Equations"
- Irene Arias - Universitat Politecnica de Catalunya, "Scaling laws in complex material behavior"
- María del Mar Artigao Castillo - Escuela Politécnica Superior de Albacete, "Performance analysis of parallel algorithms fornonlinear time series analysis"
- Bruno Juliá Díaz - Dept. de Estructura i Constituents de la Materia, Universitat de Barcelona, "Dynamical Coupled-channel Analysis of Excited Baryons"
- Gerardo Delgado - Departamento de Física Atómica, Molecular y de Agregados Instituto de Física Fundamental Blas Cabrera, "Theoretical simulations in gas-phase clusters and liquids"
- Pablo Cerda Duran - Max-Planck-Institute for Astrophysics (Germany), "MHD instabilities in compact objects"
- Jordi Faraudo - Departamento de Física de la Universitat Autònoma de Barcelona, "Statistical Mechanics Of Ionic Liquids Under Confinement: Molecular Simulations"
- Luis Antonio Fernández - Universidad Complutense de Madrid, "First-order transition in a three-dimensional disordered system"
- Domingo Giménez Cánovas - Facultad de Informática. Universidad de Murcia, "High performance computation of Simultaneous Equation Models"
- Vicent Giménez Gómez - Dept. Fisica Teorica Universitat de Valencia and IFIC, "Monte Carlo numerical computations of the properties of hadrons"
- Fabien Godeferd - Laboratoire de Mécanique des Fluides et d'Acoustique. Ecole Centrale de Lyon, France, "High resolution numerical simulations of homogeneous turbulence with complex effects"
- Manuel María Gonzalez Alemany - Facultad de Fisica de la Universidad de Santiago de Compostela, "First-principles calculations for the electronic structure of semiconductor nanowires"
- Jorge Íñiguez, ICMAB-CSIC, "Multifunctional oxides"
- Pilar Hernández - Instituto de Fisica Corpuscular UV/CSIC, "Non-perturbative aspects of QCD in flavour physics"
- Thilo Knacke - Institut für Strömungsmechanik und Technische Akustik (ISTA), Technische Universität Berlin, "Numerical simulation of airframe noise"
- Asensi Oliva Llena - CTTC (Centre Tecnològic de Transferència de Calor), UPC , "Direct Numerical Simulation Of Turbulent Flows In Complex Geometries"
- José E. Roman - Universidad Politécnica de Valencia, "Scalability of Eigensolvers and SVD solvers in the SLEPc Library"
- Ángel Rubio - Universidad del País Vasco, "A dynamic landscape from femtoseconds to minutes for excess electrons at ice-metal interfaces"
- Ángel Rubio - Universidad del País Vasco, "Spectroscopic properties of biomolecules, nanostructures and extended systems (ETSF activity)"
- Juan Jesús Ruiz-Lorenzo - Departamento de Fisica, Universidad de Extremadura, "Critical behavior in three dimensional spin glasses in presence of magnetic fields"
- Javier Jiménez Sendín - Universidad Politécnica de Madrid, “Simulation of Turbulent Boundary Layers”

- Gabriel Staffelbach - European centre for Research and Advanced Training in Scientific Computation, "Towards Large Eddy Simulation of an industrial gas turbine"
- Vassilis Theofilis - School of Aeronautics. Universidad Politécnica de Madrid, "Global instability analysis of the trailing vortex system in the wake of commercial aircraft"
- Daniela Tordella - Politecnico di Torino (Italy), "Anisotropy and asymptotics in the mixing of shear-free homogeneous turbulent fields"
- Andreas G. Yiotis, Michael E. Kainourgiakis, Athanassios K. Stub, Institute of Nuclear Technology & Radiation Protection, "A Lattice-Boltzmann study of immiscible two-phase flow in pore networks"
- Markus Uhlmann, CIEMAT, Madrid - "Fully-Resolved Direct Numerical Simulation of Turbulent Channel Flow With Suspended Solid Particles"

Chemistry and Material Science

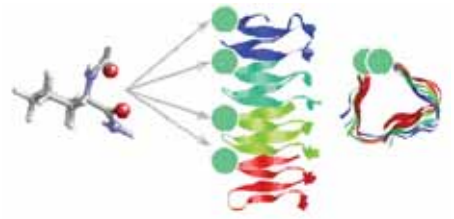
- Regla Ayala Espinar - ICMSE-CSIC, "Investigation of the Intrinsic Connectivity of Metal Aquaions and Polyoxoanions in Aqueous Solutions by means of Ab initio MD simulations"
- Regla Ayala Espinar - ICMSE-CSIC, "Solution Chemistry of Radioactive Po(IV) and Th (IV) ions: insights from ab initio molecular dynamics"
- G. C. Boulougouris and D. N. Theodorou - Department of Materials Science and Engineering. National Technical University of Athens, "Atomistic simulations of atactic polystyrene in the glassy state"
- Carles Bo - Institute of Chemical Research of Catalonia (ICIQ), "Computational modeling of nanocages: giant polyoxometalates"
- Sofia Calero Diaz - Department of Physical, Chemical and Natural Systems, University Pablo de Olavide, "Development of force fields for simulations of substrates and reaction intermediates-photocatalyst-zeolite interactions"
- Albert Cirera - Departament d'Electrònica. Universitat de Barcelona, "Modeling for NanoElectronics"
- Avelino Corma - Instituto de Tecnología Química UPV-CSIC, "Selective hydrogenation of nitroaromatics catalyzed by gold"
- José C. Conesa - Instituto de Catálisis y Petroleoquímica, CSIC, "DFT calculation of defects and electron localization at redox-active oxide surfaces"
- Victor Cruz - Instituto de Estructura de la Materia. CSIC, "Rheological and crystallization processes of metallocene based polymers by molecular dynamics simulations"
- L. Michel Espinoza-Fonseca - University of Minnesota, "Molecular dynamics simulations of the full-length M1 muscarinic acetylcholine receptor"
- Javier Fernandez Sanz - Universidad de Sevilla, "Computational modeling of Ru/HfO2 interface"
- Alberto García Vela - Instituto de Matemáticas y Física Fundamental, "Large scale simulations of solvation effects in the structure and dynamics of weakly bound clusters"
- Gregory Geneste - Ecole Centrale Paris, "Ab initio simulation of ionic conductors for solid oxide fuel cells"
- German Ignacio Sastre - Instituto de Tecnología Química (UPV-CSIC), Universidad Politécnica de Valencia, "Brønsted acidity of chabasite zeolite"

- Francesc Illas - Institut de Química Teòrica i Computacional & Departament de Química Física, Universitat de Barcelona, "Unraveling the molecular mechanisms of heterogeneous catalysis by combination of computational modeling and controlled experiment in model systems"
- Alfonso Jaramillo - Ecole Polytechnique, "Computational design of biosensors for explosives detection"
- Nuria López - Institut Català d'Investigació Química, " Computational high-throughput screening for the selective production of NO on platinum group metal surfaces and alloys from the degradation of ammonia on Ir nanostructured crystals: structure sensitivity " "The role of copper oxide nanostructures and their self-assembly on the initial stages of Cu oxidation" "The Chemistry of RuO2(110) in Selective Oxidations"
- Feliu Maseras - Institut Català d'Investigació Química, "DFT modeling of reactivity in an ionic liquid"
- Fernando Martín García - Universidad Autonoma de Madrid, "Two-photon double ionization of helium above and below the threshold for sequential ionization"
- Petr Nachtigall - Institute of Organic Chemistry and Biochemistry. Academy of Science of Czech Republic, "Theoretical investigation of metal-exchanged zeolites"
- Juan J. Novoa - Dept. Quimica Fisica, Universitat Barcelona, "Accurate methods for the theoretical prediction of polymorphic crystalline materials of technological interest"
- Gianfranco Pacchioni - Dipartimento di Scienza dei Materiali, Università di Milano, "Metal clusters on oxide ultra-thin films: the way towards new materials with unprecedented properties"
- Silvia Picozzi - CNR-INFM (Italy), "Ferroelectricity and magnetism in RMnO3 : Coupling mechanisms from ab-initio studies"
- Ramon Reigada Sanz - Universidad de Barcelona, "Molecular dynamics simulations for the study of mitochondria Cardiolipin membrane properties"
- Ramon Reigada Sanz - Universidad de Barcelona, "Effects of Cholesterol and headgroup charges on the structural properties of cell membranes"
- Octavio Roncero - Instituto de Matemáticas y Física Fundamental (CSIC), "Quantum non-adiabatic reactiondynamics"
- Eliseo Ruíz - Universitat de Barcelona, "Magnetic Properties of Large Single Molecule Magnets"
- Enrique Sánchez Marcos - Dept. Química Física, Universidad de Sevilla, "CPMD Study of Planar Metal Complexes of Pd(II) and Pt(II) in Solution"
- Miquel Solà - Universitat de Girona, "Chemical reactivity of D3h-C78 (Metallo) Fullerenes: Regioselectivity Changes Induced by Sc3N and Y3N encapsulation"
- Mariona Sodupe Roure - Dep. Quimica, Universitat Autonoma Barcelona, "Ab initio simulation of amorphous silica surface and its interaction with biological molecules"
- Marcel Swart - Institut de Química Computacional, Universitat de Girona, Institució Catalana de Recerca i Estudis Avançats (ICREA), "Parallel scaling of the Amsterdam Density Functional (ADF) program"
- Frederik Tielens - Université Pierre et Marie Curie, "Quantum Chemical Study of Self Assembled Monolayers of Mixed Thiols on Noble Metal and Metal Oxide Surfaces"

Carlos Alemán
Universitat Politècnica de Catalunya

Tubular Nanostructures Based on ProteinMotifs

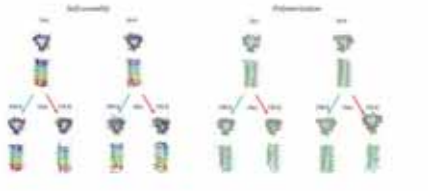
The effect of replacing natural amino acids by non-proteogenic residues in, β-helix building blocks (residues 131-165 of the 1krr) has been evaluated using extensive molecular dynamics (MD) simulations. Four different types of non-proteogenic amino acids have been considered for substitution: (i) one dehydroamino acid, (ii) two D-amino acids, (iii) one, β-amino acid and (iv) two α,α-dialkylamino acids. The results indicate that the ability of these amino acids to stabilize small building block motifs is site-dependent. The suitability of a synthetic amino acid such as 1-aminocyclohexane-1-carboxylic acid (Ac6c) to stabilize nanotubes made of self-assembled and covalently linked repeats of both 1hv9 and 1krr was investigated by using MD. Results lead us to conclude that, when replacing a natural residue located in the flexible loops of helical β-motifs by Ac6c, the stability of both the building blocks and nanotubes is enhanced.



Insertion of a synthetic amino acid in loop regions of nanoconstructs based on β-helical motifs

Atomistic molecular dynamics (MD) simulations have been used to examine different aspects of tubular nanostructures constructed using protein building blocks with a β-helical conformation. We considered two different neutral protein building blocks, which were extracted from the protein data base: residues 131-165 of E. coli galactoside acetyltransferase (1krr) and residues 296-329 of N-acetylglucosamine-1-phosphate uricyltransferase GlmU, C-terminal domain from E. coli (1hv9).

They were used to compare the relative stabilities of the nanotubes made of self-assembled and covalently linked repeats. Results show nanotubes constructed by linking building blocks through covalent bonds are very stable. The team also tested the effect of the change in the charge distribution in the inner core of the self-assembled 1krr nanotube, concluding that it is possible to generate de proper conditions for charge transfer inside these nanotubes by introducing different histidine ionization states in selected positions of the internal core of the construct, in addition to specific mutations with charged amino acids that altogether will allow the formation of coherent networks of aromatic ring stacking, salt-bridges, and hydrogen bonds.



Structure of self-assembled and polymerized nanotubes obtained from both 1krr and 1hv9 at the beginning and after 10 ns of MD simulation

Publications

N. Haspel, D. Zanuy, J. Zheng, C. Alemán, H Wolfson, R. Nussinov. "Changing the Charge Distribution of β-Helical-Based Nanostructures Can Provide the Conditions for Charge Transfer", Biophys. J. 2007, 93, 245-253.

D. Zanuy, F. Rodríguez-Ropero, N. Haspel, J. Zheng, R. Nussinov, C. Alemán. "Stability of Tubular Structures Based on β-Helical Proteins: Self-Assembled versus Polymerized Nanoconstructs and Wild-Type versus Mutated Sequences". Biomacromolecules 2007, 8, 3135-3146

D. Zanuy, F. Rodríguez-Ropero, R. Nussinov, C. Alemán. "Testing ,–helix motif stability by targeted substitutions with non-proteogenic amino acids: A Molecular Dynamics study". J. Struct. Biol. 2007, 160, 177-189.

Jaume Bonet
Structural Bioinformatic's Lab. Biomedical Informatics Research Unit, Parc de Recerca Biomèdica de Barcelona

Aligned profiles with multiples environments and methods: Selection of the best parameters

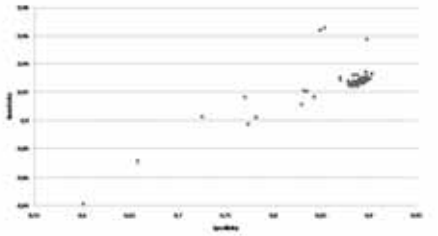
The comparison of multiple sequences might provide clues about the structure and function of a protein family. Sequence-profile or profile-profile alignment is important not only for protein annotation but also for comparative modelling. Due to this importance, several methods have been designed in order to obtain profiles of multiple sequence alignments. In spite of these advances, many errors are still found on the alignment of sequences in comparative modelling. Accurate sequence alignments are crucial in the regions of 20-30% pairwise sequence identity, where most often methods fail to correctly align these sequences.

The aim of this project is to combine the improvements obtained from 13 different methods of profile-profile alignment. The results will be used to create a database of sequence profiles of domains.

The team has completed the first section of the project and assigned the best scoring relation between similar methods. This way the group has calibrated between them the two variants of both COMMPASS and PICASSO methods, the three methods based on the sum of pairs and the four methods based on Pearson correlation. The best parameter combinations have been obtained by comparing our alignments with gold standard alignments and evaluating both sensitivity and specificity.

The team defined a family-calibration, a superfamily-calibration, a fold-calibration and a global-calibration for each group depending on the type of relation between the two aligned profiles (global-calibration does not take SCOP classification into account). Each calibration has two optimal solutions per group, which means that we have 16 combinations of optimal solutions when combining all the methods.

The team is calculating the best parameter combination between the different methods for each profile-profile relation. From which the team has completed several combinations of parameters for both family and fold analysis.
The other part of the project is developing a database that will contain profiles for almost 3 million proteins, a prediction of their domains, and interactions among them.



Parameters benchmarking of weighted combination of methods for family-calibration. It can be seen that range of results cover more than 0,3 points of specificity and 0,12 of sensibility

The whole database of domains and the server for profile-profile alignment is intended to serve as a powerful tool for further research on the proteomics field. The group expects to provide the scientific community with a fast and versatile tool for the research on the proteomics field. The database, with millions of precomputed protein alignments, will be accessible by the scientific community via a web server. This fast access to the results can save a lot of time and computational resources to the users, while the profiles can be used for computing more reliable protein alignments. Additional aspects of interest of this project are the development of a method for predicting protein domains and protein interactions. The future perspectives of this project are multiple: once the database and the method is constructed, both the method and the database can be extended for other research in protein analysis regarding protein sequence. The existence of such a complete database offers many possibilities not only for the external researches accessing this data, but also for further development and improvement on the method we use.

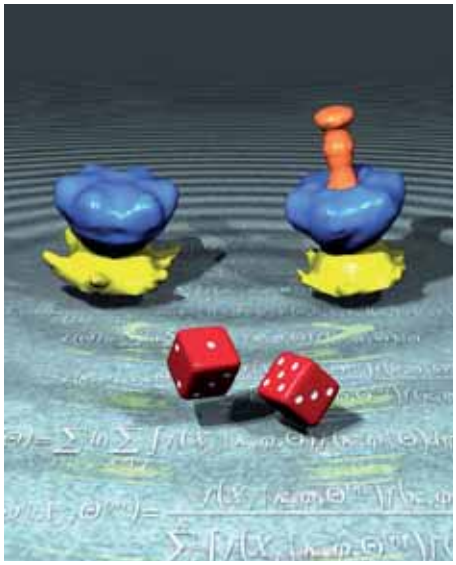
The database, that in the previous report contained the blast searches for nr40 (sequences with less than 40% of homology), nr60 and has been recently updated to nr90.

José María Carazo
Centro Nacional de Biotecnología – CSIC

Maximum-likelihood classification of structurally heterogeneous electron microscopy data

Many processes in the living cell are performed by very large macromolecular complexes, called molecular machines. Similar to daily-life machines, these complexes typically use relative movements of distinct parts of their machinery to carry out their functions in the living cell. In principle, cryo-electron microscopy allows visualization of flexible macromolecular assemblies in their various functional states. However, the inability to classify noisy projection data from structurally heterogeneous samples has posed serious limitations on this technique. The team is developing new classification methods based on maximum-likelihood principles. The fundamental novelty of this approach lies in the formulation of statistical models for the experimental noise in the data. In 2007, the team has provided a convincing proof-of-principle, showing that maximum-likelihood classification may be used to classify structurally heterogeneous electron microscopy data without depending on prior knowledge about the structural variability in the sample. Furthermore, the group formulated an improved statistical model to better describe the experimental situation of correlated noise. Using this improvement, we were for the first time capable of visualizing 3D density for double-stranded DNA sticking out of large T-antigen dodecamers.

The obtained data sets may contain up to billions of data points, and the proposed approach may take several months of CPU to classify a single experiment. In an editorial comment on the publication in Nature Methods, Dr. Sigworth called our application "perhaps the most audacious application of the expectation-maximization algorithm ever performed". Without the increasing supercomputing capabilities at MareNostrum, it would not be feasible to apply this type of algorithms to the tremendous problem of classification of structurally heterogeneous cryo-electron microscopy data sets. Therefore, the team also notes the importance of a related activity that was launched in 2007, where several experimental electron microscopy groups have joined up to apply these new algorithms to some of their most challenging biological problems.



Carbon dioxide adsorbed in MOR type zeolite at 300K and 1000 KPa

Robert Castelo
Univ. Pompeu Fabra, Barcelona

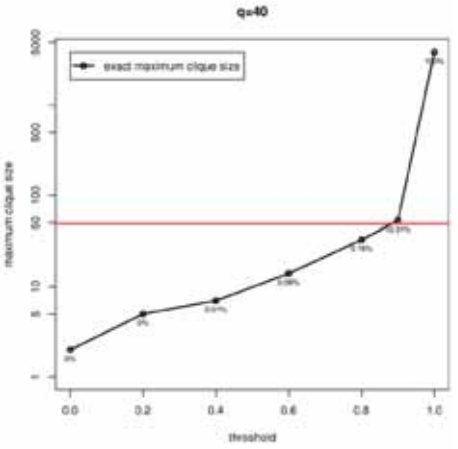
Simulation and learning of large biomolecular networks using graphical Markov mod

Microarray data probe simultaneously thousands of elements along the genome in a smaller number of experimental conditions. The resulting expression data matrix has thus a dimension that precludes the direct application of standard statistical methods for learning multivariate models of the networks of interactions among the probed elements. We are parallelizing the methods we have developed for learning these models, which are computationally demanding and therefore require supercomputing environments.

The results of this project will have an impact in the way co-expression networks can be reverse-engineered from microarray data. Currently most of the methods in the literature for this purpose learn bivariate models of these networks which are unable to distinguish direct from undirect co-expression associations. The use of the methods for learning mutlivariate models, like the ones being developed in this project, overcome this limitation and will be of great help to unravel the regulatory program that we observe through microarray experiments.

The current methodology allows us to assess whether the available data allows one to recover a multivariate model with reasonable reliability and, in such a case, enables that learning process by means of the so-called qp-graphs learned with our methods.

By using a supercomputing environment as MareNostrum we can try to tackle the reverse-engineering of multivariate models of co-expression networks for thousands of probed elements from a microarray expression experiment. Such a dimension would be infeasible to approach outside such an environment.



Plot obtained from breast-cancer microarray data on 3883 genes and 49 samples (West et al., PNAS, 2001). The plot shows the dimension (y-axis) of the networks resulting of applying different thresholds (x-axis) on the non-rejection rate of every pair of vertices. The red horizontal line indicates the available number of samples. A usable network should have a dimension smaller than the number of samples while the lower the threshold the larger the probability of wrongly removing interactions. For this data we observe that we need a threshold of 0.8 indicating that the underlying network might not be sufficiently sparse for the available data. The non-rejection rates were calculated in MareNostrum in about 1 hour using 80 processors while this would require about 2 days in a non-parallel machine

Albert Compte

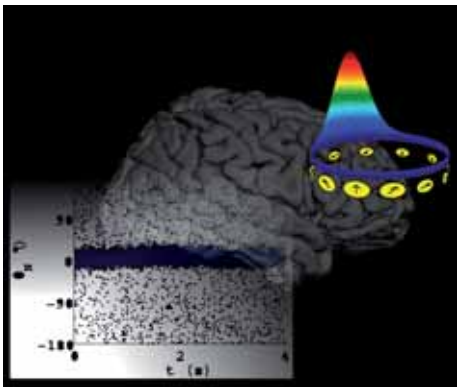
Institut d'Investigacions Biomèdiques August Pi i Sunyer (IDIBAPS)

Exploring the specificity of the relationship between cortical network function and biological simulation parameters with a particle swarm optimization algorithm

Traditionally, computational neuroscientists generate computer implementations of neural circuits that perform specific brain functions, such as vision, decision, memory, attention, etc. while relying on the tacit assumption that the nervous systems of all individuals use the same mechanisms to accomplish the corresponding function. However, recent findings in small networks in invertebrates or in anatomically detailed neuron models have shed doubts on this usual assumption. These investigations argue against a biological predefinition of mechanisms, and rather support a biological quest for function with many different possible (qualitatively different) mechanistic implementations. The team attempts here the exploration of this situation for current state-of-the-art large biological network models of cortical function. The team studies the compactness in parameter space of network models able to perform a specific neural computation (working memory, attention, sensory normalization,...), seeking to find out whether there are many qualitatively different network architectures that sustain similar activity, and how they differ from each other.

Apart from the biological insight that emerges for each specific neural function, this research activity will allow to develop and test a new methodological approach to biological neural network modeling. This approach relies on the usage of an optimization algorithm to explore the large parameter space of these neural network simulations searching for constellations of parameters that allow the network to perform the desired function. Such a search was typically accomplished by manual trial-and-error. The use of a supercomputer like MareNostrum, with its enormous computational power, allows us to carry out this search efficiently. The team can then analyze questions that were beyond earlier methodological approaches, such as: how many different scenarios are there given our assumptions? In what aspects do they differ? How could we discard or validate these different scenarios experimentally?

The team has focused so far on the phenomenon of working memory. This psychological capacity was studied computationally extensively and there are a number of biophysical models available. The group choses one of these models and asked whether the same basic assumptions could subserve a whole family of similarly operating networks. The team ran the search for these different networks in 2007 and we are now analyzing the results. The group has obtained 24 different networks that are able to replicate the basic phenomenology of neurophysiological experiments in the prefrontal cortex of awake behaving monkeys performing a working memory task. Preliminary inspection of the various networks reveals that there are qualitatively distinct network organizations that can accomplish similar operations. The team is in the process of analyzing quantitatively the network solutions and prepare the corresponding publication.



Xavier de la Cruz
Parc Científic de Barcelona

Molecular Dynamics Simulation of the Folding/Unfolding Mechanism of Apoflavodoxin

Apoflavodoxin from Anabaena is a α/β, globular protein with 169 residues (pdb code: 1FTG). Apoflavodoxins display a classic α/β, fold, comprising a parallel five-stranded central, β-sheet and a small three-stranded, β-sheet surrounded by five α-helices. Apoflavodoxin is an interesting model to investigate the folding/unfolding mechanism by both experiment and computational simulation.

The aim of this project is to study the structural and energetic aspect of apoflavodoxin transition state and intermediate under the urea and thermal denaturation. In order to thoroughly understand the folding/unfolding event of apoflavodoxin at atomic level, the team performed several long term (at least 500 ns) MD simulations under natural and denaturation conditions (urea and thermal denaturation) using a variety of force fields: CHARMM, AMBER and OPLS. Additionally, ϕ-guided molecular dynamics simulations based on structural experimental results helped to drive the protein structure towards the thermal intermediate and urea transition state, respectively.

Thanks to the increasing supercomputer capabilities of MareNostrumó it is feasible to simulate so much extensive trajectories. The results obtained from the simulations of the thermal unfolding show that the unfolding mechanism is being complicated by the existence of a thermal intermediate with a similar structure to the native protein, where most of the secondary structure domains are maintained, except for the loop corresponding to the long-chain flavodoxins. The result correspondent to the simulations of the chemical denaturation suggest also the presence of a transitory intermediate, different from the thermal one, where some of the native secondary structure domains are unstructured. Longer simulations will lead to a more unfolded structure of apoflavodoxin and will offer the possibility of studying the lifetime and characteristics of these interesting intermediates.

Native structure

Thermal denaturation
(500 ns, NAMD/Charmm)

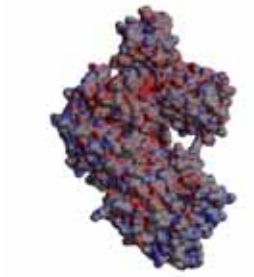
Urea denaturation
(300 ns, NAMD/Charmm)

Natalia Díaz
Universidad de Oviedo

Computational Modelling of Matrix Metalloproteinases: Influence of the Hemopexin-like domain in the MMP-2 enzyme

The computational work carried out in the BSC is framed into a long-term research project devoted to the study of both the matrix metalloproteinase enzymes (MMPs) and their most relevant substrates, the collagen molecules. The MMPs are a family of structurally-related, zinc- and calcium-containing enzymes that play a central role in all physiological processes requiring tissue turnover and remodelling. However, their expression is also known to increase in various inflammatory, malignant and degenerative diseases, which converts these enzymes in potential drug targets for the treatment of some of these prevalent pathologies. Besides the catalytic domain, the MMPs present a second domain with a hemopexin-like structure that is essential for the collagenolytic activity performed by these enzymes. To analyze the structure of this C-terminal fragment and its interaction with the catalytic domain in the full-length MMP-2 enzyme, we have performed several molecular dynamics (MD) simulations of the fully solvated systems. The MD trajectories complement structural information from X-ray crystallography and provide some clues about the "mechanical" mode of action of the MMP-2 enzyme in order to bind and process a complex macromolecule like collagen.

Ribbon model of the full-length MMP-2 enzyme after 66 ns of MD simulation in aqueous solution. Zn(II) and Ca(II) ions are shown as magenta and green CPK spheres, respectively



Molecular surface mapped by electrostatic potential

Publication

N. Díaz and D. Suárez "Molecular Dynamics Simulations of Matrix Metalloproteinase 2: The Role of the Structural Metal Ions" Biochemistry, 2007, 46, 8943-8952.

Hernán J. Dopazo
Centro de Investigación Príncipe Felipe

From Historical Gene Pattern to Darwinian Molecular Processes. Towards a complete catalogue of adaptative events ocurring after gene duplication in the human phylome

The origin of organismal complexity is generally thought to be tightly coupled to the evolution of new gene functions arising subsequent to gene duplication. Under the classical model of evolution of duplicated genes most copies degenerate by accumulating deleterious mutations (pseudogenization or nonfunctionalization), while the other retains the original function. On rare occasions, one duplicate may acquire a new or a related adaptive function (neofunctionalization) resulting in the preservation of both members of the pair. In spite of its popularity, the classical model fails at moment to explain the high number of duplicate genes observed in nature. Alternatively, the duplication-degeneration-complementation model (DDC) assumes that degenerative mutations (most occurring in regulatory regions) facilitate rather than hinder the preservation of duplicate functional genes. Under this model, the fates predicted by the classical model are indeed considered and a new one is possible if each daughter gene adopts part of the function of their parental gene (subfunctionalization or specialization). The failure of the classical model rest on the simplistic view of gene structure. Genes often have several functions, each of which may be controlled by different DNA regulatory elements controlling tissue-specific expression patterns. Since the changes of gene expression after gene duplication appear to be the rule rather the exception and seems to occur quickly after gene duplication, the high number of duplicated copies observed in species does not represent a theoretical problem for the DCC model.

In the current project the group aims to define events of neofunctionalization and subfunctionalization by specialization using the information derived from the Human Phylome project previously developed in MareNostrum supercomputer. The group aims to obtain a systematic, reliable and statistically significant description of adaptive processes occuring in all the duplicated genes of the human genome. After our previous project in MareNostrum, the team defined the full set of orthologous and paralogous genes of the human genome in a phylogenetic context. The main question to solve is a major questions in molecular evolution, namely: What is the realtive importance of positive selection in paralogous gene evoltion? Using the full set of orthologous and paralogous genes we can assess the relative numbers of gene differentiation by positive selection after duplication.

After finishing the runs, the team obtained the first results of the project searching for the assymetic distribution of the selective constraints at different times of duplication origin.

Gloria Fuentes
Centro Nacional de Investigaciones Oncológicas

RAS superfamily and the interactions with their effectors: functional specificity

Ras genes code for small GTPases that act as GDP/GTP-regulated molecular switches involved in many biological pathways. Conformational changes allow them to interact with regulators and effectors.

Structural techniques have partly unraveled the Ras:effectors interaction mechanism. However, this set of PPIs is redundant and does not represent all partners. Possible Ras binding partners detected in vivo and reported in databases also span other protein families. So far, the studies carried out to rationalize the specificity of Ras proteins towards their effectors have been based only in this set of Ras:effector crystal structures.

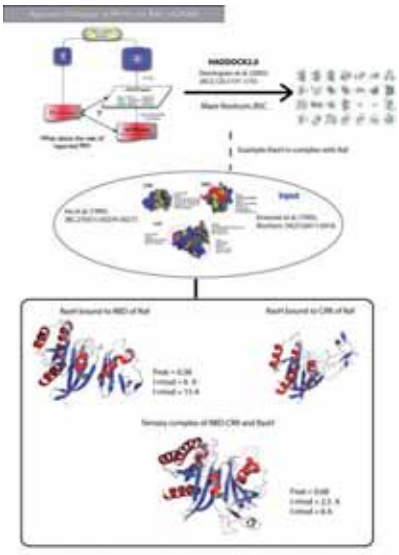
The team has extended this to a large-scale bioinformatics and computational study, including driven-docking of Ras:effectors for which no complex structure is available but biological data supports complex formation.

During this period the group screened several Ras:effector associations, trying to scan the whole Ras superfamily and understand the specificity for each subfamily. Although more detailed study and analysis is needed, certain important points already surface. The accuracy of the models obtained after docking strongly depends on the input data. When only bioinformatics information is available, the team obtained models of medium-accuracy (test-runs were also carried out for already-solved complexes). These models, and especially the putative mutations obtained from them, can serve as leading points for molecular biologists to either confirm or reject the solutions.

When the team adds experimental information, the complexes modeled get very close to the crystal structures (for RasH:RAF1, an Fnat of around 0.7 was found; see figure). In these cases, we identified a high number of cross-talking between the Ras pathways, due to sharing effectors. Another fast conclusion obtained is the necessity to move from the one-domain-biology to the full-length and "sociology-biology" to better understand the mechanisms governing biology. Regarding the previous example, we see that RasH has a high tendency to bind to the RAF1 kinase using two domains (RBD and C2), as previously reported in vivo, and unlike the in vitro complex solved by crystallography that only includes RBD in the preparation of the structure.

High-throughput proteomics has yielded detailed lists of proteins present in a cell. However, little was known about the interaction of these proteins. Emerging experimental techniques are bringing this possibility. This information on protein-protein interactions could be translated into atomic models from which to obtain putative mutations (to disrupt/strengthen interactions, alter specificity, etc) as well as provide template structures for the "visual proteomics" projects.

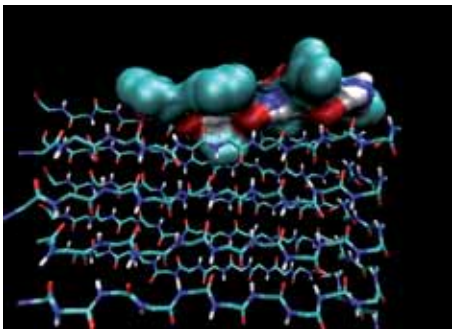
To achieve a challenge like that, algorithms are already available, but this will require a large number of computational resources and time. This is the point where MareNostrum could serve as an indispensable tool. Although the algorithm used in this approach, HADDOCK2.0, was not the most suitable for the requirements of MareNostrum, some changes were done and future work on the optimization of the program will help to achieve this putative mutation map and template structure library.



Ernest Giralt
Institut de Recerca Biomèdica (IRB Barcelona)

Evolutionary Algorithms and de Novo Peptide Design

The program “Evolutionary structure de Novo Peptide Design Algorithm” (ENPDA) has been developed to design peptide inhibitors against an user defined target. The implementation of different kind of evolutionary techniques is necessary to tackle the huge search space. The team has used a ß-amyloid fibril model as a target for peptide drug design. ß-amyloid fibrils are an important target related with Alzheimer's disease. The ENPDA software attempts to evolve individuals by applying natural evolution principles. The goal of our evolutionary process is to obtain good individuals, peptides, that bind to the ß -amyloid fibril target. In order to measure the binding energy ENPDA uses docking calculations.



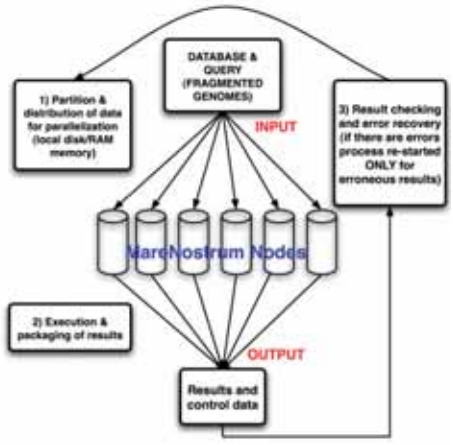
De novo peptide design were performed with ENPDA using a basis set of hydrophobic amino acids (Phe, Ala, Val, Leu). The genetic algorithm was run for 30 generations. The best peptide was obtained for FVLFFF

Roderic Guigó
Parc de Recerca Biomèdica de Barcelona

Use of TBLASTX to find regions of homology among multiple large-size full genomes

The predictive power of many bioinformatic tools makes use of similarities between genomes, which can be detected computationally using the intensive algorithm TblastX. In the R. Guigó Genome Bioinformatics group at the "Centro de Regulación Genómica" (CRG) in Barcelona the team used MareNostrum (MN) to run TblastX to find regions of homology (in the form of High-Scoring pairs -HSPs-) between full genomes (i.e. Mouse vs. Human). Running TblastX to find potentially conserved regions between different species is an essential component of the homology-based gene prediction tool SGP which has been developed by the group. Generally TblastX comparison among species with large genomes, such as Human and Mouse, would require 7-10 days on a 20-25 processor grid. However, MN´s processing speed and especially parallelization potential allows the same work to be performed in approximately 12 hours (on 256 CPUs and excluding queuing time). This is important because it allows to execute TblastX to find homologies among many different genomes at the same time, in a reasonable time frame, which would be impossible to achieve locally or using a smaller computer grid. This, in turn, allowed the group to develop and improve SGP for large genome species to a level which would be unattainable by using a smaller grid. In past the team used a MN-optimized version of the TblastX algorithm to look for orthologous regions between different assemblies of *H. sapiens* and *M. musculus*, to compare an older version of the cow genome against previous assemblies of H. *sapiens* and *M. musculus* and to look for matches between the rat genome and older assemblies of the Human genome. The team also extended our TblastX comparisons to include analyzing assemblies of the chimp, rhesus monkey, rabbit, and other mammals that are of interest in our studies. The group also continuously update our more standard full-genome comparisons (i.e. Mouse vs Human, Rat vs Human, Cow vs Human or Mouse) as new

genome assemblies become available. Finally, the team was involved in a collaboration to annotate the current version of the Bovine genome (Btau3). The SGP homology-based gene prediction program is to be one of the tools employed in this annotation and for this purpose the team will be running TblastX comparisons among different mammalian genomes against that of the cow, in order to try and optimize the performance of SGP. Moreover it is expected that a new cow assembly will be available within the next few months and we expect to have to re-run TblastX of this updated version of the genome against other mammalian genomes. SPG homology-based annotations of the Mouse, Rat, Human, Cow and Chicken ,many of which obtained with the help of MN, can be seen both at the golden path (UCSC - http://genome.ucsc.edu/cgi-bin/hgGateway) genome browser and as local DAS annotations (http://genome.imim.es:8080/das/) to the ensembl web browser (http://www.ensembl.org). As previously mentioned the group hopes to extend the annotations to several new mammalians species and new assemblies of already available genomes.



TblastX execution pipeline diagram

Publication
SGP homology-based annotations obtained using TblastX: comparison data obtained at MN: Identification and analysis of functional elements in 1% of the human genome by the ENCODE pilot project. The ENCODE Project Consortium. Nature 447, 799-816 (14 June 2007)

Francisco Javier Luque
Universidad Barcelona

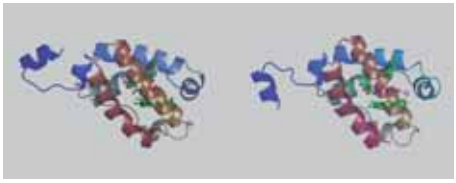
Unraveling the molecular mechanisms of ligand migration in Mycobacterium tuberculosis truncated haemoglobin N

Mycobacterium tuberculosis, the causative agent of human tuberculosis, is forced into latency by nitric oxide produced by macrophages during infection. In response to nitrosative stress *M. tuberculosis* has evolved a defence mechanism that relies on the oxygenated form of "truncated haemoglobin" N (trHbN), formally acting as NO-dioxygenase, yielding the harmless nitrate ion.

Extended molecular dynamics (MD) simulations allowed us to unravel the molecular mechanisms that control diatomic ligand diffusion through the apolar tunnel system. Our results pointed out that O2 migration in deoxy-trHbN is restricted to a short branch of the tunnel, and that O2 binding to the heme drives conformational and dynamical fluctuations promoting NO migration through the long tunnel branch. This is achieved by modulating the conformation of residues TyrB10 and GlnE11, which regulate the dynamical behaviour of helices B and E.

MD simulations were also successful in deciphering the mechanism involved in the eggression of the nitrate anion. The results indicate that formation of the product promotes a large structural change in the active site, which favors the entrance of water molecules, whose interaction with the nitrate anion facilitates breaking of the corrdination to Fe(III). In addition, a new eggresion pathway to the bulk solvent was identified.

Overall, the simulation results suggest that trHbN has evolved a dual-path mechanism for migration of O2 and NO to the heme active site and for fast eggresion of the nitrate anion, which ensures an efficient NO detoxification.



Publications

A. Bindon-Chanal, M. A. Martí, D. A. Estrín, F. J. Luque Dynamical Regulation of Ligand Migration by a Gate-Opening Molecular Switch in Trunacted Hemoglobin-N from Mycobacterium tuberculosis. J. Am. Chem. Soc. 2007, 129, 6782-6788.

M. A. Martí, A. Bidon-Chanal, A. Crespo, S.-R. Yeh, V. Guallar, F. J. Luque, D. A. Estrín Mechanism of Product release in NO Detoxification from Mycobacterium tuberculosis Hemoglobin N, J. Am. Chem. Soc. In press

Sara Marsal

Institut de Recerca Hospital Universitari Vall d'Hebron

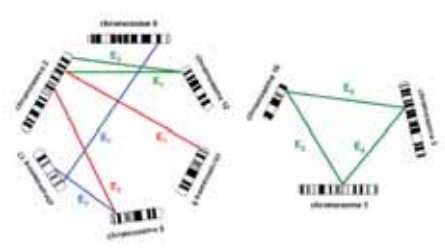
Whole genome epistatic modelling in Rheumatoid Arthritis and Chronic Inflammatory Arthritis

Rheumatoid Arthritis is a chronic inflammatory disease that affects 1% of the population worldwide. The aetiology of RA is unknown, but several family aggregation and twin studies clearly show that there is a heritable component of the disease. Part of this genetic component of susceptibility has been consistently associated to the HLA class II locus variation. The remaining 50-75 % of the genetic component includes several other genomic regions that are more being difficult to identify either due to their lower penetrance or by acting through more complex genetic models. One of such complex models is epistasis, in which combinations of genes yield more information on the disease than the sum of the information from each individual gene.

Genomewide genotyping has recently enabled the transition from candidate gene studies (i.e. genes selected based on –often limited- biological knowledge), to a systematic evaluation of the complete genome. New candidate genes of genomic regions are being added to the genetic architecture of complex diseases. Thus, genomewide scans are also a fundamental tool to resolve a fundamental question in any particular human disease: is there a genetic epistasis susceptibility component? However, answering this question still confronts several difficulties. Two of the most important obstacles for genomewide analysis for epistasis are the efficiency of analytical algorithm used and the need of a vast computational power.

The team has performed a genomewide scan for Rheumatoid Arthritis in 400 patients and 400 controls in the Spanish population. 317,503 Single Nucleotide Polymorphisms (SNPs) have been genotyped per individual amounting a total of 254e6 genotypes. Using the computational power of MareNostrum the team has been able to rapidly test and optimize several epistasis algorithms in the genomewide scale. These include Multifactor Dimensionality Reduction

and Constructive Induction analysis algorithms. Using MareNostrum the team has been able to perform an exhaustive analysis for epistasis and determine a group of gene-gene interactions that are strongly associated to i) Rheumatoid Arthritis ii) Highly erosive Rheumatoid Arthritis and iii) Chronic Inflammatory Arthritis susceptibility. These analyses have identified new relevant loci for RA susceptibility which, through main effect analysis, would have been discarded. Also, the present study downsizes the relevance of HLA region in the epistatic dimension and emphasizes the need to perform exhaustive genomewide epistasis scans in the study of RA and, by extension, of any particular human disease.



Top epistatic interactions identified through exhaustive genomewide analysis of 317,503 SNPs in 400 patients and 400 controls. Interacting genomic regions are connected by colored lines (i.e. green: susceptibility to RA, blue: susceptibility to highly erosive RA, red: susceptibility to Chronic Inflammatory Arthritis). Some genomic regions are shared by different epistatic pairs, suggesting the existence of higher order genetic networks

Publication

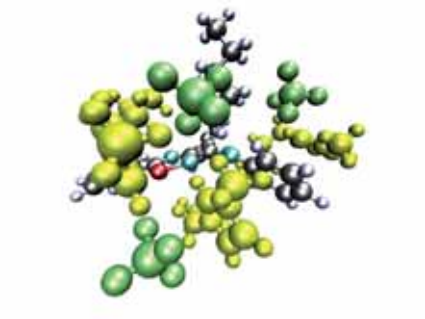
Julià A, Ballina J. Cañete et al. "Genomewide Association Study of Rheumatoid Arthritis in the Spanish population" Submitted.

Feliu Maseras
Institut Català d'Investigació Química

DFT modeling of reactivity in an ionic liquid

Room temperature ionic liquids (RTIL) have generated tremendous enthusiasm in recent years as a new type of solvents. They are viewed as an alternative to the highly contaminant nature of organic solvents often used in the chemical industry. RTIL's possess a very low vapor pressure, and are easier to separate, thus providing a cleaner and more sustainable option. The precise effect of the RTIL environment in chemical reactivity remains largely unexplored from a computational point of view, and it seems difficult to treat with the continuum approaches often applied to more conventional solvents.

The team has applied the powerful computational resources of the Barcelona Supercomputing Center to the problem. In particular, the team has analyzed what would be a reasonable density functional theory (DFT) approach to describe the effect of the presence of the ionic liquid [BMIM][BF4] on the energy barrier for the amine-assisted SN 2 intramolecular rearrangement of the Z-phenylhydrazone of 3-benzoyl-5-phenyl-1,2,4-oxadiazole. The results are of similar quality to those obtained in the reproduction of the barrier in a conventional solvent as water. Analysis of the results furthermore indicates how the ionic solvent lowers the barrier with respect to the value in vacuum. The cation and the anion of the solvent interact strongly with the charge centers that appear in the rate determining transition state, and thus lower its energy with respect to the reactants. The study also suggests that explicit treatment of two ion pairs is a much better solution than use of one, because of the overefficient stabilization associated to the case when a single ion pair is considered. The result of this first investigation of reactivity in an ionic liquid is encouraging and opens the path to apply this same computational approach to study the reactivity of other chemically relevant processes in room temperature ionic liquids.



Explicit introduction of two ion pairs provides a first reasonable estimation of the effect of an ionic liquid on chemical reactivity taking place in this solvent

Publication
F. Bessac, F. Maseras; "DFT modeling of reactivity in an ionic liquid: How many ion pairs?", J. Comput. Chem., in press.

Milagros Medina
Universidad de Zaragoza

Action mechanism of flavoenzymes: a MD Study

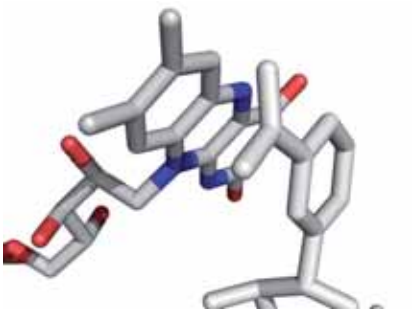
The goal of this project is to increase the knowledge of the parameters that maintain reactions involving flavoproteins, in particular those participating in electron transfer processes.

Mechanism of interaction and electron transfer between FNR and its coenzyme, NADP+; In biological systems many vital functions depend on electron transfer processes where flavoproteins are involved due to their unique ability to mediate two-electron transfer processes with those involving a single electron. Ferredoxin-NADP+ reductase (FNR) is a flavoenzyme that during the photosynthesis catalyses the reduction of NADP+ to NADPH by accepting electrons from Photosystem I via ferredoxin (Fd) or flavodoxin (Fld). Although the overall mechanism of this reaction is well known, the mechanisms of electrons and hydride transfer are not well understood. This includes the hydride transfer from the FNR flavin to NADP+ in one step to produce NADPH, as well as the previous placing of the reactive centres of FAD and NADP+ in adequate conformation for hydride transfer is still not understood. Comparative MD simulations of the wild-type and Tyr303Ser FNR forms are being carried out in order to study the mechanism of reorganization of the FNR-NADP+ interaction to achieve a functional hydride transfer model. Additionally, the importance of the 2'P of NADP+/H in determining FNR coenzyme specificity versus NAD+/H has been stated by analyzing the role of the residue Y235 of Anabaena FNR in adequate coenzyme binding and orientation for hydride transfer. MD simulations with Y235F or Y235A FNR mutants confirm the importance of the stacking interaction between Y235 and the 2´P of NADP+. The results are consistent with experimental data.

Flavodoxin: a model for determining the flavin properties within the protein environment. The team has experimentally produced a series of FMN analogues that have been used to

reconstitute Anabaena Flavodoxin previously depicted from its FMN cofactor. The reconstituted Flavodoxins have been experimentally characterized. The effect produced on the flavin oxido-reduction properties and flavin binding affinity depends critically on the modification introduced into the protein. In silico models have been produced and a comparative molecular dynamics simulations study of the wild-type and 3-methyl-FMN, 7-demethyl-8-Cl-FMN, 7,8-diCl-FMN, 7-demethyl-8-Cl-FMN and 7-Cl-8-demethyl-FMN reconstituted flavodoxins in the oxidized, semiquinone and reduced states has been inititated. This required the previous Determination of the force field parameters of the oxidized, semiquinone and reduced states for FMN and each one of the FMN analogues: 3-methyl-FMN, 7-demethyl-8-Cl-FMN, 7,8-diCl-FMN, 7-demethyl-8-Cl-FMN and 7-Cl-8-demethyl-FMN).

The FAD synthetase mechanism. To clarify the mechanism of action of the C. ammoniagenes FAD synthetase and the analysis of the binding order of its 4 substrates MD simulations of the three structural modelled structures obtained for this protein have been carried out. The obtained data show the presence of high flexible regions, suggesting where substrate binding might take place during the enzyme catalytic mechanism.



Putative optimal orientation between the flavin ring of FAD in FNR and the nicotinamide portion of the NADP+ coenzyme for hydride transfer

Communications

I. Lans, S. Frago and M. Medina. Contribution of the FMN electronic distribution to the conformation of the isoalloxazine environment in Anabaena Flavodoxin: a simulation analysis. Poster. International Network on Protein Engineering Centers, INPEC 2007. Jaca (Spain) June 2007

I. Lans, S. Frago, M. Medina. Computational study of Anabaena flavodoxin by point changes in the flavin ring of the FMN cofactor Poster. Trends in Transient Interactions Between Biological Macromolecules. Sevilla (Spain) May 2007.

Arcadi Navarro i Cuartiellas
Universitat Pompeu Fabra

Genomic Distribution of Ancestral and Recent Natural Selection in the Human Genome

Increasing evidence about the action of natural selection at the genomic scale has highlighted the interactions between natural selection and function that shape the adaptation of humans to their environments. Our knowledge, however, is far from complete. For example, most studies focus on coding regions and thus we ignore how adaptation is distributed in the genome. Another limitation is that most studies have difficulties in coping with complex demographical histories and tend to make simplifying assumptions. Our 2007 activities were centred in these two related areas. First, we analyzed the molecular footprint of ancestral and recent selection in human introns using a Maximum Likelihood (ML) method that makes use of human-chimpanzee alignments. And, second, we studied how certain neutrality tests, commonly used to detect selection perform under a wide range of demographic scenarios.

As for the first issue, we achieved the first genome-wide ML estimation of divergence in human introns and coding regions and, thus, the first list of introns for which there is evidence of positive selection in some of their sites (in both our lineage and that of the chimpanzee). Our results in that area will be completed during 2008 by using a complementary ML method that allows increasing statistical power by using multiple alignments from various species. As to the second, we obtained a comprehensive study of the behaviour of the most widely used statistical tests.

Publications

Marquès-Bonet, T., J. Sanchez-Ruiz, R. Khaja, L. Armengol, N. Lopez-Bigas, J. Bertranpetit, M. Rocchi, E. Gazave, and A. Navarro, 2007. On the association between chromosomal rearrangements and genic evolution in humans and chimpanzees. Genome Biology 8: R230.

Gazave, E., T. Marques-Bonet, O. Fernando, B. Charlesworth and A. Navarro, 2007. Patterns and rates of intron divergence between humans and chimpanzees. Genome Biology 8:R21.

Ángel R. Ortiz
Centro de Biología Molecular "Severo Ochoa", CSIC-UAM

Including solvent effect and receptor flexibility in virtual screening via rescoring techniques

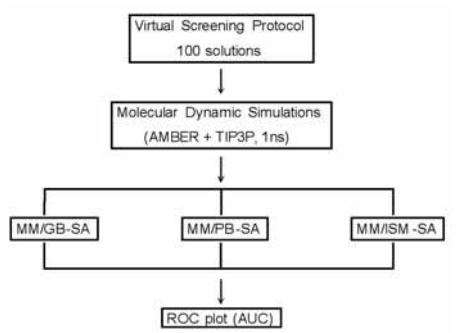
Docking and virtual screening are routinely used tools in the search for, discovery of, and improvement of drug molecules. Despite the advances in both computer algorithms and power, it seems that we have arrived to a plateau. There are at least three main reasons for this: a) the huge universe of chemical structure, b) a reliable method to include solvent effects into the scoring functions in a fast and accurate way, and c) the inherent flexibility that all the proteins/enzymes present. The first issue could be alleviating in principle by the use of precompiled and already synthesized molecule from different vendors. Solvent and flexibility are much more complicated and challenging tasks.

In a typical virtual screening workflow, these last two effects are not taken into account properly at early stages mainly due to computational limitations. Rescoring of selected poses with more accurate scoring functions in addition to molecular dynamics calculations are the usual way to include solvation and flexibility, respectively, once the docking was performed.

There is little knowledge about the convenience of applying molecular dynamic simulations and accurate solvation models on dynamics results as a tool for a better enrichment in virtual screening environment. The scarce results indicate a target specific effect and the dominant role played by the accuracy of the docking algorithm employed.

Within this project we have addressed this question studying the influence of flexibility (via molecular mechanics minimization and molecular dynamics trajectories), and solvent effect (PBSA, GBSA, ISMSA) on several target (AChE, fXa, ERa, and CDK2) using results obtained from previous virtual screening experiment. The best 100 molecules for each target were selected and submitted to 1 ns of non restrained molecular dynamics simulation. Solvation calculations were performed over

snapshots taken from the trajectories and then averaged. The results obtained after the application of the different protocols were analysed using ROC plot technique. Initial results have been presented at the VIII Jornadas de Bioinoformática, last February in Valencia.

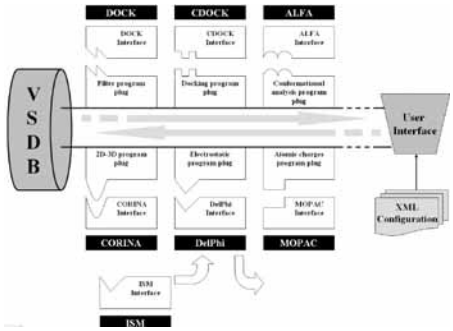


VSDB: A platform for virtual screening computations

The use of computer-based techniques to aid in the discovery of new drug candidates is a commonly employed strategy today. In this context, virtual screening is an emerging technology that tries to find out, from a pool of thousand or even millions of compounds, only those with high probability to be classified as leads. The engine underlying virtual screening is in most of the cases a docking program. To get success in a docking experiment, and also in virtual screening, two main elements are needed: an efficient sampling algorithm, able to account for all possible ligand-receptor orientations (configurations or poses); and an accurate scoring function to discriminate, among all the configurations, the one that correspond to the native pose of the ligand within the binding site of the receptor.

The group is developing a computational, flexible, and fully automated platform to perform virtual screening experiments. It combines all the needed steps to generate a short list of candidates beginning from a database of molecules with 2D structure. It is intended to fill an existing gap in docking and VS fields related to the storage and management of the data. The platform was developed in C/C++ programming languages providing good execution times, great functionality and versatility. The database management system is performed in MySQL using MySQL++ package which offers an object oriented interface with the database.

The aim of this project was to port and test this virtual screening system in MareNostrum. The technical objectives have been fully accomplished. The team successfully implemented a MySQL based relational database within MareNostrum. Also, all the programs needed for the correct implementation of our VSDB were compiled and are running normally. It was also needed to develop some codes in order to use the GRID superscalar programming environment, which was done successfully. Finally, the team used 128, 256, and 400 processors during 72 h periods.



An efficient conformational sampling method for Homology Modeling

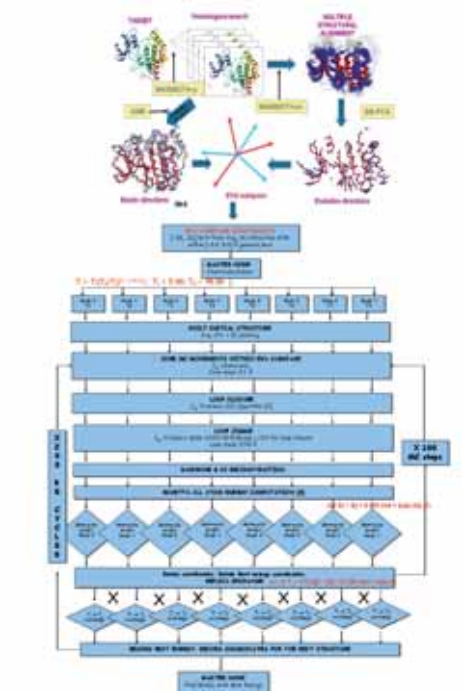
Predicting the structure of a protein is a keystone in Computational Biology. While solving the problem “ab-initio” still faces huge theoretical and computational difficulties, “comparative modeling” techniques are continuously improving towards the task to build accurate 3D models even for relatively distant homologues of already known protein structures.

All the comparative modeling techniques try to solve two very hard problems: the choice of the best template structure, through reliable alignment techniques, and the 'a posteriori' energy refinement. The team concentrated on the second problem, since it has been reported

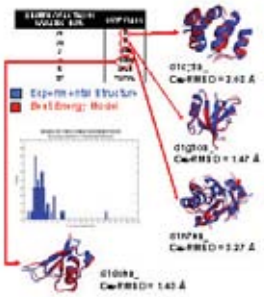
that even for a perfect initial alignment the refinement step is more likely to cause degradation of the final model rather than improvement. In general the limitations of refinement are mainly due to the inaccuracy of the free energy function adopted, on one side; and the difficulty to sample properly the high dimensional and rugged free energy landscape, on the other side.

A new refinement strategy was developed by the group in order to tackle the sampling problem. The method creates a reduced sampling subspace by combining the evolutionary favored directions along the members of homologous protein structures, with the subspace defined by the lowest frequency anisotropic normal modes, up to a total of 50 dimensions. This subspace is as accurate as to represent the cores of most of the proteins within 1 Å Cα-rmsd, and as reduced as being effectively sampled by Replica Exchange Monte Carlo simulations (REMC).

The group implemented the REMC sampling in a parallel Fortran77 program.The team tested it first using a Go-like energy function based on the Rmsd from the native structure plus a large amount of frustration to make the sample problem more difficult. The team is using the Rosetta all-atom energy function. The figure below summarizes our last implementation of the protocol.



The group tested the last version of the refinement protocol simulations on 57 ASTRAL40 protein domains of different SCOP classes, using 8 temperatures (replicas) per system. The preliminary results are summarized in the second figure. In this figure, the quality of the modeled protein cores, for the best energy models is shown as a histogram of the Cα-rmsd distribution (modeled cores versus experimental structure), together with the optimal structural superpositions (best energy modeled core onto experimental structure) and the corresponding Cα-rmsd for a member of each SCOP class.



The team is improving the protocol to assess the quality and convergence of the simulations using Rosetta's energy, through different criteria, both pure statistical and derived from first principles in statistical physics. Hence the team needs to test multiple simulations in multiple processors and different temperatures, for many protein structures. Without the massive computer facility and support of RES at the IAC node in La Palma, the team could never achieve those highly demanding computational tasks.

Manuel Palacín
Parc Científic de Barcelona

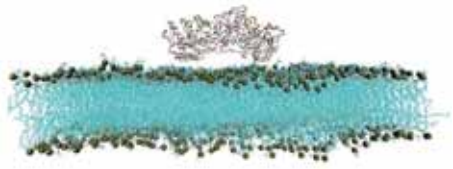
Study of 4F2hc ectodomain-induced membrane curvature by means of MD

Heteromeric Amino acid Transporters (HATs) are composed of two subunits: a polytopic membrane protein, (the light subunit) and a disulfide-linked N-glycosylated type II membrane glycoprotein (the heavy subunit), that appears to be essential only for trafficking to the plasma membrane. Two types of heavy subunit (4F2hc and rBAT) and 10 types of light subunit have so far been identified.

Two different architectures of human 4F2hc ectodomain have been recently solved. The structure of human 4F2hc ectodomain provides a model for homodimerization and electrostatic interaction with plasma membrane: monomer (monoclinic crystals) and a homodimer (orthorrombic crystals). Overexpression of human 4F2hc in heterologous expression systems results in the formation of homodimers linked by a disulfide bridge involving residues Cys109. This allows to build-up a model for 4F2hc insertion in the membrane, where the bottom surface of the 4F2hc homodimer has a relevant patch of positive charged residues, suggesting an electrostatic interaction with the polar heads of phospholipids.

Using NAMD and Molecular Dynamics the team aims to model the association of the monomer and dimmer of 4F2hc ectodomain on the plasma membrane surface. Thanks to the increasing supercomputing capabilities such as MareNostrum, it is feasible to treat such big systems, containing more than 740.000 atoms.

Molecular dynamics of the dimmer of 4f2hc ectodomain showed that it was stable along the time, independently of the presence or not of the crystallographic Zn ion situated between the two monomers. The effect of this dimeric structure over a mixed and asymmetric membrane composed by POPC, POPE and POPS was also studied by molecular dynamics, reaching 15 ns of simulation. The results suggest that the membrane begins to suffer a depression in the zone where the dimmer was situated.



View of the system after 15 ns of simulation. Water molecules are removed for clarity

Florencio Pazos
Centro Nacional de Biotecnología (CSIC)

Prediction of Protein Interaction Specificity

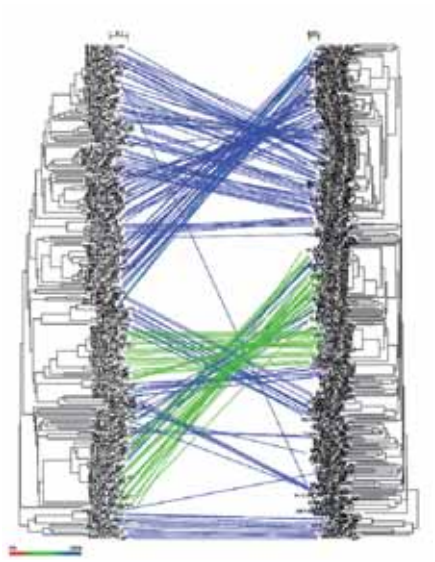
The biological function of many proteins can only be understood in the context of their relationships with others. For this reason, in recent years many experimental and computational techniques were developed with the aim of deciphering the network of protein interactions for a given proteome (interactome).

One of the computational techniques for predicting and studying protein interactions widely accepted by the community is based on the consistent relationship found between protein interactions and similarity of phylogenetic trees. The hypothesis that explains this relationship states that physically or functionally interacting proteins are subject to similar evolutionary pressure and forced to adapt to each other, both factors resulting in similar evolutionary histories, which are in turn reflected in similar trees.

In order for two trees to be compared, a mapping between their leaves has to be established (set of links between the leaves). Hence, having a common rationale behind, this mirrortree approach has two main angles. Either this mapping is known (for example implicit in the orthologous relationships) and the tree similarity according with it is calculated to asses the possible interaction between the two families, or the interaction is known and the consequently (expected) high similarity is used to look for the right mapping (the pairings between the members of both families). This situation is particularly common in eukaryotic organisms where there are many cases of large families of interacting paralogues (e.g. a family of ligands and their corresponding receptors) for which only one or a few pairs of interacting proteins have been experimentally determined, and where the goal is to decipher the entire set of interactions between the two families.

The way in which these methods work is by exploring different sets of relationships between two families of interacting proteins on the basis that the correct mapping will be that which maximizesthe similarity between the trees. These methods use an heuristic (Monte Carlo) approach to explore the space of solutions (possible mappings) since the exhaustive exploration is unfeasible. Due to their intrinsic heuristic nature, these methods do not ensure the global best solution to be found, and they are easily trapped within local sub-optimal solutions. To partially overcome this problem, these methods are run several times in the search for a consensus between the different analyses, commencing each execution from a different point in the solution space. All this make that these methods are highly CPU-demanding, what hindered their assessment in large sets of interacting families.

In this project, the team developed a variation of these methodologies wich is able to incorporate information regarding orthologues, or any other assignment of proteins to "classes" that may restrict possible mappings (avoiding pairings between proteins of incompatible classes, i.e. between proteins of different organisms or of different cellular compartments). These constraints speed up the Monte Carlo search and improve the results. Moreover, this increasing in speed, together with the computing power of the BSC allowed to test, for the first time, this class of methodologies in large datasets of interacting proteins in order to statistically asses its performance and its dependence on the characteristics of the input data. We tested the new method on a large set of 604 protein domains (forming 488 interacting pairs) obtaining and accuracy around 80% correct pairings in the most favourable cases. The group also analysed in detail the results of the method for a well defined case of interacting families, the sensor and kinase components of the Ntr-type two-component system, for which up to 98% of the pairings predicted by the method were correct.



Predicted mapping between the sensor and kinase components of the Ntr-type two-component system. The color of the links indicate their confidence

Ruben Pérez
Universidad Autónoma de Madrid

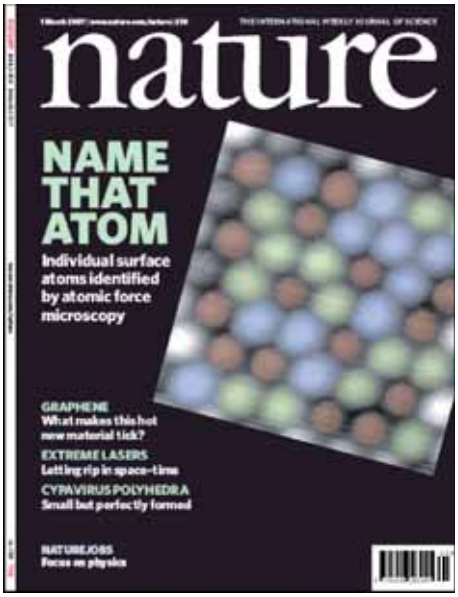
Interaction of Atoms and Molecules with metals and metallic oxides characterized by first-principles calculations and simulations of surface imaging techniques

The common purpose of this activity is to gain insight into the interaction of atoms and molecules with metals and metallic oxides combining first-principles simulations with state-of-the-art experimental techniques. In this broad field, we focus on some paradigmatic examples --including tip-sample interactions in Atomic Force Microscopy (AFM), electronic and mechanical characterization of organic/metal interfaces, structure and properties of 1D structures on oxide surfaces, conductance quantization in clean and contaminated nanocontacts, and stress-strain characteristics in alkaline-earth tungstates for device applications— that are relevant from both a basic perspective and in prospective technological applications. Our theoretical approach combines first-principles total energy calculations with the theoretical simulation of different surface science experimental techniques (like LEED and AFM) that are used to characterize these systems.

Significant progress has been achieved in some of these areas. We have continued our characterization of the catalytically relevant TiO2(110) surface.The simulations of the LEED-IV data have shown that a recently prop osed model for the (1x2) reconstruction (Park et al. Phys. Rev. Lett. 96, 226105, (2006)) where Ti atoms are located on interstitial sites with Ti2O stoichiometry is not consistent with the experimental results, that favored the Ti2O3 added row model. Furthermore, we have explored the possible presence of soft modes in the usual (1x1) reconstruction, where these low-energy distortions could explain the additional contrast observed in recent, detailed STM measurements.

In the case of metallic nanowires, we have completed a first-principles study of the evolution of the mechanical and transport properties of clean and contaminated Au

nanowires during the whole breaking process, combining DFT and Green's function methods. The presence of adsorbed atomic impurities introduces significant changes in the conductance, providing a quantitative explanation for the new peaks found in the conductance histograms. The enhanced chemical reactivity, leading to the dissociation of the molecular species, can be traced back, through the analysis of the local density of states,to both the reduced coordination and the applied tensile strain.



Our first-principles simulations for the tip-sample interaction have contributed to the development of a protocol for the chemical identification of individual atoms on surfaces with the Atomic Force Microscope

Regarding dynamic AFM, our combination of quantitative force spectroscopy experiments with first-principles simulations of the tip-sample interaction has paved the way for the extension of the single-atom characterization and manipulation capabilities of AFM. Our simulations have unveiled and put on a firm quantitative basis the atomistic mechanisms involved in the lateral manipulation of single tightly-bound atoms on semiconductor surfaces. Furthermore, we have developed a protocol for the chemical identification of individual atoms on surfaces.

Publications

M. Blanco-Rey, J. Abad, C. Rogero, J. Méndez, M. F. López, E. Román, J. A. Martín-Gago, and P. L. de Andrés, "LEED-IV study of the rutile TiO2(110)-1x2 surface with a Ti-interstitial added-row reconstruction", Physical Review B 75, 081402(R) (2007)

Y. Sugimoto, P . Jelinek, P. Pou, M. Abe, S. Morita, R. Perez and O. Custance. " Mechanism for Room-Temperature Single-Atom Lateral Manipulations on Semiconductors using Dynamic Force Microscopy", Physical Review Letters, 98, 106104 (2007).

Y. Sugimoto, P. Pou, M. Abe, P. Jelinek, R. Perez, S. Morita and O. Custance, "Chemical identification of individual surface atoms by atomic force microscopy", Nature, 446, 64-67 (2007).

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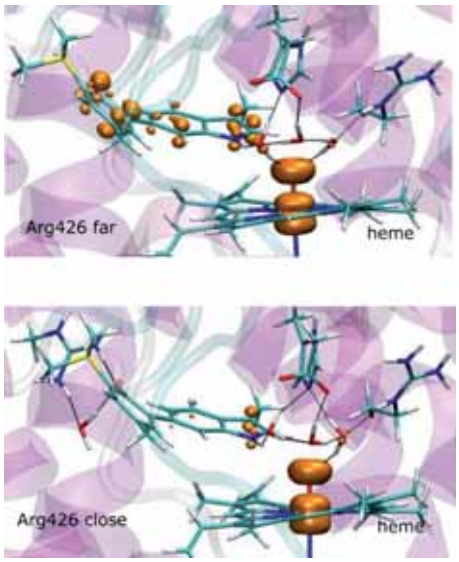
Unraveling the reaction and drug activation mechanisms in Mycobacterium tuberculosis catalase-peroxidase by means of Car-Parrinello QM/MM simulations

The Mycobacterium tuberculosis catalase-peroxidase (MtKatG) is a multi-functional enzyme which activates isoniazid (INH), the front line drug to treat tuberculosis. The precise knowledge of the enzymatic mechanism is of fundamental importance in understanding both the activation process of the drug and the significance of enzyme mutations responsible for drug resistance. In this project the team models these mechanisms by means of Car-Parrinello QM/MM molecular dynamics simulations, in comparison with monofunctional catalase and peroxidase enzymes. During 2007 the group characterized the protonation state of reaction intermediates of catalase and catalase-peroxidases, as well as the mechanism of its formation. It was found that the catalytic power of one single water molecule is crucial to lower the energy barrier of the reaction in Horse radish peroxidase. In catalases, a relation was found between the protonation of the radical intermediate and the occurrence of electron transfer from the protein. Instead, the location of the unpaired electrons in catalase-peroxidase depends on the flipping motion of a residue that is not in direct contact with the active site. Unraveling the relation between this versatility of the reaction intermediate with drug activation is our next goal. Because of the large number of atoms to be treated quantum mechanically (about 250), this investigation required the usage of a large number of MareNostrum processors. This investigation is performed in collaboration with the experimental groups protein crystallography.



Electronic structure of the principal species of the catalytic cycle of catalase-peroxidase in the ative site region obtained from Car-Parrinello QM/MM calculations (from reference 3)

Publications

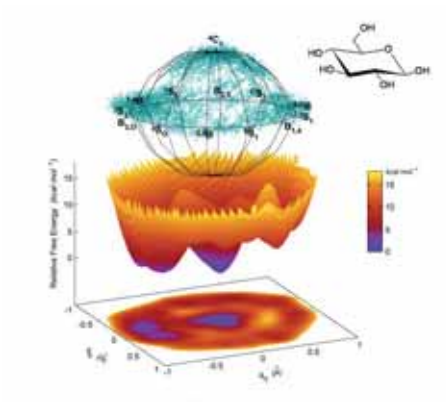
E. Derat, S. Shaik, C. Rovira, P. Vidossich, M. Alfonso-Prieto, "The effect of a water molecule on the mechanism of formation of Compound 0 in HRP". J. Am. Chem. Soc. 2007, 129, 6346-6347.

M. Alfonso-Prieto, A. Borovik, X. Carpena, G. Murshudov, W. Melik-Adamyan, I. Fita, C. Rovira, P. C. Loewen, "The structures and electronic configuration of compound I intermediates of Helicobacter pylori and Penicillium vitale catalases determined by X-Ray crystallography and QM/MM DFT calculations". J. Am. Chem. Soc. 2007, 129, 4193-4205.

P. Vidossich, M. Alfonso-Prieto, X. Carpena, P. C. Loewen, I. Fita, C. Rovira, "Versatility of the electronic structure of compound I in catalase-peroxidases (KatGs)". J. Am. Chem. Soc. 2007, 129, 13436-13446.

Activation of glycoside hydrolases by specific carbohydrate-protein interactions

The activity is aimed at deciphering the mechanisms of substrate specificity in glycoside hydrolases (GHs), the enzymes responsible of the hydrolysis of glycosidic bonds in carbohydrates, means of ab initio QM/MM molecular dynamics simulations. Recent structural studies show that the substrate changes conformation upon binding to the enzyme. Computer simulation represent a powerful aid to the identification of the substrate distortion, since it allows to investigate directly the native substrate-bound enzyme. During the last two years the team has investigated the dynamics of the carbohydrate-protein interaction using the Bacillus 1-3,1-4-beta-glucanase enzyme as a test case. This study has revealed that one part of the substrate undergoes a ring distortion upon binding to the enzyme that favors the enzymatic reaction. By means of ab initio metadynamics simulations we showed that the distortions occurring in beta-glucoside hydrolases can be rationalized from the conformational free energy landscape of one sugar unit (see picture). The next goal is to predict specific modifications of these enzymes that could affect its catalytic activity, as well as designing experiments to test these predictions. Thanks to the MareNostrum it is feasible to do this project, in which a large number of atoms needs to be treated quantum mechanically. This investigation is performed in collaboration with the experimental group of Biotechnology of the Universitat Ramón Llull.



Trajectory of the metadynamics simulation projected on the conformational sphere of beta-D-glucopyranose. The reconstructed free energy landscape is shown below

Publications

X. Biarnés, A. Ardèvol, A. Planas, C. Rovira, A. Laio, M. Parrinello, "The conformational free energy landscape of beta-D-glucopyranose. Implications for substrate preactivation in beta-glucoside hydrolases. J. Am. Chem. Soc. 2007, 129, 10686-10693.

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Campus Universidad Autónoma

Analysis of large three-dimensional electron microscopy data sets by computationally intensive algorithms

Many processes in the living cell are performed by very large macromolecular complexes, called molecular machines. Similar to daily-life machines, these complexes typically use relative movements of distinct parts of their machinery to carry out their functions in the living cell. One of the emerging experimental techniques to study these flexible complexes is cryo-electron microscopy. However, as this technique yields data sets that may contain billions of data points, the image processing involved is computationally extremely intensive. Therefore, in this activity several experimental cryo-electron microscopy research groups (which are at the forefront of structural biology in Spain) joined with the aim of applying novel image processing algorithms to their experimental studies. In particular, the separation of distinct conformational states of the flexible complexes under study would be prohibitive without the computing resources available at the BSC. However, with the use of MareNostrum, for two projects of the participating groups a successful classification of their experimental data could be performed. The first case concerned the characterization of the complex formation between human chaperone CCT and the chaperonin called Hsc70. The second case concerned the structural characterization of a DNA-repair complex (between DNA ligase IV and Xrrc4).

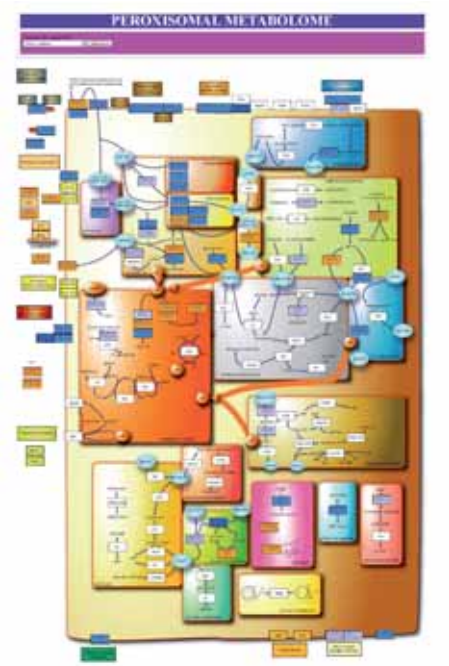
Agatha Schlüter
Institut d'Investigació Biomèdica de Bellvitge

Peroxisomal Metabolome Characterization and Evolutionary Origen

The peroxisome is a dynamic cell component that plays a key role in several metabolic routes, notably the oxidation of fatty acids and oxidative stress. The importance of peroxisomes for normal mammalian development and growth is underlined by the existence of severe inherited diseases in humans, the peroxisomal disorders, often fatal. However, knowledge on organelle biogenesis, metabolic functions and their key players, and the evolutionary history of peroxisomes is still incomplete. Full understanding of peroxisomal metabolic networks is limited because only a few of the estimated peroxisomal proteins have been identified experimentally, due to technical limitations. The objectives are: i) Identification of novel peroxisomal components, and novel key players of peroxisome metabolic networks; ii) searching the ancestors of peroxisomal enzymes and providing clues about the biological events or pressures that forced the generation of the organelle.

The team generated and integrated the peroxisomal metabolome data according to the following data sets: a) Orthology. The group proved a set of 46 eukaryotic complete genomes with our data core (an ensemble of 103 proteins, from man and yeast, which the team had previously curated as truly peroxisomal proteins, collected and organized in different pathways in www.PeroxisomeDB.org. The results were 2331 new peroxisomal proteins in the 46 full sequenced genomes that will be included in PeroxisomeDB b) Peroxisomal targeting signals (PTS). Identification of proteins bearing the targeting signals: PTS1, PTS2 o PEX19BS using available predictors that we have developed and integrated in PeroxisomeDB. The team identified 1126 proteins with PTS in the 46 new genomes c) Peroxisomal protein domains. The group identified the presence of 185 specific protein domains, found to be exclusively peroxisomal in the 46 new genomes. d) In the resulting peroxisomal metabolome, the team designed 137 HMM (Hidden Markov model) profiles for searching the ancestors of peroxisomal enzymes

in 353 bacterial and 28 archaea genomes, which led to the identification of more than 50.000 related proteins. By using the phylogenetic tools (MrBayes) the team defined which ancestors might have transferred, at once or sequentially in the evolution, the different peroxisomal enzymes or routes that constitute the peroxisome today.



Wolfgang Wenzel

Research Center Karlsruhe

De-novo protein folding and structure prediction with free-energy forcefields

Protein structure prediction and the elucidation of the protein folding process remain important grand computational challenges with many application in the life-sciences. In the last years the team has developed models and algorithms which permit reproducible and predictive folding of small proteins (up to sixty amino acids) from random initial conformations using a free-energy approach. The group exploits Anfinsons thermodynamic hypothesis that many proteins are in thermodynamic equilibrium with their environment under physiological conditions. The unique three-dimensional native conformation of the protein can then be predicted as the global optimum of a suitably free-energy model. Using efficient stochastic optimization methods, the global optimum of the complex protein thee-energy surface can be found orders of magnitude faster than by traditional simulation techniques.

The team has parameterized an all-atom free-energy forcefield for proteins (PFF01/02), which is based on the fundamental biophysical interactions that govern the folding process. The group has also developed, or specifically adapted, efficient stochastic optimization methods (stochastic tunneling, basin hopping, parallel tempering, evolutionary algorithms) to simulate the protein folding process. Forcefield and simulation methods are implemented in the POEM (Protein Optimization with free-Energy Methods) program package.

With this approach the team was able to predictively and reproducibly fold more than a dozen proteins in simulations starting from random initial conformations.

During the period of the present activity, the team performed simulations of the helical protein 1ENH and the mixed protein 1OPC and obtained further insights in the mechanism of protein folding. In particular, the group was able to demonstrate that the protein folding in silico is consistent with the “all-or-none” principle known from the melting experiments.

This fact, being of fundamental importance, will help to develop more efficient search algorithms for de-novo protein structure predictions.
Using the computational power of the MareNostrum permits to extend the scope of the approach to describe novel aspects of protein structure simulation that cannot be addressed with laboratory scale computational resources.

Publications

A. Verma, S. M. Gopal, J.S.Ooh, K.H. Lee, and W. Wenzel. All atom de-novo protein folding with a scalable evolutionary algorithm. J. Comput. Chem. 28, 2552 (2007)

A. Verma, S. M. Gopal, A. Schug, J. S. Oh, K. Klenin, K. H. Lee, W.Wenzel. Massively parallel all atom protein folding in a single day. Proceedings of the 2007 ParCo Conference, Jülich

A. Verma and W. Wenzel. Predictive and reproducible de-novo all-atom folding of a - hairpin loop in an improved free energy forcefield. J. Phys: Cond. Matter 19, 285213 (2007).

Srinivasa M. Gopal and Wolfgang Wenzel. All atom folding studies of a DNA binding proteinin a free energy forcefield. J. Phys: Cond. Matter 19, 285210 (2007).

José Luis Álvarez Pérez
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Numerical Simulation of Emissivity of Soils and Ocean

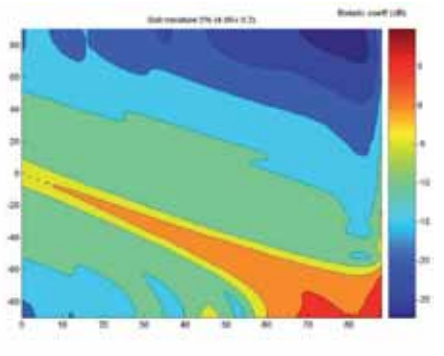
The problem of analyzing and modeling the scattering and emission phenomena at microwave frequencies for Earth surface natural targets that can be described as rough surfaces has been the objective of this project. It amounts on previous experience both in numerical simulation methods and actual data acquisition. The problem has been approached by using the method of moments (MoM) based not only on compactly supported functional bases but on global support. The traditional MoM does not rely on completeness of functional bases, but on achieving a reasonably accurate solution for a given set of functions and in the sense of minimizing the norm of the residual error. Due to the symmetry of the problem, bases introducing alternative Hilbert space structures for the solution space have also been used in the work performed at MareNostrum. In particular, a basis of separable functions corresponding to a cylindrical system of coordinates produce Bessel functions as a spectral representation in the same way as a Cartesian system produces a basis of plane waves.

The main results of the simulations performed with MareNostrum summarizes as follows:

1) In terms of the scattering coefficients, a MoM based on the Hilbert space basis of Bessel functions provides a 0.1-dB accuracy and makes it possible to reduce to a 10% of the number of functions in a pulse + Dirac deltas basis of a traditional MoM.

2) In terms of emissivity, results can be kept above 99% accuracy by using a Bessel functional basis as small as the 15% of the pulse + Dirac deltas basis.

3) We have obtained a comprehensive sample of results for a great number of situations in terms of roughness level, autocorrelation value, soil humidity and ocean salinity, which cover all those parameter space regions that are explained by classical analytical methods as well as others that are beyond the reach of these asymptotic models.



Example of the bistatic scattering coefficient from nadir incidence to grazing angles where interesting phenomena dealing with surface waves can be observed

Publication

Alvarez-Perez, J. L., Vall-llossera, M., Nieto-Borge, J. C., Comparison of different separable basis functions for the application of the Method of Moments on rough surface scattering, International Geoscience and Remote Sensing Symposium, IGARSS 2007, 23-28 July, Page(s):81 – 84, 2007.

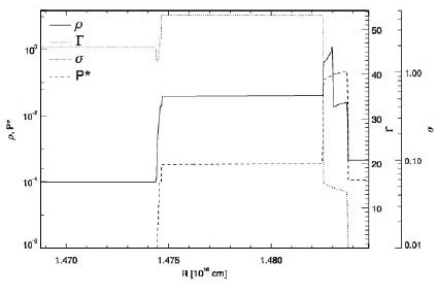
Miguel Ángel Aloy
Universidad de Valencia

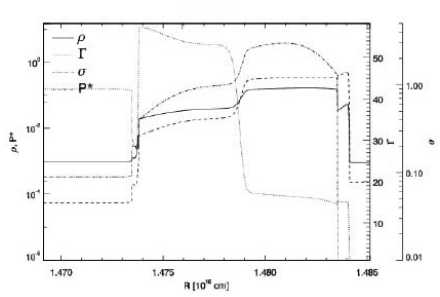
Explaining blazars and gamma-ray bursts with numerical relativistic magnetohydrodynamics

The general purpose of the research is to study the variability properties of relativistic outflows, focusing on the implications to the observed light curves of rapidly varying compact sources of non-thermal radiation such as gamma-ray bursts (GRBs) and blazars. To study them the group uses the so-called internal shock model, (applied to blazars and to the prompt phase of a GRB) and the external shock model (applied to the GRB afterglow phase). Internal shocks are generated by collisions of dense shells in a relativistic outflow whose velocity is nonuniform, while the interaction between the shell and the interstellar medium generates external shocks in the later stages of a GRB. Relativistic shocks accelerate particles to very high energies, and the radiation which is observed on Earth is caused by the synchrotron radiation emitted by these particles gyrating in the magnetic field behind the shocks. The team computes the evolution and synthetic observations using a sophisticated relativistic magnetohydrodynamic, finite volume code MRGENESIS which enables to perform high resolution simulations of magnetized shell evolution and collision under extreme conditions generated by the relativistic outflows of GRBs and blazars (velocities very close to the speed of light, high density and pressure contrasts, highly magnetized outflows). Parallel computation on the RES computers enables to properly capture physics of blazars and GRBs, follow the evolution for a sufficiently long time and run a large enough number of models in order to be able to improve our understanding of the connection between the observed radiation and the not directly observable magnetohydrodynamic properties of relativistic outflows.

During the past year, the team has used the computers of the RES to perform high-resolution (several millions of computational zones) numerical studies of the transition from the prompt to the early afterglow phase of GRBs. The afterglow is modeled as the radiation from a relativistic shell expanding into a homogeneous external medium. The team hase studied the difference between the ?reball (unmagnetized shell) and the Poynting-?ux dominated (magnetized shell) models. So far, only one-dimensional simulations have been performed since they are extremely expensive. The reason being that the simulations have to cover the propagation of relativistic shells for more than two decades in radius (from 1014 cm to 1017 cm) and, at the same time, it is necessary to resolve magneto-fluid scales of the order of 1012 cm. In the context of the early optical afterglow, the group has shown analytically that even a moderate magnetization of the ?ow can suppress the existence of a reverse shock, and thus explain the apparent paucity of the optical ?ashes (a very characteristic signature of GRBs that can be detected using optical telescopes) for a large number of early afterglows.

The team has currently performing simulations to study the formation and suppression of relativistic shocks in detail. To study the later phases of the afterglow we aim to determine the in?uence of the initial shell magnetization on the energy content, transfer of energy from the shell to the forward shock, and the long-term ?ow structure. The group has developed a novel scheme for treating non-thermal processes in relativistic magnetohydrodynamic simulations. This scheme is used to compute multi-wavelength light curves from numerical simulations. The aim is to study the in?uence of the initial magnetization on the short- and long-term light curves.





Snapshots from relativistic hydrodynamical simulations of a spherical, non-magnetized (σ0 = 0; top panel) and magnetized (σ0 = 1; left panel) shell that decelerates interacting with external medium of density 10 cm?3 . The total energy of the shell is E = 1051 erg, its initial width Δ0 = 1014 cm and bulk Lorentz factor y0 ? 50. P? (dashed line), ρ(solid line) stand for the gas pressure and (lab frame) density respectively (in arbitrary units). With increasing radius, one can clearly see the reverse shock, contact discontinuity and forward shock located at r ? 1.483 · 1016 cm

Publications

Mimica, P., Giannios, D., Aloy, M. A., "An RMHD study of transition between prompt and afterglow GRB phases", accepted. To appear in Proceedings of the conference "Supernovae: lights in the darkness", October 3-5, 2007, Maó (Menorca).

Aloy, M. A., Mimica, P., "Ultrarelativistic out?ows associated to progenitors of Gamma-Ray Bursts", accepted. To appear in Proceedings of the conference "Supernovae: lights in the darkness", October 3-5, 2007, Maó (Menorca).

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Galaxy transformations through interactions, mergers and accretion

Understanding the transformations that occur when galaxies interact and merge can only be done with numerical simulations, due to the extreme non-linearity of the physical processes taking place during interactions. Processes include gravitational tidal fields, hydrodynamics, and star formation. In numerical models of galaxy interactions, accuracy is limited by the spatial resolution, which determines the accuracy of the resulting maps, as well as the accuracy of the gravitational potential, and, hence, the dynamics. This Activity uses RES supercomputers to reproduce such processes at higher resolution than is feasible on standard desktop computers. The team runs models with 1.5 million particles using the code Gadget2.

Line-of-sight velocity distributions (LOSVDs) in the cores of elliptical galaxies provide fossil records of the processes that delivered mass to the galaxy cores. When an LOSVD is asymmetric, the easiest interpretation is that a disk of stars, formed from deposition of gas in the center, is superimposed on top of the overall spheroidal mass distribution. Previous studies by the group showed that mergers with purely elliptical galaxies of unequal masses also lead to asymmetric LOSVDs. The demonstration of this process requires a very detailed modelling of the nuclear dynamics of the merging galaxies. During 2007, an extensive battery of models for the merger of elliptical galaxies with varying the nuclear density contrast have been run. Analysis is in progress.

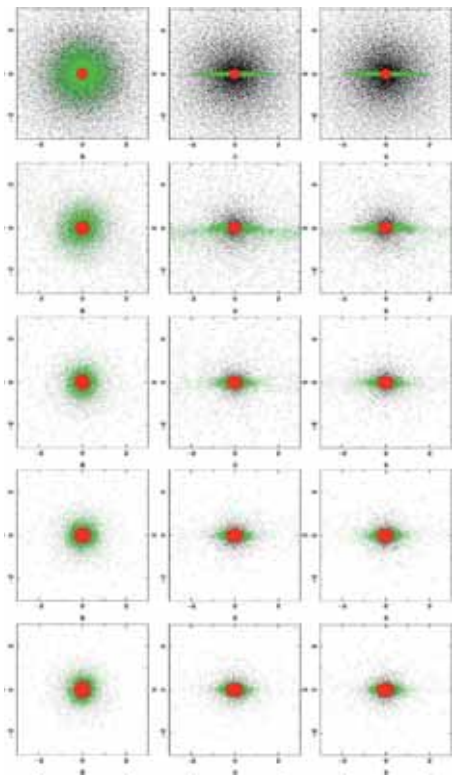
In previous years, the group studied the evolution and the growth of central bulges of spiral galaxies during interactions. In 2007, activity has extended in two directions. First, to the domain of very small bulges. Second, toward the inclusion of a gaseous medium in the description of the merging galaxies.

The group has studied the merger origin of intracluster light. Simulations of mergers between two elliptical galaxies with three different 'stellar' populations plus a dark matter

halo have been run. Models cover different orbital initial conditions as well as a variation in the initial dark-to-luminous mass ratio. The análisis is complete and a paper is near submission.

The group has also addressed tidal harassment of disk galaxies due to interactions with cluster galaxies. The initial conditions are several different models of disk galaxy with varying bulge-to-disk mass ratio. A number of tidal interactions have been run in each model. The final snapshot in each tidal interaction has been analysed and compared with observations.

In preparation for merger models involving disks with a gaseous component, the Kuijken-Dubinski (1995) model has been extended with the addition of a disk of gas, using the SPH formalism. Stability tests show that the system is stable for up to 2 Gyr, making it suitable for merger experiments.



Destruction of the disk and dark matter halo of a disk galaxy due to harassment with companion galaxies in a cluster environment. Each row presents the end point of a tidal interaction. The three panels display orthogonal views. Black dots are halo particles, green are disk particles and red are bulge particles. Differences between the various models reflect differences in internal structure of the model galaxias and of the intracluster orbit

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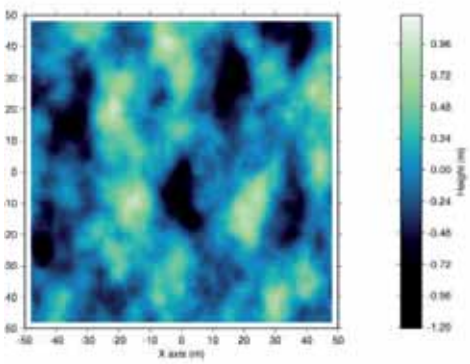
Scattering of navigation satellite signals on realizations of the sea surface

The signals emitted by the Global Navigation Satellite Systems (GNSS) can be used as sources of opportunity for observation of the Earth, similarly to bi-static radar measurements. The concept, called GNSS-Reflections (GNSS-R) or PAssive Reflectometry and Interferometry System (PARIS) provides wide coverage, given by the multiple GNSS reflections that can be captured simultaneously: 4 to 13 satellites of the American Global Positioning System (GPS) are visible from any spot on Earth, and this number keeps increasing with the recovery of the Russian GLONASS system, and the future European and Chinese GALILEO and COMPASS constellations. The concept is also attractive for its relatively low cost (only the receivers must be deployed), and it suitability to be embarked in a Space-based mission is under study.

Some Ocean surface properties can be obtained with a receiver able to collect the GNSS signals scattered by the Ocean. The sea surface roughness is estimated by the analysis of the returned signal-power, whereas other geophysical parameters such as sea surface salinity and mean geocentric height (sea level) might require phase-based analysis. The power-features of the signal (signal-to-noise ratio, shape of the received waveform) can be numerically modeled in standard PC, even for Space-borne scenarios. Nonetheless, the modeling of phase-observables as collected from Space requires integration of the scattered signal over a finely sampled grid on large particular realizations of the Ocean surface. The code to simulate phase-observables works on single PCs, for air-craft scenarios. Transition to parallel and supercomputing architectures is thus necessary to contribute assessing the performance of the concept from Space-based platforms. The activity conducted during two quarters of 2007 has been the adaptation of our existing serial code to run in parallel at MareNostrum.



The model integrates of the order of 5000 squared kilometers of particular realizations of the sea surface at squared decimeter sampling. The first step is to generate the surface grids, such as the pictured above, zoom into a 0.01 squared kilometer

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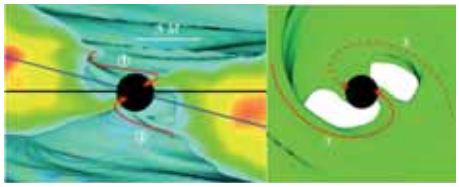
Bar-mode Instability in rapidly Rotating Magnetized Polytropes

The original aim of the project was the study of the bar-mode instability of magnetized neutron stars. Following an agreement with the personnel from the Barcelona Supercomputing Center (BSC) this original project had to be reconsidered due to the unexpected low efficiency found in our numerical code cosmos++ when run in MareNostrum. This issue was indeed totally unexpected since it could not be foreseen in all test simulations performed with this code in supercomputers of architecture similar to MareNostrum. These tests, which were conducted before submitting the proposal at BSC, did not show the poor scaling on Mare Nostrum. The main conclusion of further testing, once access to MN had been accepted and could compare timing data between MareNostrum and the other clusters was that, up to 64 processors the scaling of cosmos++ in both MareNostrum and other clusters were lineal but, however, MN was a factor of two slower than other machines. The low scaling of our code was due to the third party software called Hypre used in cosmos++ to solve Poisson's equation for the gravitational field.

Therefore, after reaching an agreement with the personnel from BSC on the possibility to redirect the use of our allocation, the team was able to use the bulk of it to conduct fully relativistic magnetohydrodynamic numerical simulations of tilted accretion disks around rapidly rotating black holes. These simulations revealed dramatic differences from comparable simulations of untilted disks. First, the symmetry of the disk was notably broken in the vicinity of the black hole. Instead of aligning with the symmetry plane of the black hole the disk is strongly warped. Accretion of matter onto the black hole occurs predominantly through two opposing plunging streams that start from high latitudes with respect to both the black-hole and disk midplanes (see figure). The plunging orbits start from a slightly larger radius than for untilted disks, leaving a larger than expected evacuated volume around the black hole. Another unique feature of the tilted disk is that it precesses due to a torque from the rotating black hole. The precession frequency is nearly constant throughout the simulation and matches well with the range of low-frequency quasi-periodic oscillations observed in many Galactic black-hole X-ray binaries.

The group also began work implementing and utilizing a "cubed-sphere" grid (see figure), which will allow us to simultaneously resolve the midplane and polar regions of accretion disk simulations. This new grid will permit to answer such critical questions as: 1) Does a jet form from a tilted black-hole accretion disk as it does from an untilted one? and 2) If a jet does form, what is its orientation? There are two principle models for jet formation from black hole accretion disks, and they give different predictions with regard to the orientation of the jet. One model has the jet drawing its power from the spin of the black hole, which would orient it perpendicular to the black-hole symmetry plane. In the second model the jet draws its power from the angular momentum of the disk. In this case we would expect the jet to be perpendicular to this disk. In our simulations this would also mean that the jet would precess with the disk; precessing jets are observed in Nature.



(Left) Zoomed in view of the inner region of a tilted accretion flow revealing two opposing, high-latitude streams of material connecting the disk to the horizon (indicated by arrows). (Right) Top view of the plunging streams connecting the tilted accretion disk with the black-hole horizon

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Large Numerical Simulations for Dark-Enery Surveys

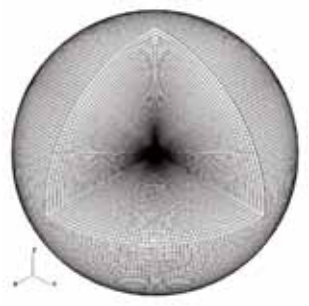
There is growing observational evidence supporting that the human being live in a universe dominated by dark-energy, a form of energy filling the universe that counteracts gravity on cosmological scales, and causing the universe to expand in an accelerated way.

Understanding the nature of dark-energy has deep implications not only for astrophysics and cosmology, but also for particle physics. This problem has been widely recognized by the scientific community as one of the most important open questions in physics.

There is now huge investment in new cameras, detectors and telescopes with the goal of mapping the large-scale structure of the universe at high redshift in order to probe dark-energy properties. There is a clear need to match this effort with a significant improvement in the theoretical predictions regarding the growth of structure in universes dynamically dominated by dark-energy.

The team is using the largest supercomputer in Europe, MareNostrum, to develop the largest simulations to date to study the process of large-scale structure formation in dark-energy dominated cosmologies with unprecedented detail. These simulations are called the MareNostrum-Institut de Ciencies de l'Espai (MICE) Simulations.

In particular, the group has used a massively parallel code, GADGET (see http://www.mpa-garching.mpg.de/gadget/) running on up to 512 processors to simulate the gravitational interaction of up to 2048^3 (i.e, about 10000 million) dark-matter particles in cosmological volumes of thousands of cubic giga-light-years. This iscomparable to the size of the entire observable universe. We are making use of these simulations to build realistic mocks of future galaxy surveys, such as the DES, PAU, VHS, DUNE, or upcoming cosmic microwave background experiments such as the ESA PLANCK satellite mission, in which our group is actively involved.



Comparison of traditional spherical-polar grid (top) and cubed-sphere grid (bottom).

Publications

C. C. Lindner & P. C. Fragile, A Numerical Study of Jets from Tilted Black-Hole Accretion Disks, AAS, 211, 48.09 (2007)

P. C. Fragile, C. C. Lindner, P. Anninos, & J. Salmonson, A Numerical Study of Jets from Tilted Black-Hole Accretion Disks, ApJ, in preparation

P. C. Fragile & C. C. Lindner, What Determines the Orientation of Jets Ejected From Accreting Black Holes?, ApJ, in preparation

J. A. Font, P. C. Fragile, P. Anninos, K. Camarda, & J. Salmonson, Bar-Mode Instability in Rapidly Rotating Magnetized Polytropes, ApJ, in preparation

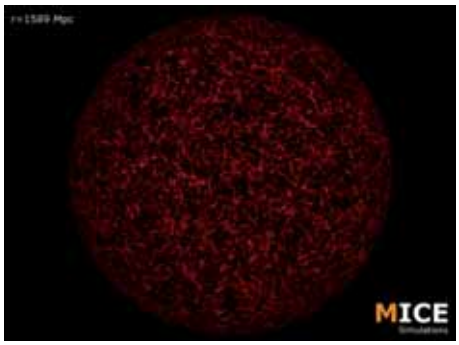
The development of these simulations is essential for the optimal scientific exploitation of these astronomical surveys.

On the other hand, galaxy surveys provide a large-scale view of the universe that typically has a limited line-of-sight or radial resolution. This can be modelled by picturing the universe as a set of concentric spherical shells around the observer, i.e, an onion-like structure. This is what we call the "Onion Universe".

Using the lightcone output of our MICE simulations, the team has built a set of angular maps that mimic this onion-like structure. The onion maps are a highly compressed version of the raw data (ie. a factor >1000 smaller size) providing a new and powerful tool to exploit large scale structure observations.

The team investigated two basic applications of these maps that are especially useful for constraning dark energy properties. Firstly, the team has measured the baryon acoustic oscillations (BAO) in the matter power spectrum, a basic cosmic distance ruler that can be used to constrain the geometry and matter-energy content of the universe. Secondly, the group has built all-sky maps of the weak lensing distortion, i.e, a measure of the deflection of light emitted by distant cosmological sources by the intervening matter in the universe.

Weak lensing maps give a measure of the growth rate of structure in the universe and they probe dark-energy properties and can differenciate between theories of gravity on the largest observable scales.



Il sky dark-matter distribution at 5.8 million light-years (or a comoving distance of 1589 Mpc/h) from earth. The angular map results from a projection of a spherical layer of the matter distibution in the lightcone with a radial width of about 80 million light-years

Publications

"The Onion Universe: all sky lightcone simulations in shells", P.Fosalba, E.Gaztanaga, F.Castander, M.Manera, 2007. arXiv:0711.1540 (submitted to MNRAS).

"Cosmology and Structure Formation", PhD Thesis, Marc Manera. Supervisor: E.Gaztanaga,University of Barcelona, June 2007.

Juan García Bellido
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Gravitational waves from preheating after inflation

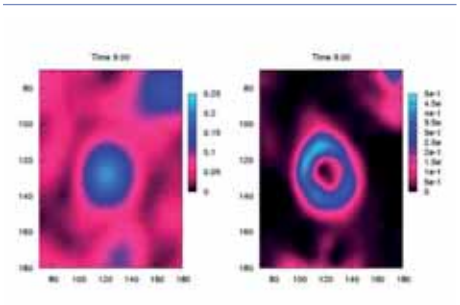
This scientific program involves the study of the creation and evolution of a background of Gravitational Waves created during a very early stage of the evolution of the universe, known as Reheating. After inflation ended the Universe was empty but the coupling between the inflaton and the other fields gave raise to the creation of particles. The production of those particles occured in a very violent way, through the nucleation and subsequent collision of large concentrations of energy density in the form of bubble-like structures moving at relativistic speeds.

The team has used MareNostrum to make runs of the main parallel codes that the team has written in order to study the generation of the stochastic background of gravitational waves after inflation, whose time evolution was determined by the successive stages of reheating.

The resources of MareNostrum have been crucial, since one of the main problems in our research is to fit the physical spectrum within the window of the periodic boundary lattices the group uses for the simulations.

Being able to run our code in paralell, the team could obtain a lattice box large enough without compromissing the resolution of our simulations, such that the numerical results were fully under control both in the IR and UV parts of the spectra.

From reheating, the produced gravitational waves would propagate unimpeded to us. The group has found that the fraction of energy density today in these primordial gravitational waves could be significant for GUT-scale models of inflation, although well beyond the frequency range sensitivity of gravitational wave observatories like LIGO, LISA or BBO. However, the team has also simulated low-scale models, and found that it could still produce a detectable signal at frequencies accessible to BBO or DECIGO interferometers. The discovery of such a background would open a new observational window into the very early universe, where the details of the process of reheating, i.e. the Big Bang, could be explored. Moreover, it could also serve in the future as a new experimental tool for testing the Inflationary Paradigm.



Publications

A stochastic background of gravitational waves from hybrid preheating. Authors: Juan Garcia-Bellido, Daniel G. Figueroa Published in Phys.Rev.Lett.98:061302,2007. e-Print: astro-ph/0701014

A Gravitational Wave Background from Reheating after Hybrid Inflation. Authors: Juan Garcia-Bellido, Daniel G. Figueroa, Alfonso Sastre Accepted in Phys.Rev.D e-Print: arXiv:0707.0839 [hep-ph]

A new gravitational wave background from the Big Bang. Authors: Juan Garcia-Bellido, Daniel G. Figueroa Accepted in the Proceedings of JGRG17 Conference, Nagoya (Japan) e-Print: arXiv:0801.4109 [gr-qc]

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SPECFEM3D

Modeling of seismic wave propagation resulting from large earthquakes in the three-dimensional (3D) Earth is of considerable interest in seismology because analyzing seismic wave propagation in the Earth is one of the few ways of studying the structure of the Earth's interior, based upon seismic tomography. The field of numerical modeling of seismic wave propagation in 3D geological media has significantly evolved in the last few years due to the introduction of the spectral-element method (SEM), which is a high-degree version of the finite-element method that is very accurate for linear hyperbolic problems such as wave propagation, having very little intrinsic numerical dispersion. In addition, the mass matrix is exactly diagonal by construction, which makes it much easier to implement on parallel machines because no linear system needs to be inverted. Here we implement the SEM on MareNostrum. The team shows that on 2166 of its IBM PowerPC 970 processors the group can simulate seismic waveforms accurately up to a maximum frequency of 0.5 Hertz based upon message passing with MPI.

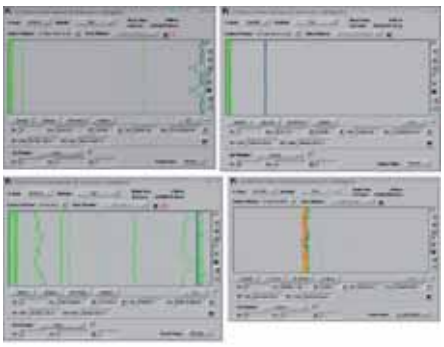
The SEM combines the flexibility of the finite-element method with the accuracy of the pseudospectral method. It uses a mesh of hexahedral finite elements on which the wave field is interpolated by high-degree Lagrange polynomials at Gauss-Lobatto-Legendre (GLL) integration points. Here we are interested in differential effects on very high frequency (0.5 Hertz) seismic phases when they propagate inside the solid inner core of the Earth, therefore to significantly reduce the computational cost the gropu suppresses the crust of the Earth and replace it with an extended upper mantle, and convert the whole mantle from elastic to acoustic, thus reducing the problem in that part of the model from a vectorial unknown to a scalar unknown, i.e. reducing memory usage and CPU cost by a factor of roughly three in 3D. In the acoustic mantle and crust we solve the acoustic wave equation in terms of a fluid potential. The team keeps a (much more expensive to solve) elastic anisotropic medium in the inner core only. In that small part of the mesh we also model seismic attenuation (i.e., loss of energy by viscoelasticity), which has a significant impact on the cost of the simulation because memory requirements increase by a factor of roughly 2 and CPU time by a factor of roughly 1.5.

The total number of spectral elements in this mesh is 323 million, which corresponds to a total of approximately 21 billion global grid points (the “equivalent” of a 2770 x 2770 x 2770 grid), since each spectral element contains 5 x 5 x 5 = 125 grid points but with points on its faces shared by neighboring elements. This in turn also corresponds to approximately 21 billion degrees of freedom because a scalar unknown is used in most of the mesh (everywhere except in the inner core of the Earth, as mentioned above). Such simulations use a total of approximately 2.5 terabytes of memory. The mesh files, created once and for all by our in-house parallel mesh generator, are stored on the local disk of each blade of MareNostrum to avoid overloading the parallel GPFS file system with very large files that are only written once and then read back once at the beginning of the simulation.

The SEM solver is based upon a pure MPI implementation. The team first performed a ParaVer analysis of the code on 96 processors (Figure 1). The figure shows that in version 3.6 of SPECFEM3D, the number of L2 cache misses was very different between mesh slices, thus inducing severe load imbalance. In version 4.0, L2 cache misses have been drastically reduced and very well balanced. The number of instructions executed is also very well balanced. As a result, useful duration of the calculations is well balanced as well. In total, the group gains a huge factor of 3.3 in terms of wall-clock time. This shows that the IBM PowerPC 970 is very sensitive to cache misses because the same run performed on an Intel Itanium and also on an AMD Opteron cluster shows a factor of “only” 1.55 to 1.60.

For the final runs, the team computed 50600 time steps of the explicit time integration scheme of the SEM algorithm in 60 hours of wall-clock time on 2166 processors (being the only user running on the corresponding

dedicated blades). Total memory used was 2.5 terabytes. The code performed well and performance levels obtained were very satisfactory. The eophysical analysis of the seismograms is currently under way.



ParaVer analysis of the code on 96 processors, from processor 1 at the top of each picture to processor 96 at the bottom. Top left: In version 3.6 of SPECFEM3D, L2 cache misses were very poorly balanced between mesh slices, thus inducing severe load imbalance. In version 4.0 (top right), L2 cache misses (represented on the same horizontal scale) have been drastically reduced and very well balanced. The number of instructions executed is also very well balanced (bottom left, blue line). As a result, useful duration of the calculations (bottom right, in orange) is well balanced as well

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Heisenberg Spin Glasses: Large Lattices at Low Temperatures

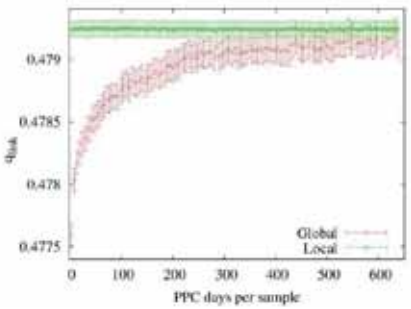
Spin-glasses are disordered magnetic alloys with very unusual behaviour. Interest in spin glasses goes far beyond just this class of materials, however, because they provide a convenient model system from which to derive a unified theory of the glassy state (glass is one of the most common, yet mysterious states of condensed matter). Interest in spin glasses also extends outside of condensed matter physics because there has been a fruitful exchange of ideas between the spin glass community and researchers in other branches of science such as computer scientists working on combinatorial optimization. Simple analytical approximations predict that spin glasses have a finite temperature transition, but whether this actually occurs (or is an artefact of the approximations used) has remained unclear, at least for a variety known as "Heisenberg spin glasses". The advent of a new generation of simulation algorithms, finite-size scaling analysis and parallel computers have mean that, at last, the team can make a serious attempt to fully understand the phase transition in Heisenberg spin glasses.

This investigation was started in MareNostrum in early 2006. In a first stage, the team reached the unexpected conclusion that, in three dimensions, the phase transition is somewhat marginal. The extreme Kosterlitz-Thouless limit (the low temperature phase does not display a "glassy" ordering, but slowly decaying correlations for distant apart spins) could not been discarded. This shocking result was made possible by the large computing power available in the MareNostrum, and by the realization that simulation tools borrowed from high-energy physics where extremely effective in this problem. The combination of this two factors allowed to obtain equilibrium results for unprecedently large systems (namely, cubic lattices of side L=32).

During 2007 the team has worked with the MareNostrum to extend this result in two directions:

1) The Heisenberg spin-glass is an ideal limit, in the sense that all physical systems have some degree of anisotropy in their interactions. The team has investigated the effects of small anisotropies, finding that our previous results were stable with respect to this perturbation.

2) The ongoing investigation, that will last a significant part of 2008, is concerned with the precise nature of the phase transition in the ideal limit of a purely isotropic system. This requires obtaining equilibrium configurations on even larger systems and at even lower temperatures. Extending previous research in either of the two directions is a dramatic computational challenge. Thanks to the combination of the most advanced algorithms (parallel tempering and overrelaxation), and the parallel computations made possible by the MareNostrum, the team is reaching equilibrium on enormously large systems, such as lattices with side L=48 (see figure). Fully conclusive results will be reached by slightly extending the time duration of these simulations, and by simulating a larger number of disorder realizations (called samples).



Time evolution (in Power PC days) of the quantity known as "q_link" at our lowest temperature. Interestingly, q_link can be computed in either of two alternatives ways. One of them (green symbols),converges to the equilibrium value very fast. Yet, q_link can be alsocomputed by taking into account the global spin-glass ordering (red symbols). The coincidence of the two alternative computations is the strongest known thermalization test. Reaching equilibrium in a single computer (i.e. without parallel omputation), would takes almost twoyears while the team can reach it only in 8 days in the MareNostrum (persample). In fact, since one needs to reach equilibrium for several instances of the problem (50 samples in this plot), the total computing time needed was the equivalent of 87 years of a singlecomputer

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Daniel Guirado Rodríguez
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Polarimetry of Light Scattered by Irregular Particles

The group was focused on the study of circular polarization of light scattered by randomly built aggregates. A small but non-zero degree of circular polarization (DCP hereafter) has been persistently observed for light scattered by dust grains in comets. The accuracy of the observations is, in general, quite low, especially for measurements of comet Halley, where the errors are of the order of the mean values, or even larger.

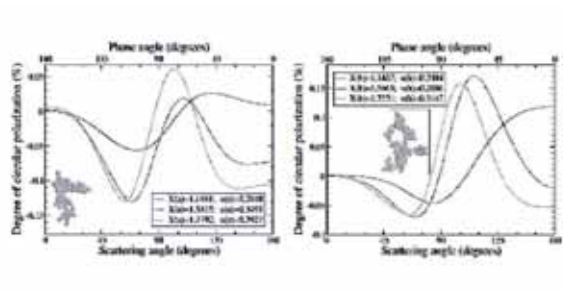
In previous works the team conducted a systematic study of the DCP of light scattered by model asymmetrical particles. There the group used two artificially asymmetrical aggregates of identical spheres (monomers) and calculated the DCP curves, i.e., the DCP as a function of the scattering angle for several sizes, refractive indices and numbers of monomers of the aggregates. The team obtained a DCP of up to 2\%. From the results of that work the group inferred the following: when the substructure (monomer or group of monomers) producing the asymmetry of the aggregate is comparable in size to the wavelength, some principal peaks appear in the DCP curve. These peaks reduce their amplitude when the aggregate becomes larger than the wavelength, but always remain at about the same scattering angles. Also the number of principal peaks keeps constant when varying the size of the aggregate. When the size of the aggregate is increased in such a way that the diameter of each monomer becomes of the order of the wavelength, secondary peaks appear in the DCP curve. The number of these peaks increases while increasing the size of the aggregate, and their positions change. Finally, when making an average of the DCP curve over a size distribution the secondary peaks contribution is canceled out when these peaks are summed up and only principal peaks remain, because they always contribute in the same sense at the same positions.

From these conclusions, the team derived that aggregates built in a random way may also produce a significant DCP of scattered light if the substructure producing the asymmetry of the

particle is comparable in size to the wavelength of scattered light. The main goal of the present work is to study what is the order of magnitude of the DCP of light scattered by randomly built aggregates. If too small, the group could directly rule out real asymmetrical aggregates as producing most of the circular polarization in comets, but if it is of the order of the observations, the team should proceed with a systematic study of several geometries, sizes and refractive indices.

For the generation of the aggregates the group implemented a cluster-cluster aggregation (CCA) method in a Fortran code. For all calculations the team used the T-matrix superposition method for aggregates made of spherical monomers. The results depend somewhat on the accuracy parameters of the code,and the team needed very accurate results because the group expected to obtain small values of the DCP. So, the team changed the accuracy parameters until the results became stable. Some of the calculations were also performed using a parallel implementation of the DDA method for checking. All calculations were performed in the MareNostrum supercomputer, at the Barcelona Supercomputing Center.

Two different shapes were used for the aggregates (see figure). The team will denote by x the size parameter of the monomers of the particle, and by X the volume equivalent size parameter of the whole aggregate. As seen in the figure, single scattering of unpolarized light by randomly built optically inactive particles in random orientation can produce values of the degree of circular polarization comparable to the observed values for light scattered in comets.



The degree of circular polarization as a function of the scattering angle for different collections of randomly oriented randomly built aggregates differing in volume equivalent size parameter

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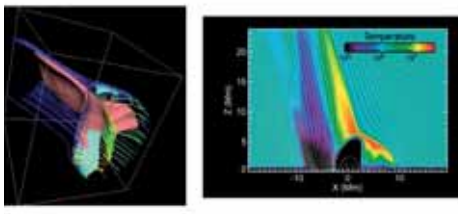
Eruptive phenomena in the atmosphere of the Sun and cool stars

The Sun is a highly active star. The solar atmosphere is continually modifying its structure and appearance, in a futile search for magnetic and dynamical equilibrium. As part of that activity, gigantic eruptions take place, many of which cause enormous amounts of mass to be hurled from the Sun to the interplanetary space, sweeping the Earth in their way toward the outer planets and causing important disruptions in the Earth's surroundings. In other cases, the eruptions cause subatomic particles (e.g., protons) to be accelerated in the solar atmosphere to velocities nearing the speed of light part of which propagate in the heliosphee. In either case, the eruptions are not only spectacular and interesting physical phenomena; they are important also for practical reasons since they may cause problems in the radio communications in the Earth, can jeopardize space missions, put in danger the lives of the astronauts, etc. Eruptions of these types are expected basically in all stars with magnetic activity like the Sun or higher.

In many cases the eruptions result from the emergence of magnetized gases from the interior of the star. In our project we are trying to understand in depth the physics of these processes. To that end the team solves the equations of fluid dynamics and electromagnetism for the solar atmosphere using massively parallel supercomputing installations. One of the types of models the team is solving in MareNostrum is centered has special focus on the phenomena known as 'magnetic field line reconnection'. Those phenomena cause small volumes of the solar atmosphere to become extremely hot (up to tens of millions of degrees), with the hot matter then being ejected with velocities of up to 1000 km per second along the surrounding magnetic field links. Such ejections are known as X-Ray jets, since they are clearly detected with telescopes sensitive to X-Ray radiation placed on board satellite missions. In 2007, on the basis of the computational models carried out in the MareNostrum computer, the team has been

able to successfully explain a particularly interesting type of X-ray jets, namely those that appear in solar regions with magnetic field lines open to the interplanetary space (called solar coronal holes). This kind of jets have been recently shown to be a highly frequent phenomenon in coronal holes by the recently launched Hinode solar space mission. The models explain the three-dimensional shape, time evolution, velocities, densities and temperatures of these jets. In addition, the group can visualize their magnetic structure and predict how the properties of these objects depend on the preexisting structure of the atmosphere and the type of emergence from the solar interior that precedes their launch.



X-Ray jet in the solar atmosphere caused by the emergence of magnetized plasma from the interior of the star as modelled in the MareNostrum computer. Left: three-dimensional view showing magnetic field lines, and surfaces delineating the jet and the reconnection site. Right: Temperature structure of the jet seen in a two-dimensional vertical cut

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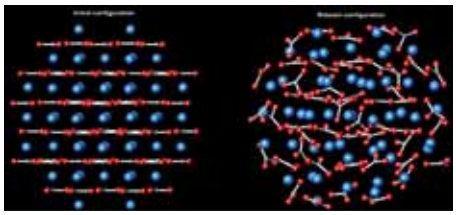
A Quantum Mechanical Approach to the Nucleation Process of Calcium Carbonate

Equilibrium relationships involving solids are based in bulk thermodynamic properties that concern ideal cr ystals of infinite size. However, real processes towards quilibrium imply development of finite mol ecular-scale entities. The configuration of these early-stage clusters and the estimation of their excess energies with respect to the ideal crystal is key to unders tand the macroscopic behaviour of a given system. As nucleation events are difficult to study ex perimentally, both because they occur spontaneously and because the nucleus size is very small, atomistic simulations are a suitable tool for understanding the early stages of crystallisation.

In the present project, starting from the ideal atomic positions in calcite, aragonite, or vaterite, the relaxation in vacuum of finite clusters of CaCO 3 has been explored. A wide variety of clusters ranging from 1 to 2000 formulae has been considered for each (calcite, aragonite, or vater ite) starting structure. With the aim of determining the influence of the cluster size on its energy and on its geometrical configuration, a series of CaCO3 clusters have been simulated and their lattice energies calculated. The cluster geometry has been fully optimized at c onstant pressure and its energy has been determined using the GULP program. In a number of cases the final configuration has been checked with good agreement using the DFT code SIESTA. Moreover, a fundamental question like the size that must have a cluster to be considered calcite, aragonite, or vaterite has been addressed from the diffraction patterns of the relaxed clusters.

Although these simulations represent not fully realistic scenarios, some results are relevant from the point of view of the polymorphic precipitation of CaCO 3 and it is a suitable basis for future studies.



Example of initial and final (after relaxation) cluster of calcite. The relaxation behaviour and the final energy per formula unit depend on the number of formulae. In this case the final configuration is partially ordered

Publications

A. Fernández González, L. Fernández-Seivane M. Prieto y J. Ferrer : From Crystals to clusters: A molecular simulation of CaCO 3 configurations. Geocimica et Cosmochimica Acta 71 (15) Supplement 1 A274 (2007)

A. Fernández González, L. Fernández-Seivane M. Prieto y J. Ferrer: Del Cristal al Cluster: Modelización Molecular de Configuraciones Finitas de CaCO 3 Macla 7, 44 (2007).

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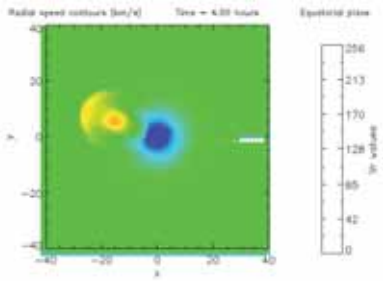
Modelling Interplanetary CME-driven shocks and solar energetic particle events

Solar energetic particle (SEP) events are an important hazard to spacecraft systems and a constraint for human activities in space. A solar-generated coronal mass ejection (CME) may produce an interplanetary shock that accelerates particles at its front. These particles propagate along the interplanetary magnetic field (IMF) lines reaching observers located elsewhere in the heliosphere. The group has been working on a compound shock-and-particle model for SEP events description. This model is composed by a 2.5 dimensional magnetohydrodynamic (MHD) model that can describe the launch and evolution of the CME-driven shock in interplanetary medium, plus a particle transport model describing the propagation of energetic particles along the interplanetary magnetic field. But 2D models have limitations and are not good enough to be used as operative tools for forecasting or nowcasting purposes.

Together with the CPA group (Centre for Plasma Astrophysics) of the Katholieke Universiteit of Leuven (Belgium), the team is working on a three-dimensional (3D) model that can simulate both the propagation of an interplanetary shock and of accelerated particles (protons or ions). The link between the two model components is the cobpoint concept (Connecting with the Observer Point). To reach this objective there are three steps to follow: (1) construct a 3D MHD model for the CME-driven shock simulation, (2) a new transport code to simulate particle propagation; and (3) an upgrading of the procedure to derive the values of plasma variables at the cobpoint. We have afforded the first step: to adapt and run a 3D MHD model developed by the CPA group (based on the Versatile Advection Code, VAC) to simulate the shock evolution from the Sun to the Earth or Mars' orbit. Our specific objective has been to study how the 3D MHD model performs in MareNostrum, taking into account that it has been only applied to less than one third of the interplanetary scenario of

interest. This spatial extension is necessary in order to be able to evaluate the particle radiation that NASA or ESA missions (such as Solar Orbiter, Solar Probe, BepiColombo or the Mars' armada) can face.

After two test activities, the team runs the 3D MHD code up to 30 solar radii (using 440 processors), the scarce time awarded allowed only two short runs. The figure displays one snapshot of 3D velocity contours projected on the ecliptic plane, 4 hours after the launch of the CME from the Sun (central white circle). The front of the shock ('the nose') is the solar wind plasma compressed region located at ~28 solar radii. The Earth is out of the picture, 215 solar radii away to the left (in the line joining the origin of Y axis with the Sun). The CME travels in 18º E direction as seen from the Sun-Earth line. The MHD strength of the shock decreases toward the wings and the CME that drives the shock is downstream the front although its angular extension is still limited (interplanetary magnetic field lines have not been plotted). The nose of the shock moves at ~200 km/s in the solar wind frame, which means ~620 km/s in space.



Snapshot of the 3D MHD simulation of a CME propagation. The plot shows radial velocity contours (colour coded) on the ecliptic plane at t = 4 hours. The CME was launched 18 degrees eastward from the Sun-Earth line. The structure of the CME is described in the text

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Gaia: preparation of the data reduction

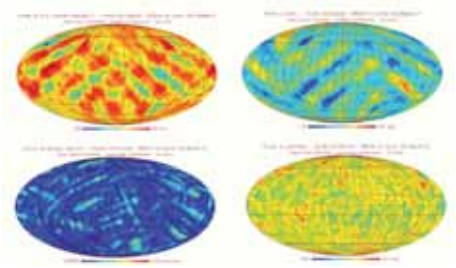
Gaia is an ambitious mission to chart a three-dimensional map of our Galaxy, the Milky Way, in the process revealing the composition, formation and evolution of the Galaxy. Gaia will provide unprecedented positional and radial velocity measurements with the accuracies needed to produce a stereoscopic and kinematic census of about one billion stars in our Galaxy and throughout the Local Group. This amounts to about 1 per cent of the Galactic stellar population.

Combined with astrophysical information for each star, provided by on-board multi-colour photometry, these data will have the precision necessary to quantify the early formation, and subsequent dynamical, chemical and star formation evolution of the Milky Way Galaxy.

In the course of Gaia's 5-year astronomical survey, about 200TB of raw information on our Galaxy will be harvested and transmitted to Earth. Sophisticated processing is needed to distill this flood of complex data into the final Gaia Catalogue of about 1000 million celestial objects. A group of more than 300 European scientists and software developers is rising to the challenge: the Data Processing and Analysis Consortium (DPAC) is already preparing for Gaia's launch in 2011. The group at the University of Barcelona (UB) is part of DPAC and has assumed the responsibility of several critical tasks in the Gaia data reduction.

On the one hand, the UB team is the coordinator of the DPAC Coordination Unit 2 (data simulations), in charge of producing simulated data for the development, testing and validation of the data reduction software. Two of its data generators are run at MareNostrum: GASS (which outputs a realistic telemetry stream) and GOG (which generates intermediate and catalogue data). Thanks to the MareNostrum computational power, the UB team has been able to generate several large datasets that have been used in 2007 in several aspects of the preparation of the data reduction. In all, about 200,000 CPU hours have been

spent and 4TB of simulated data generated in 2007. One of the crucial software modules using these datasets is AGIS (Astrometric Global Iterative Solution), the core of the Gaia astrometric solution. This module will be the key to produce the high precision astrometric results of the mission, a computational challenge both for the volume of data to be processed and the complexity of the process itself. The figure depicts the results of the convergence of this process over all the sky for one of the GASS datasets produced at MareNostrum (GASS-LSS-1-E, 10^6 objects, 5 years of observation, $72x10^6$ transits).



Sky distribution (equatorial coordinates, Mollenweide projection) of the errors of the astrometric solution obtained by AGIS using the GASS simulations produced at MareNostrum. Top left: errors in rigt ascension times cos(dec). Top right: errors in declination. Bottom left: errors in proper motion. Bottom right: errors in parallax. Data from GAIA-C3-TR-ESAC-NB-002

Publications

N. Bach, F. Raison, U. Lammers, "AGIS Validation Test Report of CY03-C2", GAIA-C3-TR-ESAC-NB-002 (2007)

J. Torra et al. "Gaia: A major step in the knowledge of our Galaxy", Highlights of Spanish Astrophysics IV, Springer-Verlag (2007)

J., Portell, J., Fabricius, C., et al., "Intermediate Data Updating Software Requirements Specifications", GAIA-C3-SP-UB-JT-003 (2007)

Y. Isasi, E. Masana, "GASS Software Requirements Specifications", GAIA-C2-SP-UB-YI-005 (2007)

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The MareNostrum Numerical Cosmology Project: Grand Challenge simulations of structure formation in the Universe

The MareNostrum Numerical Cosmology Project (http://astro.ft.uam.es/marenostrum) is an international collaboration between different researchers of Spain, Germany, Israel France and USA aimed at using the exceptional capabilities of the MareNostrum supercomputer to carry out grand challenge cosmological simulations of the formation of galaxies, clusters of galaxies and the large scale structures in the universe. The scientific objective is to understand the physical processes that were involved in the formation and evolution of these objects from initial conditions that are compatible with the early epochs of the Universe derived from the observations of the Cosmic Microwave Background radiation.

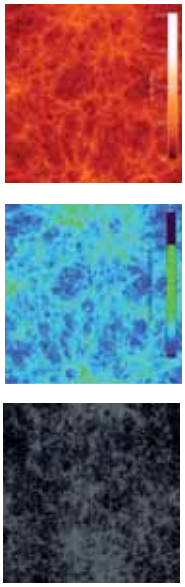
The team is currently involved in two big simulation projects:

A) MareNostrum Galaxy Formation Simulation is currently the largest simulation of early galaxy formation performed to date. It uses more than 2 billion particles to represent the different components of the matter in the universe: dark matter, gas and stars in a cubic box of 50 Mpc (150 million light years) across. The team has been using 200 blades (800 cpus) for a total of 11 million seconds wall clocktime till now. With this cpu time we have been able to evolve the simulation from a starting redshift of z=50 till z=4.9 up to now. This correspond to approximately 1.2 billion years of cosmic evolution. The evolution of the self-gravitating fluids is done by means of the parallel MPI code GADGET-2. The unique feature of this project, apart from the unprecedented numerical resolution achieved, is that the same simulations has been done alos with a different computational code, based on eulerian AMR techniques (RAMSES) by Romain Teyssier and the french HORIZON consortium starting from the same initial conditions. The comparison of these two

state-of-the-art simulation results will provide us with a unique perspective of the reliability of the results on the properties and prediction from our high redshift numerical galaxies. The group is currently investigating the observational properties of the galaxies formed in these simulations at early redshifts. The team studies the abundance of galaxies as a function of the light emitted in different wavelength and compare with the new results from real universe at early epochs from Subaru and the Hubble Ultra deep fields (z =6,5,4). The comparison of these results provides us with invaluable information on the physical conditions of the primordial galaxies. For instance, the team has discovered that there must exists a redshift dependence of the extinction by dust of the light emitted by the stars in the high redshift galaxies. The complex distribution of the gas in a filament network (see figure) is also another important issue to study. Most of the gas that is fed to the primordial galaxies come from these filaments. Therefore, knowing in detail how the galaxies gets the gas to form stars is crucial to understand how the luminosity of these galaxies evolve with time.

B) The team is also investigating the properties of clusters of galaxies formed in the concordance cosmology. The goal is to simulate a volume-limited, statistically-large sample of galaxy clusters with much higher resolution than in previous simulations. The spatial resolution of the simulations will match the superb resolution of current X-ray Chandra and XMM observations and will allow detailed comparisons with them . The simulations include metallicity-dependent radiative cooling, star formation, energy injection due to stellar winds and supernovae, and self-consistent metal enrichment and metal advection. As the team is only interested in the physical properties of clusters of galaxies, the group proceeds by selecting a volume limited sample of clusters with masses >3x1014 solar masses in a volume of 240 Mpc from a low resolution simulation and resimulate them at high resolution, using the MPI version of the N-body + Hydro AMR code called ART, developed by Doug Rudd and A. Kravtsov. The purpose is to obtain a sample of more than 100 simulated clusters which will be used to study scaling relations between cluster observable properties and their total mass, evolution of the scaling relations and, most importantly, properties of their scatter. So far we have completed more than 2/3 of the sample using the past year time allocation for this project.

These two grand challenge numerical applications are very demanding in terms of computational resources and can only be completed using CPU time allocated during several periods. The team is about to complete the two projects soon, and as it happened with the other big simulation completed in the year before, the team will start to produce scientific results and publications in the coming years.



Gas density (top) and temperature (center) in a slice cut through the whole box at z=5.2. Simulated CCD image (bottom) with 106 pixels from luminosity of stars in UBV colors

Publications

The Local Hubble Flow: Is it a Manifestation of Dark Energy? Hoffman, Y., Martinez-Vaquero, L. A., Yepes, G., & Gottloeber, S. 2007, arXiv, 711, arXiv:0711.4989

The future of the local large scale structure: the roles of dark matter and dark energy Hoffman, Y., Lahav, O., Yepes, G., & Dover, Y. 2007, JCAP, 10, 16

Is WMAP3 Normalization Compatible with the X-Ray Cluster Abundance? Yepes, G., Sevilla, R., Gottlöber, S., & Silk, J. 2007, ApJ, 666, L61

Too small to form a galaxy: How the UV background determines the baryon fraction Hoeft, M., Yepes, G., & Gottloeber, S. 2007, arXiv, 708, arXiv:0708.0229

Constrained simulations of the local universe - I. Mass and motion in the local volume Martinez-Vaquero, L. A., Yepes, G., & Hoffman, Y. 2007, MNRAS, 378, 1601

Shape, Spin, and Baryon Fraction of Clusters in the MareNostrum Universe Gottlöber, S., & Yepes, G. 2007, ApJ, 664, 117

Spin alignment of dark matter haloes in the shells of the largest voids, Cuesta, A. J., Betancort-Rijo, J. E., Gottloeber, S., Patiri, S. G., Yepes, G., & Prada, F. 2007, arXiv, 706, arXiv:0706.2775

Entropy of gas and dark matter in galaxy clusters Faltenbacher, A., Hoffman, Y., Gottlöber, S., & Yepes, G. 2007, MNRAS, 376, 1327

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Probabilistic Domain Decomposition for Partial Differential Equations

The purpose of this project is developing efficient algorithms for the numerical solution of problems in scientific computing (typically, for elliptic or parabolic partial differential equations), on parallel architectures.

The most advanced computing systems in operation to date have the use of thousands of processors, and, within few years, computers with hundreds of thousands or millions of processors will come into operation. Therefore, the algorithms the team shall obtain will be scalable, suited to grid computing and to heterogeneous computing, as well as naturally fault-tolerant. In this way, the team intends to contribute to the advancement of the performance of software, in view of the remarkable progress achieved by the hardware. These algorithms will be based on domain decomposition methods, which among the several numerical methods proposed in literature for solving boundary-value problems for PDEs, appear to be specially suited for parallel architectures. The new ingredient is that they are characterized by a domain decomposition obtained by probabilistic methods. This approach allows for a full decoupling of the original problem into a number of subproblems. Such problems can then be solved on as many independent processors, not subject to any inter-communications. Therefore, these algorithms are scalable, naturally fault tolerant and well suited to grid computing. During this period of usage of MareNostrum, the group tested succesfully scalability and performance of the algorithm by running several benchmarks up to 1,024 processors. Simultaneously, the team tried to validate our new algorithm against the most efficient numerical method for elliptic partial differential equations available these days, showing that the new one outperforms the classical one.

Publications

Acebron, J.A., and Spigler, R. "A fully scalable parallel algorithm for solving elliptic partial differential equations", Lecture Notes in Computer Science, 4641, 727- 737 (2007).

Acebron, J.A..; Duran, R.; Rico, R.; Spigler, R, " A new domain decomposition approach suited for grid computing", Lecture Notes in Computer Science, 4699, 744-753 (2007)

Acebron, J.A..; Lozano, S.; Arenas, A., "Amplified signal response in scale-free networks by collaborative signaling", Physical Review Letters, 99, 128701 (2007)

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Scaling laws in complex material behavior

The general goal of this activity is to unveil the mechanics of complex material systems through scaling laws obtained in supercomputers. These scaling laws encapsulate the net effect of small-scale phenomena in larger engineering scales, thus enabling science-based design of devices and materials and proper analysis of experiments. The investigation of such laws is often difficult or impossible experimentally, and extremely challenging numerically since several orders of magnitude spans need to be computed.

The activity has focused on the mechanics of multiwalled carbon nanotubes, a unique nanostructure holding promise in a number of nano-structured materials and devices. The MareNostrum supercomputing platform, together with coarse-graining methods for atomistic systems, have allowed us to routinely analyze the nonlinear response of nanotube systems containing over 30 million atoms, an essential capability in investigating scaling laws. Two studies have emerged from the simulations on MareNostrum.

1. Multiwalled carbon nanotubes: the thicker, the softer

Size matters for the mechanics of multiwalled carbon nanotubes (MWCNTs). It has been known for some time that MWCNTs often wrinkle under deformation exhibiting the so-called rippling deformation pattern, which makes MWCNTs much softer (cf. Figs. 1-2). Through large-scale multiscale simulations the team has characterized with a power law the softer wrinkled response, and showed that the transition strain between the super-stiff behavior attributed to MWCNTs and this softer regime scales as the inverse of the tube diameter. Thus, the tera Pascal Young's modulus can be fully exploited in devices and materials only for moderately sized tubes. Similarly, in interpreting experiments or designing devices, the classical Euler-Bernouilli beam theory can only be applied to such tubes. The elasticity of thicker tubes is nonlinear, typically display mixtures of wrinkled and unwrinkled sections, and often exhibit hysteretic mechanical behavior.

2. Mesoscopic models for the mechanics of multiwalled carbon nanotubes

On the basis of the previous study, the group proposes to model thick multiwalled carbon nanotubes as beams with non-convex curvature energy. Such models develop stressed phase mixtures composed of smoothly bent sections and rippled sections. This model is also motivated by experimental observations. The model is analyzed, validated against large-scale simulations, and exercised in examples of interest. It is shown that modelling MWCNTs as linear elastic beams can result in poor approximations that overestimate the elastic restoring force considerably, particularly for thick tubes. In contrast, the proposed model produces very accurate predictions both of the restoring force and of the phase pattern.

Fig 1. 35-walled CNT in torsion, deformed shape (top), Gaussian curvature map (middle, green is zero, red is positive, blue is negative), and energy density map (bottom, red is high, blue is low)

Fig 2. 40-walled CNT in pure bending, deformed shape (top), Gaussian curvature map (middle), and energy density map (bottom). The same color scale as in Fig. 1 applies

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Performance analysis of parallel algorithms fornonlinear time series analysis*

In difierent flelds of science and engineering (medicine, economy, oceanography, biologic systems, etc) the False Nearest Neighbors (FNN) method has a special relevance for determining the minimal embedding dimension. In some of these applications, it is important to provide the results in a reasonable time, thus the execution time of the FNN method has to be reduced.

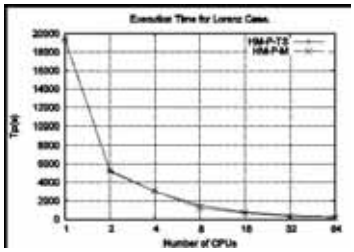
Two kind of parallel implementations have been optimized and analyzed in two visits to BSC-CNS (January and April). In particular, two parallel implementations based on time series (HM-P-TS and HM-P-M) for hybrid memory architectures, and two based on embedding dimensions (DM-S-TS1stD and DM-P-M1stD) for distributed systems have been studied. A \Single-Program, Multiple Data" (SPMD) paradigm is employed using a simple data decomposition approach where each processor runs the same program but acts on a difierent subset of the data.

The computationally intensive part of the method is mainly within the neighbors search and therefore this task is parallelized and executed using from 2 up to 64 processors.The accuracy and performance of the parallel approaches are then assessed and compared to the best sequential implementation for computing the FNN method, which appears in the TISEAN project, in terms of execution time, speed-up and e–ciency. For this analysis have been used three dynamical systems: Lorenz, Hénon and Rössler.

The results indicate that the two parallel implementations for hybrid systems, when the method is run using 64 processors, are between 75 and 95 times faster than the sequential one. The time saving with 64 processors on the MareNostrum supercomputer compared to the best sequential implementation is around 115% to 145%. Fig. 1 shows the results obtained for the Lorenz case of study. Results for the other kind of implementations are considerably worse.

This work has been partially supported by the Spanish CICYT project CGL2004-06099-C03-03/CLI and by the Castilla-La Mancha project JCCM-PCI-05-0191

a)



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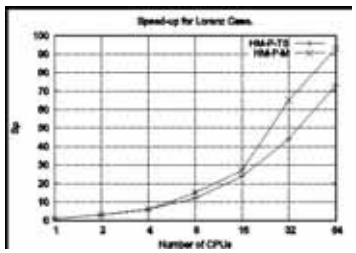

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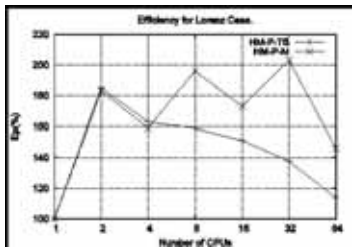

Lorenz case of study. (a) Execution time. (b) Speed-up. (c) E–ciency

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Dynamical Coupled-channel Analysis of Excited Baryons

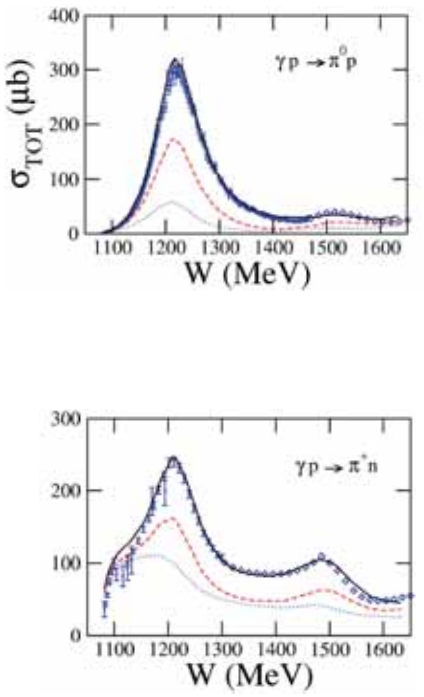
The main goal of the project was to map out the quark substructure of low lying baryons, e.g. nucleons, Delta (1232), etc. To do so we made use of a Dynamical coupled-channels model to analyze the existing experimental database of both hadronic reactions, pion-nucleon, eta-nucleon, and the single and double meson photo and electroproduction datatabase, notably the extensive recently collected data at Jefferson Laboratory.

In the first half of 2007, the team accomplished the first main task of our project, namely to successfully build a pion-nucleon coupled channels model up to 2 GeV center of mass energy. The construction of the model required heavy parallel computations which were mostly carried out at the BSC. These are mostly computations needed to perform chi2 fits of the extant experimental data.

In the second half of 2007, the team studied single pion production data keeping fixed the strong interaction part mentioned above and varying only the electromagnetic coupling of nucleon and resonances. We obtained a model up to 1.65 GeV center of mass energy. The construction of this model also required parallel computations.

During the same period the team focused on the reaction pion nucleon?eta nucleon, and refined the model described in to account for the existing differential cross section data for this reaction. The team will report on this effort which has also greatly benefited from the time allocations at the BSC.

The project is deeply related to the effort being carried out by the Excited Baryon Analysis Center, EBAC at Jefferson Laboratory (http://ebac-theory.jlab.org). The following team or researchers participates on this project: J. Durand (CEA/Saclay), T.-S. H Lee (Argonne National Laboratory), A. Matsuyama (Shizuoka University), B. Saghai (CEA/Saclay), T. Sato (Osaka University), and L.C. Smith (U. Virginia).



The figure depicts the total cross sections for single pion photoproduction using the model developed ini. The solid line corresponds to the full model, the dashed curves are obtained from turning off all the intermediate meson-baryon channels except the pion nucleon channel in the the loop integrations. The dotted curve is obtained by neglecting the loop-integrations in the pion-nucleon only calculation. Experimental data obtained using the SAID database. The diamonds correspond to the SAID solution

Publications

Dynamical coupled-channel model of meson production reactions in the nucleon resonance region
A. Matsuyama, T. Sato, T.-S. H. Lee, Physics Reports 439 (2007) 193-253.

Dynamical coupled-channel model of pi N scattering in the W <= 2-GeV nucleon resonance region.
B. Julia-Diaz, T.-S.H. Lee, A. Matsuyama, and T. Sato, Physical Review C 76, 065201 (2007).

Dynamical coupled-channels effects in pion photoproduction, B. Julia-Diaz, T.-S.H. Lee, A. Matsuyama, T. Sato and L.C. Smith, submitted Physical Review C (2007).

Gerardo Delgado

Departamento de Física Atómica, Molecular y de Agregados Instituto de Física Fundamental Blas Cabrera

Theoretical simulations in gas-phase clusters and liquids

The project contains two research lines within the frame of gas-phase clusters and liquids:

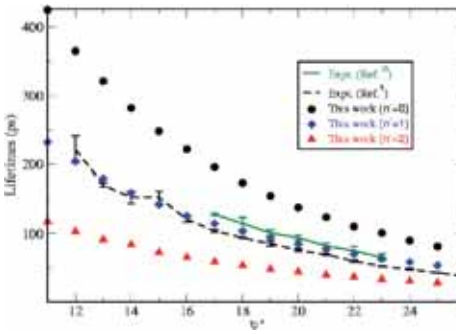
1) Structure and dynamics of molecular vdW clusters: contruction of reliable potential surfaces based on ab initio methodology and nuclear dynamics calculations in order to assign the exeprimental signatures of different isomers of Rgn - XY clusters, (Rg=rare gas, XY=diatomic molecule).

2) Molecular dynamics (MD) simulations of liquid water: MD calculations using realistic potentials to study how structural changes at a molecular level influence macroscopic properties of water and aqueous solutions. The results obtained:

1) Bound and resonance state calculations were carried out for van der Waals clusters formed of a dihalogen molecule and rare-gas atoms. Such calculations were performed using ab initio CCSD(T) potential surfaces for the ground and the first excited electronic state of HeI2 complex. The results obtained are compared with the experimental data available and the quality of the surfaces is verified. Such surfaces are of particular interest in the study of, both the solvent properties of superfluid helium and the relaxation dynamics of impurities (e.g. dihalogen molecules) embedded in He nanodroplets and interpretation of recent experimental data

2)Molecular dynamics calculations for liquid water were carried out using parallel versions of MOLDY and GROMACS codes.

These simulations are performed using two different potential models and the viscocity coefficients (bulk, shear and longitudinal) of liquid pure water are computed and compared with experimental data. The understanding of the structure and dynamics of water and aqueous solutions is crucial for all aspects of solution chemistry and for the behaviour of biological macromolecules.



Publications

A. VALDÉS, R. PROSMITI, P. VILLARREAL, G. DELGADO-BARRIO, D. LEMOINE and B. LEPETIT. "Vibrational Predissociation Dynamics Study of HeI$_2$(B) cluster" J. Chem. Phys., 126, 244314 (2007).

M.P. DE LARA-CASTELLS, R. PROSMITI, D. LÓPEZ-DURÁN, G. DELGADO-BARRIO, P. VILLARREAL, F.A. GIANTURCO, and J. JELLINEK. "Spectral simulations of polar diatomic molecules immersed in He clusters: Application to the ICl(X) molecule" Phys. Scripta, 76, C96-C103 (2007).

Pablo Cerda Duran
Max-Planck-Institute for Astrophysics (Germany)

MHD instabilities in compact objects

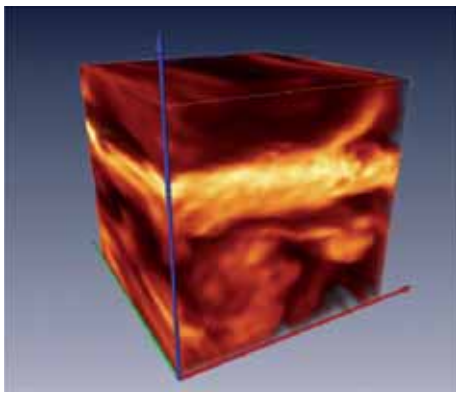
The team performed local magneto-hydrodynamics simulations of the magneto-rotational instability (MRI) and the Kelvin-Helmholtz instability (KHI) in the astrophysical context of compact objects. The aim was to solve the still open question of whether the magnetic field is able to grow substantially under the conditions of the astrophysical scenarios considered (compact objects) or not. The team performed a study of the growth rates in comparison with linear analysis estimates and of the saturation process. To asses the results we performed high resolution 3D MHD simulations and checked the resolution and box size effects in the simulations. The group used for this task a MHD Eulerian code using the state-of-the-art numerical techniques appropriate for this problem, namely Riemann solvers in conjunction with CT schemes for the magnetic field.

The simulations of the KHI allowed to establish a physical mechanism for the saturation of the growth of the instability and the amplification of the magnetic field. Simulating the instability with parameters similar to neutron star mergers, we found saturation field strengths of the order of 1016 Gauss. Thus, the team confirmed the lower range of values estimated based on global simulations by Price & Rosswog.

In simulations of the MRI in stellar post-collapse models, the team found that the instability indeed grows, leading to strong field amplification and angular-momentum transport. The group confirmed the presence of the instability under a rather wide range of physical parameters. The growth times are similar to the evolutionary time scales of post-bounce supernova cores.

Thus, the results indicate that the MRI and, hence, magnetic fields may affect the evolution of supernovae. On the other hand, the simulations, performed using only rather low numerical resolutions, which restrict to small volume boxes and do not yet allow to draw final conclusions. They, however, allowed to identify promising models for further, more refined investigation using higher resolutions.

Thanks to the supercomputing capabilities of MareNostrum the team was able to perform the simulations needed to investigate the effect of extremely small length-scale instabilities in global simulations of compact objects.



Magnetic field strength inside the shearing box for the MRI

Publications

M. Obergaulinger, P. Cerda-Duran, and E. Mueller, "Local simulations of the magneto-rotational instability in core-collapse supernovae", in preparation.

M. Obergaulinger, M.A. Aloy, and E. Mueller, "Local simulations of the magnetized Kelvin-Helmholtz instabilities in neutron stars mergers", in preparation.

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Departamento de Física de la Universitat Autònoma de Barcelona

Statistical mechanics of ionic liquids under confinement: molecular simulations

The modeling, understanding and prediction of the electrostatic properties of nanostructured ionic soft materials is a extremely challenging problem, requiring only affordable using world leader Supercomputing centers. In our previous projects, the team has investigated different soft materials in contact with electrolyte (surfactant layers, biomimetic membranes, macroions and nanoparticles,...) showing the high performance of Marenostrum in Molecular Dynamics simulations of these systems.

In the present project, the group has advanced a step further, investigating the structure of a novel ionic system which broad applications in green chemistry, the so-called room-temperature ionic liquids (IL). ILs are neutral mixtures of positive and negatively charged ions with large size and geometric asymetry which form a strongly interacting coulomb liquid at room temperature. They represent a novel class of liquids with surprising thermodynamical and electrical properties very attractive for a number of practical applications: solar cells, electrochemical sensors, and activated carbon or carbon nanotube – based supercapacitors. In all these applications, ILs are confined in nanoscale pores. Ionic liquids confined in a nanoporous structure display a different behavior with respect to the bulk . In particular, the structural charge arrangement and ionic mobility inside the pores are determinant for the electrochemical performance of all these devices based on IL-embedded porous materials. The objective of this activity is to understand the different microscopic effects leading to the thermodynamic behavior of ILs in confined environments. In particular, we have performed molecular dynamics simulations of a model ionic liquid (1,3-dimethylimidazolium chloride) confined in narrow pores of nanometer size (between 3 – 7 nm). These simulations are highly time consuming due to the sluggish dynamics of the ions inside the pore. The team has found extremely high correlation times, typically between 2-10 ns (depending on the density of the liquid). Each simulation requires an equilibration of about 1000 CPU-hours in a small system with only 500 ions (cations+anions). Since simulations need to be performed up to much larger times in order to perform proper equilibrium averages and also larger systems are desirable, it is clear that these simulations are near the limit of the technical capabilities of Molecular Dynamics Simulations in HPC.

These molecular dynamics simulations have demonstrated that the dynamics and structure of ionic liquids under confinement is much more rich and complex than was previously expected. The mobility of both anions and cations is highly reduced as compared to the bulk IL even for pores as large as 7 nm. This fact reflects the high degree of structuration induced by the confinement, enhanced by the high anisotropy in size between the cation and the anion. This effect also translates in the production of a high voltage drop between the confining walls and the center of the pore ("ferroelectric" effect induced by confinement). These simulations in MareNostrum have made possible to demonstrate that the charge distribution in these systems has extremely high correlation times (between 2-10 ns), so many previous studies cannot be considered as providing true equilibrium information. This important result could be essential to understand the present controversies between previous simulation results (and also different experimental results).

Publication

Title: Orientational transitions of anisotropic nanoparticles at liquid-liquid interfaces Author(s): Bresme, F; Faraudo, JOURNAL OF PHYSICS-CONDENSED MATTER Volume: 19 Article Number: 375110 Year 2007

Title: Electrostatics of phosphatidic acid monolayers: Insights from computer simulations, Faraudo, J; Travesset, A. COLLOIDS AND SURFACES A-PHYSICOCHEMICAL AND ENGINEERING ASPECTS Volume: 300 Issue: 3 Special Issue: SI Pages: 287-292 year 2007

Title: Phosphatidic acid domains in membranes: Effect of divalent counterions, Faraudo, J; Travesset, A. BIOPHYSICAL JOURNAL Volume: 92 Issue: 8 Pages: 2806-2818 Year 2007

Title: The many origins of charge inversion in electrolyte solutions: Effects of discrete interfacial charges Faraudo, J; Travesset, A. JOURNAL OF PHYSICAL CHEMISTRY C Volume: 111 Issue: 2 Pages: 987-994 Year 2007

Title: On the influence of solute polarizability on the hydrophobic interaction Bresme, F; Wynveen, A. JOURNAL OF CHEMICAL PHYSICS Volume: 126 Issue: 4 Article Number: 044501 Year 2007

Luis Antonio Fernández
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First-order transition in a three-dimensional disordered system

Most of phase transitions in Nature are of first order: the energy, pressure, magnetic field, etc. change abruptly. Also, most of natural systems are disordered to some degree. Hence one should ask what happens to a system undergoing a first-order phase transition on a perfect sample if one increasingly deteriorates the quality of the sample at hand.This is not only a fundamental open problem in Statistical Mechanics, but one with practical implications for instance in the field of highly correlated electron systems (such as high temperature superconductors or colossal agnetoresistance oxides).

At an intuitive level, one expects that disorder will weaken the phase transition. Actually, it does more than intuition would expect. In two space dimensions, it is known that the slightest concentration of impurities pulls the phase transition into continuous (second order) kind. Disorder acts as a fairly strong perturbation. In three dimensions there is no theoretical reason to forbid a first order transition at finite impurity concentration.

The team considers the three dimensional four states Potts model that present a strong first order phase transition between ferromagnetic and paramagnetic phases. The scope is to determine if there exists a finite dilution degree where the first order character is preserved.
The Monte Carlo simulation of first order phase transitions is a very involved problem because of the presence of the Exponential Critical Slowing Down: the typical evolution time diverges exponentially at the transition with the system size. This have prevented the possibility of working with large lattice sizes (previous work only have been capable of simulate up to 15625 spins lattices).The team has employed a recently developed method that opens the possibility of equilibrating systems with more than a million of spins.

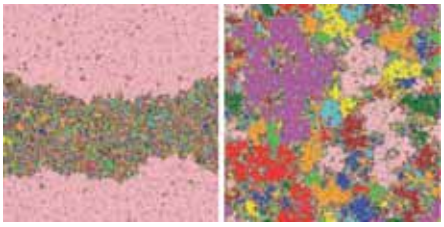
The method allows to compute the system entropy as a function of the energy, from which,

one can directly measure the energy gap (latent heat) or the energy of the phase coexistence interface (surface tension). The group has obtained very precise measurements of these quantities as a function of the dilution degree.

The team has observed that the latent heat reduces fastly when increasing dilution up to a point where it becomes zero. However the apparent critical dilution is strongly dependent of the lattice size. In fact, it becomes smaller when the lattice size is increased. The crucial point is to compute the infinite-volume value (thermodynamical limit). Fortunately, sophisticated techniques such as the Finite-Size scaling analysis allow to compute the extrapolation, if the statistical quality of data is good enough. We have obtained very precise data from lattices with linear size in the range 16 - 128 that show that a first order transition remains for a narrow dilution interval.

The study of first order transitions with Monte Carlo simulations is a classical challenge, that we show can be addressed with the developed methods. This opens the possibility of facing the study of many interesting physical problems. Work is in progress to extend the procedure to very different systems such as structural glasses and frustrated magnetic systems.

The Monte Carlo studies of diluted systems require long simulations in many disorder configurations. The use of a large supercomputing facility, such as MareNostrum, to carry out this kind of simulations is crucial in two aspects: the large computer power available, and the facility of managing a large amount of of simulation jointly.



A small amount of dilution changes a first order transition to second order. We illustrate this phenomena with two sample configurations of the ten-states Potts model in two dimensions, without dilution (left) and with a 5% of site dilution (right).

Domingo Giménez Cánovas
Facultad de Informática. Universidad de Murcia

High Performance Computation of Simultaneous Equation Models

Simultaneous Equation Models are used in different fields. In some cases the systems to study are very large and it is necessary to solve them with efficient parallel programs in large computing systems. The development of parallel algorithms for SEM is analysed.

MareNostrum has been used to experimentally study the scalability of algorithms of type Indirect Least Square (ILS) and Two Step Least Square (2SLS). Because 2SLS has higher computational cost and must be used in the solution of some of the equations in the systems, new algorithms for the 2SLS method have been developed and compared with the previous ones.

Techniques to automatically obtain satisfactory models were analyzed. For this reason it is necessary to solve a large number of potentially large SEMs, which must be done in a large computational system.

Publication

José-Juan López-Espín, Domingo Giménez: Solution of Simultaneous Equations Models in high performance systems. Parallel Processing and Applied Mathematics, Gdansk, Poland, September 9-12 2007. To be published in LNCS.

José Juan López Espín: Algoritmos de pasos de mensajes para modelos de ecuaciones simultáneas. Reunión sobre Optimización de Rutinas Paralelas y Aplicaciones. Murcia, June 12-13 2007.

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Dept. Fisica Teorica Universitat de Valencia and IFIC

Monte Carlo numerical computations of the properties of hadrons

The data analysis of the forthcoming LHC collider and B-factories requires an accurate understanding of the strong interaction between quarks in hadrons. QCD is the field theory that describes these forces. Unfortunately, some aspects are still obscure. To clarify them and perform reliable predictions one has to resort to non-perturbative methods, in particular to large scale numerical simulations in a discretized version of the continuum QCD theory: the so-called lattice QCD (LQCD).
The aim of our project is to perform realistic simulations of LQCD with 3 and 4 dynamical fermions by running at light quark masses, with a pion mass lower than 300 MeV, in lattice boxes of at least 2 fm^3. The team uses an efficient formulation of LQCD, the maximally twisted mass QCD, that amounts to adding a twisted mass term to the standard Wilson-Dirac operator.

The European Twisted Mass (ETMC) is a big international collaboration on large scale dynamical LQCD numerical simulations with twisted fermions. Using MareNostrum (MN), BGL, ApeNext and Altix, we have shown that twisted fermions offer a number of advantages when tuned to maximal twist:

1. Automatic O(a) improvement is obtained by tuning only one parameter.

2. The renormalization mixing pattern is significantly simplified.

3. The twisted mass provides an infrared regulator that allows to obtain substantially smaller quark masses compared to standard Wilson fermions.

From our Nf=2 dynamical simulations, we precisely measured the pseudoscalar mass and decay constant. When confronted with chiral PT theoretical predictions, the group obtained accurate values of the low energy constants,

F= 121.3 (7) MeV l3=3.44(8)(35) l4=4.61(4)(11)

The team has also calculated the average up-down and strange quark masses and the light meson pseudoscalar decay constants,

m_ud(2 GeV) = 3.85(12)(40) MeV

m_s (2 GeV) = 105(3)(9) MeV

f_K/f_pi = 1.227(9)(24)

The future and more promising project is to start Nf=4 dynamical simulations on MN which will take into account the quantum effects of the strange and charm quarks.

Only by using supercomputers like MareNostrum, BG/L, ApeNext and Altix, could the ETMC perform simulations at three different values of the lattice spacing a<0.1 fm with two dynamical degenerates light quarks in the range of pseudo scalar masses 300 < m_PS < 550 MeV using an improved HMC algorithm. Moreover, the next project, the simulations with 4 dynamical quarks, are feasible only on massive parallel computers like MareNostrum.

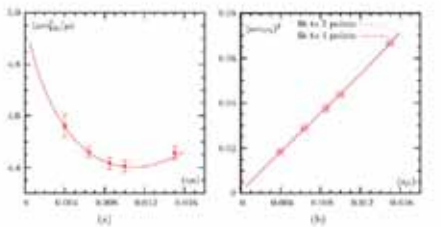

Figure 2: In (a) we show $(am_{PS})2/(a\mu)$ as a function of $a\mu$. In addition we plot the χPT fit with Eq. (5) to the data from the lowest four μ-values. In (b) we show $(am_{PS})^2$ as a function of $a\mu$. Here we present two χPT fits with Eq. (5), one taking all data points and one leaving out the point at the largest value $a\mu = 0.015$. In both figures (a) and (b) we show finite size corrected (L→∞) data points

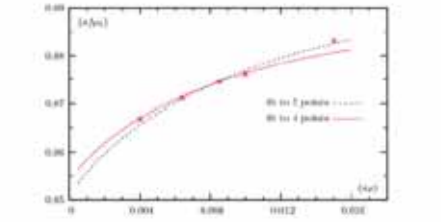

Figure 3: We show a f_{PS} as a funtion of $a\mu$ together with fits to χPT formula Eq 6. We present two fits, one taking all data and one leaving out the point at the largest value $a\mu = 0.015$. We show finite size corrected (L→∞) data points

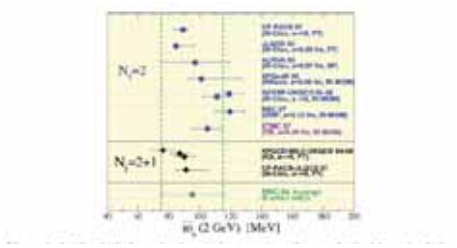

Figure 4: Lattice QCD determinations of the strange quark mass obtained from simulation with N_f = 2 [17]-[23] and N_f =2+1[14, 24, 25, 26] dynamical fermions. The PDG 2006 average from lattece only [27] is also shown for comparison

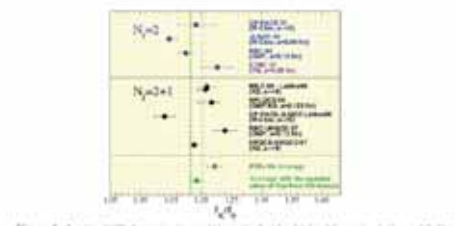

Figure 5: Lattice QCD determinations of the ratio f_K / $f\pi$ obtained from simulations with N_f = 2 [17, 18, 28] and N_f =2+1+[25], [29]-[30] dynamical fermions. The results are also compared with the PDG 2006 average [27] and with the average based on the updated determination of V_{us} from K_{L3} decays [34]

Publications

"Dynamical twisted mass fermions with light quarks". Ph. Boucaud et al. (ETM Collaboration) Published in Phys.Lett.B650:304-311,2007. e-Print: hep-lat/0701012

"Light quark masses and pseudoscalar decay constants from N(f)=2 Lattice QCD with twisted mass fermions". By European Twisted Mass Collaboration (B. Blossier et al.) e-Print: arXiv:0709.4574 [hep-lat] Submitted to Nucl. Phys. B

Plenary talks to the XXV International Symposium on Lattice Field Theory, held in Regensburg from July, 30 to August, 4, 2007.

"Lattice QCD with two light Wilson quarks and maximally twisted mass". Plenary talk. Presented by Carsten Urbach for the ETMC. To be published in PoS(Lattice 2007). e-Print: arXiv:0710.1517v1 [hep-lat]

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High resolution numerical simulations of homogeneous turbulence with complex effects

Isotropic turbulence receives a continuous effort for an increasingly refined description since Kolmogorov proposed his theory, but homogeneous turbulence subjected to complex effects still represents a great challenge, from its largely modified dynamics with respect to isotropic turbulence. Instances of distorted turbulence by external body forces or mean shear are present throughout natural and industrial flows. Geophysical flows are submitted to the effect of the Earth's rotation, when dealing with synoptic scales, and scales smaller by a few orders of magnitude may be affected by density or temperature stratification, either stabilizing, or destabilizing in convective flows. Moreover, these oceanographic and high altitude flows, or the atmospheric boundary layer, are all subjected as well to mean flow distortion such as shear. In this project, the team focuses on the effects of stable stratification and solid body rotation on the dynamics and the structure of homogeneous turbulence.

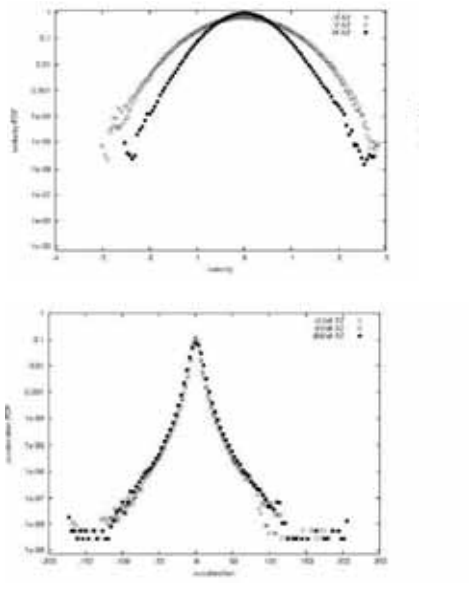
The team uses a pseudo-spectral code to perform high resolution Direct Numerical Simulations of turbulent flows in a stably-stratified and rotating fluid, to characterize the three-dimensional structure of anisotropic turbulence and its anisotropic Lagrangian properties. Cigar-like structures appear in rotating turbulence, while in stably stratified turbulence, a specific layered organization emerges in the flow. These two effects are in competition when both the Coriolis and buoyancy forces interact, depending on the rotation rate and the density gradient. Moreover, the turbulent diffusion properties depart strongly from the isotropic case, requiring to distinguish between the horizontal and vertical directions for one- and two-particle dispersion. The group starts by simulating a high Reynolds number isotropic turbulent flow from initial random conditions. This field is important, since it provides the startup conditions for the anisotropic rotating stratified cases. Energetic

constraints and numerical resolution constraints are imposed by the available possible number of grid points (here 1024?), and the anticipation of the development of turbulence submitted to the Coriolis and gravity forces, with an inhibited energy cascade with respect to isotropic turbulence dynamics. The thus obtained isotropic turbulent field is then impulsively submitted to rotation and stable stratification with varying parameters: a case with a ratio f/N of rotation over stratification of order 1/10, relevant for the Earth's geophysical flows at mesoscales, a rotation dominant case f/N> 1, and a non dispersive case with f/N=1. These cases correspond to low values of the Froude and Rossby numbers, typically of the order of 0.01 to 0.1, corresponding to the ratios of buoyancy (or rotating) timescale to the turbulence timescale.

The team first studies the dispersion properties of these anisotropic turbulent flows. The standard diffusion laws by Taylor are modified, and establishing their link with the anisotropic structure functions in rotating stably stratified high Reynolds number turbulence is a crucial question.

The DNS are run for as long as possible, in order to get the most information about the Lagrangian asymptotic laws. The trajectories of 100000 particles are followed during the computation, for convergence of the dispersion statistics. We compute the statistics of one-particle dispersion and two-particle separation in the horizontal and vertical directions, important for environmental flows modeling. In the rotation dominated cases, one-particle dispersion short-time ballistic tÇ laws are recovered, but at long time super-diffusivity is observed, with respect to the classical Brownian diffusion proportional to time t, in both the horizontal and the vertical directions. In the stratification dominated cases, one-particle diffusion reaches a plateau in the vertical direction, from the limitation of available potential energy, and in relation with the thin layering of the Eulerian velocity field. For the two-particle separation, one observes an intermediate linear stage in between the ballistic and Brownian stages, with a t? behavior. However, the duration of this stage is related to the strength of the the stratification and rotation, as well as to the Reynolds number, in a complex way. This is attested by the non universal scaling which is found for the one- and two-particle vertical and horizontal diffusion laws.

Second, the group observes the structure of the flow by visualizations, and by computing moments of the velocity and acceleration fields, in addition to directional integral length scales. The latter show a strong increase of the correlation length along the rotation axis in the rotation dominant cases, and a strong reduction of this vertical correlation length in the stratification dominant ones. Considering probability density functions (pdf) of the velocity components, and of the Lagrangian acceleration components, we observe an unexpected result: whereas, as expected from the visualizations, the pdfs of the velocity components are anisotropic, with the vertical one differing sensibly from the horizontal ones, the pdfs of the components of Lagrangian acceleration do not exhibit any observable anisotropy (see the figures). This raises the question on how the Eulerian field anisotropy connects to the Lagrangian one. The group currently seeks a partial answer in the role played by the inertio-gravity waves, present in rotating stratified turbulence.



(Top) velocity components, horizontal U and V, vertical W; (bottom) Lagrangian acceleration normalized by instantaneous values to remove the influence of viscous decay. The case shown is for strongly stratified turbulence, DNS 1024?

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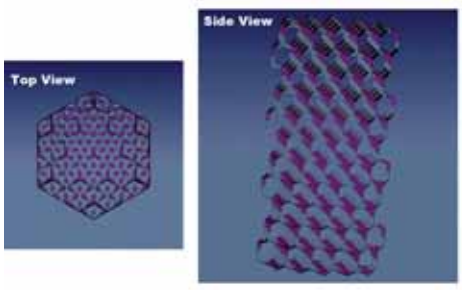
First-principles calculations for the electronic structure of semiconductor nanowires

Semiconductor nanowires are one-dimensional nanostructures that constitute ideal building blocks for highly integrated nanoscale electronics and optoelectronics. In this project the team is determining the electronic structure of semiconductor nanowires from first-principles calculations. In particular, we are using a code developed by us, the PARSEC code (http://www.ices.utexas.edu/parsec), which is devised to take advantage of high-end massively parallel computing environments such as MareNostrum.

The historical rates of improvement in productivity experienced by the semiconductor industry during the last decades are based on a continued miniaturization of silicon-based devices. However, existing materials and technologies are approaching their physical limits, which will prevent the industry from reaching similar rates of improvement. Finding new materials and technologies adequate for the fabrication of highly integrated devices in the deep nanometer regime would potentially overcome such important limitation. Among the materials investigated on this regard, semiconductor nanowires (NWs) are of special interest. One-dimensional materials like NWs are the smallest dimensional materials that can transport efficiently electrical carriers and optical excitations. Also, NWs with controlled electrical and optical properties can be synthesized for a wide variety of semiconductor species, and are known to work as functional devices like sensors, light emitting diodes, and field effect transistors. As such, NWs represent ideal building blocks for highly integrated nanoscale electronics and optoelectronics.

Despite the technological usefulness of semiconductor NWs being mostly derived from the introduction of electrical carriers in the NWs, little is known about fundamental issues behind doping these nanomaterials. For example, what is the nature of the carriers responsible for electric conductance in the doped NWs (are these states obtained by energy band engineering spatially localized or extended states?), and how size affect their electronic properties (how are the carriers affected by quantum confinement?). Answering such questions is not only important from a fundamental point of view. It is also essential to design future devices and applications based on NWs, as well as to improve characteristics of those devices already existent. Knowing the properties of NWs is a necessary step for determining the optimum working conditions of both NW-based electronic devices and opto-electronic devices.

In the current activity developed at the BSC the team is addressing issues like the ones listed above by performing first-principles calculations on doped semiconductor NWs. In particular, the team is studying NWs constructed from III-V semiconductor materials, following the enormous attention that these nanomaterials have recently attracted. The results obtained within the current Activity period are being very promising. The group has already determined the effects of quantum confinement on the characteristic properties of the impurity state introduced in a NW by p-type doping. The group knows of no previous prediction performed on any p- or n- type doped NW. Part of our results have been published in Nano Letters, the leading forum for rapid communication of nanoscale research.



Top and side view of a nanowire constructed from III-V semiconductor materials as studied within the theoretical framework

Publications
M.M.G. Alemany, Xiangyang Huang, Murilo L. Tiago, L.J. Gallego, and James R. Chelikowsky, "The Role of Quantum Confinement in P-Type doped Indium Phosphide Nanowires", Nano Letters, Vol. 7, No. 7, 1878-1882 (2007).

M.M.G. Alemany, Manish Jain, Murilo L. Tiago, Yunkai Zhou, Yousef Saad, and James R. Chelikowsky, "Efficient first-principles calculations of the electronic structure of periodic systems", Computer Physics Communications, Vol. 117, Issue 4, 339-347 (2007).

M.M.G. Alemany, Xiangyang Huang, Murilo L. Tiago, L.J. Gallego, and James R. Chelikowsky, "Ab initio calculations for p-type doped bulk indium phosphide", Solid State Communications, in press.

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ICMAB-CSIC

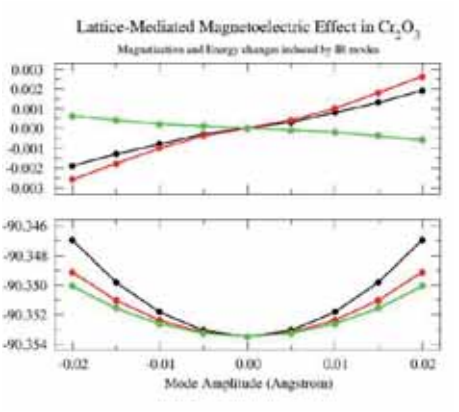
Multifunctional oxides

The team's activities in MareNostrum have been focused on the study of various multifunctional oxides. The group has worked on both the development of new first-principles methods to tackle these materials as well as on applications for particular compounds. More specifically, the team has:

1 · Developed a novel computational scheme to calculate magnetoelectric coupling parameters, which quantify the magnetic response of an insulator to an electric field, using first-principles methods based on Density Functional Theory. The new methodology was demonstrated with an application to Cr_2O_3 (see figure), an experimentally well-characterized magneto-electric compound. The new method is expected to aid the experimental search for compounds that present robust magneto-electric effects at ambient conditions. Studies of various compounds of potential technological interest are currently underway.

2 · Developed new first-principles methods for a simultaneously accurate treatment of the electronic and structural properties of ferroelectric oxides. The new methods, which relies on hybrid functionals that take advantage of novel and very accurate GGA approaches, will enable to treat, for example, metal-ferroelectric heterostructures, where having a correct description of the electronic band off-sets is crucial to predict the properties correctly. These methods open the door to realistic and accurate simulations of the materials and situations that are relevant for the behavior and performance of devices used in microelectronics and spintronics.

3 · Demonstrated the possibility of having co-existing magnetic order and ferroelectricity driven by the same chemical species. Our results for $CaMnO_3$ and related compounds correct a general misbelief in the community and open the door to many disregarded possibilities for materials design in magnetoelectric multiferroics.



Calculated response of Cr2O3, upon condensation of Infra-Red active (or polar) modes. Note that the magnetization is zero for zero mode amplitude, i.e., for the situation corresponding to a perfect anti-ferromagnetic, collinear arrangement of the spins of the Cr atoms

Pilar Hernández

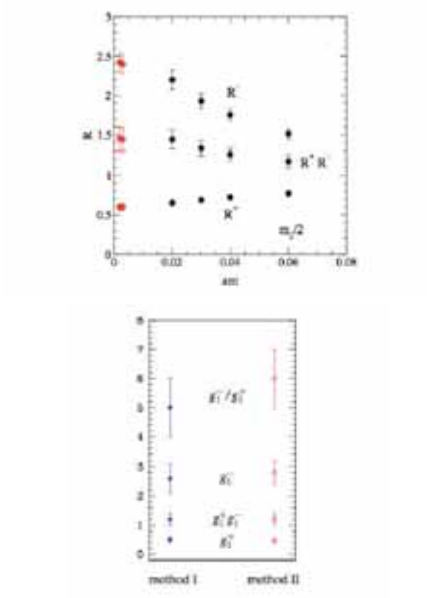
Instituto de Fisica Corpuscular UV/CSIC

Non-perturbative aspects of QCD in flavour physics

The aim of our project is to compute from first principles the amplitudes for non-leptonic kaon decays in the well-established theory of Quantum Chromodynamics, via the determination of the two low-energy couplings, g+ and g-, that control these amplitudes in the effective chiral theory. The prediction of these quantities is a very important contribution to the field of flavour physics, which tries to reveal the origin of the fundamental parameters of the Standard Model.

An unresolved problem in this field is the stricking hierarchy between the two isospin amplitudes, the so-called Delta I=1/2 rule, whose origin after many years of research remains unknown. In the time allocated to our project, the team computed these amplitudes in a particularly interesting limit of a light charm quark. The fact that the charm quark is so heavy with respect to the up, down and strange quarks has been proposed as a possible source of the hierarchy. The group has found however that a significant hierarchy remains in the case where the charm is light, challenging the old lore. This has been recently confirmed by an alternative method that relates the low-energy couplings involved in these amplitudes to the wavefunctions ot the topological zero-modes of the Dirac operator. This method has provided an independent determination that has many advantages from the numerical point of view.

During 2007 the team has also started a new project which tries to quantify the effects of the dynamical quarks, which is the most important systematic error that remains to be controlled in our previous quenched results. To do this the team will use mixed actions, in which sea and valence quarks are simulated with different regulators in order to achieve better performance.



Top: Observables obtained as a function of the quark mass. The red points have been obtained at the smallest quark masses ever reached for these quantities. Bottom: Results for the couplings, their product and their ratio with the two methods

Publications

"On K->pipi amplitudes with a light charm quark" L. Giusti, P. Hernandez, M. Laine, C. Pena, J. Wennekers and H. Wittig, Journal: Phys. Rev. Lett. 98:082003,2007.

Weak low-energy couplings from topological zero-mode wavefunctions, P. Hernández, M. Laine, C. Pena, J. Wennekers, H. Wittig, Journal: PoS LAT2007:356, 2007

Thilo Knacke

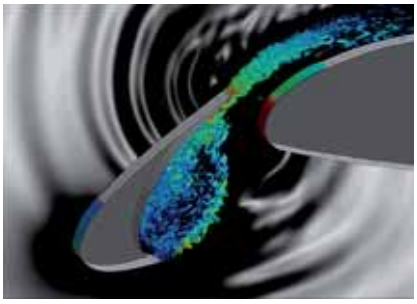
Institut für Strömungsmechanik und Technische Akustik (ISTA), Technische Universität Berlin

Numerical simulation of airframe noise

The main objective of this project is the reduction of aircraft noise by suppression of local noise sources. To assess the feasibility of reducing noise through passive and active control of unsteady pressures in the aircraft boundary layer and wake, an understanding of the flow physics is a prerequisite. The flow field simulation of the highlift system can deliver deep insight into the noise generation mechanisms which predominate under approach conditions.

The reduction of aircraft noise is an important issue for aircraft manufacturers to prevent increasing noise exposure caused by the continuous growth in air traffic. During the landing approach, the flow around deployed highlift devices is known to be a major contributor to the overall sound pressure levels perceived by observers in the distance. A good understanding of the underlying noise generation mechanisms is essential for the development of noise reduction strategies. Insight can be obtained from numerical simulation, which is well suited to provide detailed flowfield information. As the basis for the airframe noise simulation a typical 3 component high lift configuration has been selected, which is simulated under landing approach conditions in freeflight. The computational grid consists of approx. 30 million volumes and allows for resolution of both sound waves and turbulent sound sources. At the present state of the timeaccurate simulations, selfsustained unsteady turbulent motion continuously generates broadband noise and especially strong sound waves are seen emanating from the slat of the configuration.

Thanks to supercomputing facilities such as MareNostrum, increasingly complex flows of industrial relevance are becoming accessible by means of numerical simulation.



Vertical structures and sound waves surrounding the slat of a highlift system deployed in landing configuration

Publications

Mockett, C.; Greschner, B.; Knacke, T.; Perrin, R.; Yan, R.; Thiele, F.: Demonstration of improved DES methods for generic and industrial applications. In: Peng.

Michel, U.; Eschricht, D.; Greschner, B.; Knacke, T.; Mockett, C.; Thiele, F.; Yan, J.: Simulation of the sound radiation of turbulent flows with DES. In: Proceedings of the WestEast High Speed Flow Field Conference, Moscow, Russia, 2007.

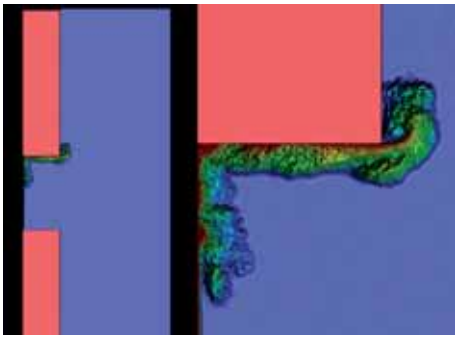
Asensi Oliva Llena

CTTC (Centre Tecnològic de Transferència de Calor), UPC

Direct numerical simulation of turbulent flows in complex geometries

Direct numerical simulation (DNS) is an important area of contemporary fluid dynamics, because its interest for improving the understanding of th e physics of turbulence and because it is an essential tool for the development of better turbulence models. Recently, relevant improvements on turbulence modeling based on symmetry-preserving regularization models for the convec tive (non-linear) term have been developed.They basically alter the convective terms to reduce the produc tion of small scales of motion by means of vortex-stretching preserving all inviscid invariants exactly. Since now, they have been successfully tested for a differentially heated cavity at high Rayleigh (Ra) numbers. At this stage, high resolution DNS results at of relatively complex geometries and configurations are of extreme importance for further progress. The main idea behind this is to assess the validity of tur bulence models in more realistic configurations, understand their limitations and finally improve them. Therefore, this is really a crucial issue since turbulence modeling ultimately becomes an essential tool for engineering applications.

To do so, we have been using the DNS code devel oped by CTTC at the MareNostrum supercomputer to carry out simulations of turbulent natural convec tion flows in open domains (see figure). The two configuration chosen are an extension of our previous work to an open cavity flow at Ra-numbers 10 10 and 3x10 10. Due to the complex behavior exhibit, an accu rate turbulence modeling of this configuration remains as a great challenge. This new DNS results shall give new insights into the physics of turbulence and will provide indispensable data for future progresses on turbulence modeling.



Instantaneous isotherms at Ra=3x1010. Left: general view of the extended domain. Right: zoom around top part of the open cavity

Publications

F.X.Trias, R.W.C.P.Verstappen, M.Soria, A. Gorobets, A.Oliva, " Regularization modelling of a turbulent differentially heated cavity at Ra=10 11", 5th European Thermal-Sciences Conference, EUROTHERM 2008, Eindhoven (The Netherlands), May F.X.Trias, M.Soria, A.Oliva, C.D.Pérez-Segarra. "Direct numerical simulations of two- and three-dimensiona turbulent natural convection flows in a differentially heated cavity of aspect ratio 4 ", Journal of Fluid Mechanics, vol.586, pp.259-293, 2007.

A.Gorobets, F.X.Trias, M.Soria and A.Oliva, ``A scalable Krylov-Schur-Fourier decomposition for the efficient solution of high-order Poisson equation on parallel systems from small clusters to supercomputers '', submitted to Computers & Fluids.

José E. Roman
Universidad Politécnica de Valencia

Scalability of Eigensolvers and SVD solvers in the SLEPc Library

Solvers for large-scale eigenvalue problems lie at the core of many computationally intensive applications. The objective is to enhance the efficiency of these solvers, by proposing modifications of the algorithms that can lead to higher megaflop rates and less overhead due to parallel execution with many processors. The improved algorithms are incorporated into the publicly available library SLEPc. The focus is on solvers for large-scale sparse eigenvalue and SVD problems that can scale to hundreds or even thousands of processors.

Eigensolvers parallelized in a straightforward way may behave well with a few tens of processors. However, the algorithms have to be tuned for allowing their use with many more processors.

For very large-scale, grand challenge applications such as those arising in nanoscience and other fields, users need to use hundreds of processors. In that case, scalability of solvers is very important in order to minimize performance degradation, thus enabling to use more processors for solving more complex problems in less time.

Furthermore, more efficient algorithms represent a better use of expensive supercomputing facitilites such as Mare-Nostrum. The team has conducted research on algorithm design so that scalability is improved while numerical robustness is maintained. The developments of the activity have resulted in eigensolvers that scale well up to 512 processors, or even more. SLEPc is currently being used in many different application areas across the world.

This research project requires to test the algorithms with a large number of processors, in order to assess the improvements in performance achieved by certain algorithmic modifications. On the other hand, it is important to perform the development and testing of new algorithms directly in the same platform that will be used by the final user.

Publications

V. Hernández, J. E. Román, A. Tomás, "Parallel Arnoldi eigensolvers with enhanced scalability via global communications rearrangement", Parallel Computing 33: 521-540 (2007).

V. Hernández, J. E. Roman, A. Tomas, "A robust and efficient parallel SVD solver based on restarted Lanczos bidiagonalization", submitted.

V. Hernández, J. E. Román, A. Tomás, "A parallel Krylov-Schur implementation for large Hermitian and non-Hermitian eigenproblems", Int. Conference on Industrial and Applied Mathematics (ICIAM), Zurich, Jul 2007.

V. Hernández, J. E. Román, A. Tomás, "Paralelización híbrida con OpenMP y MPI de métodos de Krylov para el cálculo de valores propios", XVIII Jornadas de Paralelismo, Zaragoza, Sep 2007.

Ángel Rubio

Universidad del País Vasco

Spectroscopic properties of biomolecules, nanostructures and extended systems (ETSF activity)

This project applies state-of-the-art computer simulation tools developed within our ETSF infrastructure to describe electronic excited states in complex structures, from nano-to bio-molecules and adsorbates on surfaces. The global scientific aim of is to directly address specific problems related to the ab-initio modeling of the most widely used characterization tools based on spectroscopic techniques (such as optics, EELS, angle and time-resolved photo-emission, STM, etc) applied to complex materials as nanotubes, biomolecules, molecular and nano- electronics devices, quantum dots, etc. including environment and dissipation effects. The computer tools used and developed are octopus, abinit, self.

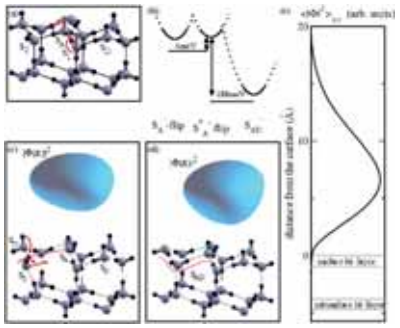
The results obtained are: i) Description of the optical and luminescence spectra biological chromophore and nanostructures for photovoltaic applications; ii)understanding the electronic and structural properties of crystalline ice-layers supported on metallic substrates; iii) Theoretical developments and test of the computing implementations of TDDFT and Many-body perturbation theory. The team has improved the scalability and parallelisation performance of the octopus code, address hybrids functional for optics and electronic structure and their implementation in the code SELF.

A dynamic landscape from femtoseconds to minutes for excess electrons at ice-metal interfaces

Excess electrons in low-dimensional water and ice structures are of general importance in atmospheric science, chemistry, biology, and astrophysics since in aqueous systems electron driven excitations, relaxations, and reactions span a wide range of energy and time scales. In bulk liquid water excess electrons are known to form a solvated complex in which the excess charge is screened and decays by geminate recombination.

In low dimensional systems like clusters or at ice surfaces the solvation process is determined by the more rigid structure of the water network. In such systems excess electrons can be localized outside the water structure in vacuum where they interact with a reactant.

Stabilization of excess electrons were studied at crystalline ice-metal interfaces by femtosecond time-resolved two-photon photoelectron spectroscopy and ab initio calculations. Following optical excitation into delocalized image potential states, electrons localize at preexisting defects which are located at the ice-vacuum interface. The stabilization of these trapped electrons is monitored continuously from femtoseconds up to minutes. This behavior is fundamentally different from liquid or amorphous solid water where excess electrons have a lower survival probability because they are screened less efficient. First principle calculations unveil the structure of the responsible orientational defects and the initial sequence of the electron induced structural modifications. Thereby, the team shed light on the collective character of the nuclear rearrangement that determines the energetics over all timescales.



(a) formation of the orientational defects SA-flip and S1-flip on the (0001)-ice surface, the reorientation / motion of the D2O molecules indicated by arrows. (b) Sketch of the energy surface of the initial reconstruction induced by the excess electron. (c) Geometry of SA-flip and the electron density of the excess electron $\phi(R)|2$ at 70% of its maximum value. The electron is bound to both DO-bonds at the neighbouring SA and SD. The arrows indicate the reconstruction of the bond network to form SAD. (d) Geometry of SAD and the excess electron density $\phi(R)|2$ as for SA-flip; the dashed line indicates new hydrogen bonds and the involved sites. (e) In-plane average of the density of the excess electron vs. the distance from the surface at SA-flip to illustrate its negligible overlap with the ice/metal system (similarly for the SAD defect). The gray horizontal lines indicate the position of the oxygen layers

Juan Jesús Ruiz-Lorenzo
Departamento de Física, Universidad de Extremadura

Critical behavior in three dimensional spin glasses in presence of magnetic fields

Nowadays a large amount of numerical, analytical and experimental studies have been done in finite dimensional spin glasses in absence of a magnetic field. For Ising spins, it is now clear the existence of a phase transition in three dimensions and above. However, the characterization of the properties of the low temperature phase is still under serious scrutiny.

On the contrary, the behavior of spin glasses under a field is really more complicated: there are no clear insights from analytical computations, simulations and experiments.

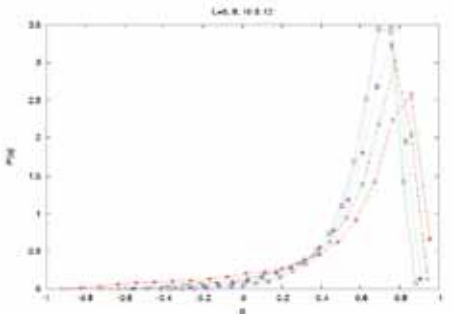
On the one hand, in the theoretical side, there are two main (competing) approaches to the model: the droplet model predicts no phase transition but the replica symmetry breaking theory predicts a higher order phase transition (third order in the Mean Field approximation). Numerically, at equilibrium, simulating small lattices, the data seem to discard a standard second order phase transition, however, out of equilibrium studies find clearly a phase transition (based in the study of violations of the fluctuation-dissipation theorem).

On the other hand, the experimental situation is also confused. Experiments in Ising models find an irreversibility line (that could be identified with a phase transition) but the authors claimthat the data are compatible with a paramagnetic phase, nevertheless the Heisenberg spin glass model shows a phase transition (droplet theory predicts a paramagnetic phase for any amount of magnetic field even for Heisenberg spins).

Monte Carlo studies of spin glass systems require long (time) simulations in many disorder configurations (replicas). The use of a large supercomputing facility is mandatory in order to obtain physical results.

In this project we have studied numerically the three dimensional Ising spin glass with binary couplings in a constant external magnetic field. The main goal of this study has been to analyze the presence of finite size effects on moderate size lattices, and in particular, if the probability distribution of the order parameter (the overlap) would have a positive support (this results is common to all the theoretical approaches).

The team has found that, even in the largest lattice simulated, the finite size effects are still large for different magnetic fields and temperatures, meaning that the group is far away of the asymptotic regime (thermodynamic limit), so the previous results based on these lattices are inconclusive.



Probability distribution of the order parameter, P(q), for all the lattice sizes simulated (L=6(red),8(black),10(yellow) and 12 (blue)) at T=0.8and h=0.4. Notice that the largest lattice simulated (L=12) still shows strong finite size effects (i.e. large tails in the negative overlap region)

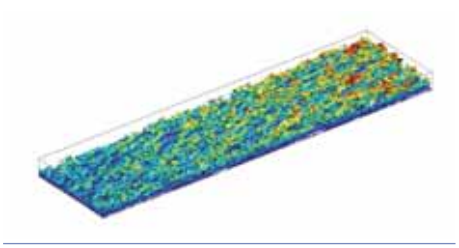
Javier Jiménez Sendín
Universidad Politécnica de Madrid

Simulation of Turbulent Boundary Layers

The goal of this project is to carry out a simulation of a Zero-Pressure Gradient (ZPG) boundary layer, at a Reynolds number high enough, and with enough development length, to serve both as an aid in the interpretation of experiments, and as a basic reference case for future Adverse Pressure Gradient (APG) simulations. The Reynolds number grows from Re_theta=600 at the entrance, to Re_theta=2000 at the exit, with a development length of the order on about 1200 initial momentum thickness. Previous simulations of these flows have either had lower Reynolds numbers or shorter boxes. This flow is a difficult one to interpret experimentally, because of the difficulty of accurately measuring the wall friction. This simulation is in the range of at least some experiments, and will therefore serve, not only as a reference case to study the physics of the flow, but as a calibration to existing experiments. The long box length is also important. One of the results of the preliminary simulations has been that most of the previous simulations were too short and probably corrupted by the inlet conditions.

Our code is coded in house. It is a Fortran MPI code, with mixed spectral/finite differences spatial discretization, and RK in time, which has been tuned for MareNostrum over the last year. It has already produced useful fluid mechanics results. The parallelization is essentially the same as in a previous channel code that ran on 2100 MareNostrum processors, in the preproduction period of that machine, and whose results are now the reference simulation for turbulence channels, worldwide. The central exchange is a global transpose that is hand coded, and that has been optimized extensively for MareNostrum.

This is a long-range activity, even if it consists of the production run of a single simulation. The full simulation will probably require about 6 Mcpu hours in 512 processors, and it is expected to finish before 2008 summer. This study is part of the long-term program for the study of turbulence physics in our group. The APG case is part of a European Strep cooperation to generate knowledge about near-wall turbulence, especially away from equilibrium (Wallturb, AST4-CT-2005-516008).



Publications

"Reynolds number effects on the Reynolds-stress budgets in turbulent channels", S. Hoyas & J. Jiménez, Phys. Fluids, to appear.

"Turbulent fluctuations above the buffer layer of wall-bounded flows", J. Jiménez & S. Hoyas, J. Fluid Mech., to appear.

"Recent developments in wall-bounded turbulence", J. Jiménez. Rev. R. Acad. Cien. Serie A, Mat. 101, 187--203 (2007)

"Vorticity organization in the outer layer of turbulent channels with disturbed walls" O. Flores, J. Jiménez & J.C. del Álamo, J. Fluid Mech. 591, 145--154 (2007).

"What are we learning from simulating wall turbulence?", J. Jiménez & R.D. Moser. Phil. Trans. Royal Soc. London. A 365, 715--732 (2007)

Gabriel Staffelbach

European centre for Research and Advanced Training in Scientific Computation

Towards Large Eddy Simulation of an industrial gas turbine

The CFD Team at CERFACS (European centre for Research and Advanced Training in Scientific Computation) specializes in ground breaking massively parallel simulations of combustion processes. The code AVBP, co-property of CERFACS and IFP (French Institut of Petroleum) used for these studies, has been ported on all available architectures and its linear scalability has been demonstrated on over 5000 Bluegene L processors. The use of numerical approaches to replace or add to the knowledge of experimental test cases of gas turbines is limited by the realistic modelisation of these devices using CFD (Computational Fluid Dynamics). One of the most marking examples is that most designs contain multiple burners (up to two dozen or more is some designs) but numerical and experimental studies often only focus on one (because of the costs, computational and financial, of building a complete set-up that just might not work). CERFACS's aim is to perform state of the art full combustion chamber simulations capable of reproducing the real behavior of turbines taking into account all the burners and all possible details. The first steps towards this type of simulation have been taking. Here AVBP was used to performe a Large Eddy Simulatin (LES) on Marenostrum on a annular combustion chamber for an helicopter prototype. All the burners, dilution jets and films as well as the complete casing are computed thus providing the first insights into the mechanisms present in the devices.The picture shows a cylindrical plane passing through the axis of all the burners colored by the temperature with velocity iso-contours. The outer casing is visible in quarters to visualize the complexity of the geometrical set-up. Preliminary results shows the first ever LES results on azimuthal acoustics and flame interaction ever done on an industrial set-up. Thus bringing us closer to a future “virtual burner”.

Vassilis Theofilis

School of Aeronautics. Universidad Politécnica de Madrid

Global instability analysis of the trailing vortex system in the wake of commercial aircraft

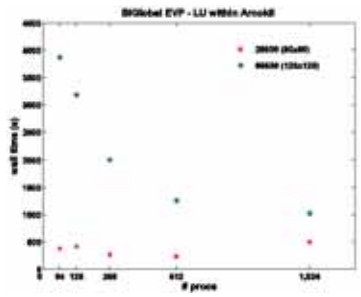
Linear instability of complex flows may be analyzed by numerical solutions of BiGlobal, partial-derivative-based eigenvalue problems (EVP).

Numerical solutions of this EVP in flows of engineering significance, such as the trailing vortex system in the wake of commercial aircraft, reveal instabilities inaccessible to simplified analyses. On the other hand, BiGlobal analysis is orders-of-magnitude more efficient than the alternative analysis methodology, namely full three-dimensional direct numerical simulation. However, the discretization of the BiGlobal EVP results in discrete matrices the size of which is well beyond the capabilities of serial platforms and solution algorithms.

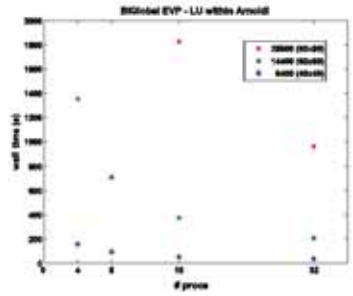
A parallel BiGlobal EVP solution methodology has been developed in 2007 and validated against serial solutions (at low resolutions). Use of the ScaLAPACK library (as part of the optimized PESSL library on the MareNostrum platform) has been made for the first time for this class of problems. Scalability tests have been performed for realistic flowfield resolutions on different platforms (own cluster comprising 128 processors, Magerit, using up to 256 processors, and MareNostrum, using up to 1024 processors). The relative merits of the different platforms have been assessed and documented in several publications, both in terms of wall-clock time and available number of processors. From a physical point of view, previously unknown instability mechanisms have been unravelled through massively parallel solution of the BiGlobal EVP.

Daniela Tordella
Politecnico di Torino (Italy)

Anisotropy and asymptotics in the mixing of shear-free homogeneous turbulent fields



MareNostrum



Local machine comprising 128 procs

Publications

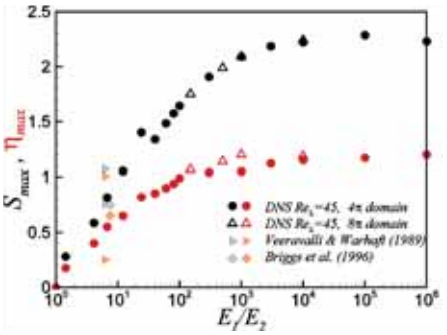
L. González, J. de Vicente and V. Theofilis (2007) High-Order Finite Element Methods for Global Viscous Linear Instability Analysis of Internal Flows. AIAA Paper 2007-3840. 18th AIAA Computational Fluid Dynamics Conference, Miami, FL, June 25-28, 2007

V. Theofilis and L. González (2007) Finite-Element Numerical Methods for BiGlobal Linear Instability Analysis of Vortical Flows. AIAA Paper 2007-4359. 37th AIAA Fluid Dynamics Conference and Exhibit, Miami, FL, June 25-28, 2007

The interaction of two isotropic decaying turbulent fields in the absence of mean shear generates the simplest kind of inhomogeneous turbulent field. This mixing is highly intermittent and has intense bursts of vorticity and strain, leading to non Gaussian velocity statistics. A set of numerical simulations between two decaying homogeneous and isotropic turbulent fields with the same integral scale and turbulent kinetic energies E_1 and E_2 has been carried out to measure the level of intermittency and anisotropy, inside the mixing layer, as a function of the energy ratio E_1 / E_2. In particular, the asymptotic behaviour in the limit for E_1 / E_2 going to infinity has been investigated. The latter asymptotic configuration corresponds to the diffusion of turbulence in a region of still fluid, the energy gradient is the maximum observable value for a fixed high energy level E_1.

It has been found that the mixing layer is intermittent for any value of the energy ratio, as shown by the large values of the velocity skewness and kurtosis. The intermittency, and the intermittent penetration in the low energy turbulent field, defined as the displacement of the maximum of the velocity skewness inside the low energy field, increases with the energy ratio to a finite asymptotic value. The maximum of the skewness is about 2.2 and the penetration is 1.2 times the mixing layer thickness. At the same time, the pressure transport is significant and remains proportional to the velocity triple moments, which are highly anisotropic, with about half of the turbulent kinetic energy flow across the mixing due to the self transport of the velocity component in the mixing direction.

A significant skewness of the transversal velocity derivative of the component in the mixing direction has been found. This small-scale anisotropy of the third order moments increases with the turbulent kinetic energy gradient which produces the mixing and is of the same order as the one observed in homogeneous shear turbulence at similar Reynolds number.



Maximum of the skewness (black-grey symbols) and intermittent penetration (red-orange symbols, $\eta_{max} = X_{max} / \Delta$, where X_{max} is the position of the maximum of the skewness and $\Delta(t)$ is the mixing layer thickness) as a function of the initial energy ratio E_1 / E_2. Comparison data are from previous laboratory (Veeravalli and Warhaft, JFM 1989) and numerical (Briggs et al}, JFM 1996) experiments

Publications

D.Tordella, M.Iovieno, P.R.Bailey, ``Asymptotic behaviour of the shearless turbulent kinetic energy mixing'', in Advances in Turbulence XI, 697-699, (Proceedings of the 11th European Turbulence Conference, Porto, 25-28 June 2007).

D.Tordella, M.Iovieno, P.R.Bailey, ``Transversal and longitudinal velocity derivative statistics in shearless turbulence'', 60th APS-DFD Annual Meeting}, Salt Lake City, 18-20 November 2007.

Andreas G. Yiotis
Michael E. Kainourgiakis
Athanassios K. Stub
Institute of Nuclear Technology
& Radiation Protection

A Lattice-Boltzmann study of immiscible two-phase flow in pore networks

Two-phase flow in porous media is a subject of significant scientific and industrial interest. It is involved in processes such as underground water flows, oil recovery, soil remediation and many more. In recent years, Lattice Boltzmann models (LBM) have been used to simulate two phase flow in porous media, and more complex two-phase processes such as viscous fingering in Hele-Shaw cells, Rayleigh-Taylor instabilities and the dynamics of liquid bubbles under gravity among others. Such works demonstrate that the lattice Boltzmann method (LBM) is a powerful tool for the computational modeling of multiphase flow problems.

In this paper the group studies the immiscible two-phase flow in porous media using the Lattice-Boltzmann model through a series of numerical simulations performed at the Barcelona Supercomputing Center. By considering a set of appropriate boundary conditions for the density distribution function defined in that model, the team account for the effect of wettability at solid-fluid interfaces and capillarity in the pores where the fluid-fluid interfaces reside. Different contact angles of the fluid-fluid interface at solid walls can be realized by taking appropriate values for the density distribution function at the solid sites of the porous domain.

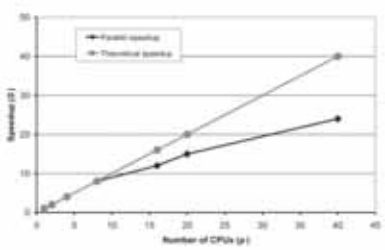
A series of numerical simulations were performed in a 2D pore network with porosity ε=0.77 and a 3D pore network with porosity ε=0.53 for various values of the initial wetting saturation S_w and fixed values of the wetting angle θ. For the 2D simulations, the dimension of the computational grid was 400x400 lattice units (L=400δx) and the size of each block of solid or void was 20x20 lattice units (n=20δx). For the 3D simulations, the computational

domain was 100x100x100 lattice units (L=100δx) and the size of each block of solid or void was 10x10x10 lattice units (n=10δx).

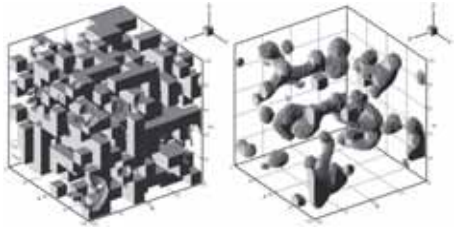
The Lattice Boltzmann model is parallelized for implementation on distributed memory computers using the Message Passing Interface (MPI) libraries. The computational domain (two and three-dimensional arrays) is decomposed in the y-direction in 2D pore networks and in the z-direction in 3D pore networks in order to take advantage of Fortran's column-major storage of multi-dimensional array elements. This scheme ensures that array elements exchanged across processors with MPI are located in continuous memory blocks.

The typical production runs were performed on 10 to 20 CPUs for 300000 to 1000000 δt. Each numerical simulation required approximately 4 to 32 hours, depending on the dimensionality of the pore network and the number of available CPUs. The parallel speedup of our model is shown in the figure. The parallel efficiency E of our LB code is greater than 0.8 on 20 CPU's and drops to 0.625 on 40 CPU's.

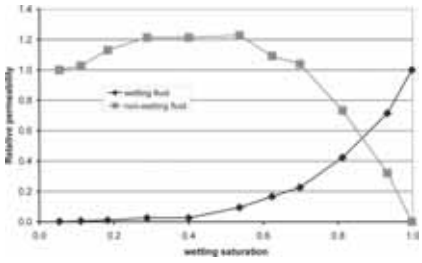
The results show that the proposed model is an ideal tool for modeling immiscible two-phase flow in porous media, due both to its ability to incorporate complicated boundary conditions at the pore walls and also capture the physical aspects of the flow in the bulk and the interfaces (see figures 2 & 3). Furthermore, the width of the fluid-fluid interfaces is kept less than 3-4 lattice units allowing for simulations in relatively low resolution porous lattices.



Parallel speedup of the LB algorithm



Phase distribution patterns in 3D pore networks of the wetting phase (left panel) and the non-wetting phase (right panel) when M=10 and Sw=0.8. The solid is not shown in these figures. D=0.05, θ=175o, G=1.0e-7, ε=0.53, κ=10-4



Relative permeabilities when M=10 in the 3D pore network. D=0.05, θ=175o, G=1.0e-7, ε=0.53, κ=10-4

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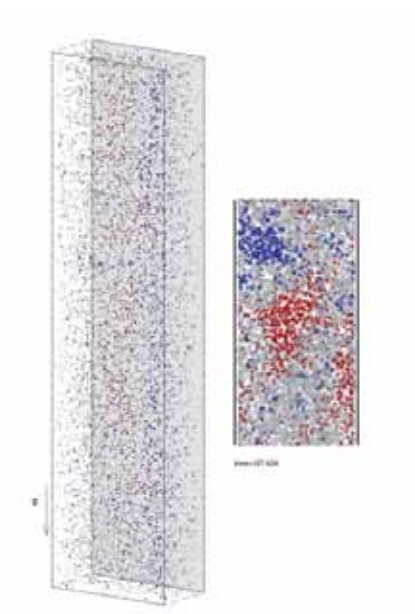
CIEMAT, Madrid

Fully-Resolved Direct Numerical Simulation of Turbulent Channel Flow With Suspended Solid Particles

In this project the group considers the problem of the motion of a large number of spherical particles suspended in an incompressible fluid. The dilute mixture is driven through a vertical plane channel by a mean pressure gradient which is sufficiently large to generate turbulent motion. The particles are of comparable size to the near-wall flow structures. In addition, the buoyancy-induced relative velocity between fluid and particles is sufficiently high in order to generate strong wakes trailing the particles (average particle Reynolds number 136). Therefore, the flow field around individual particles needs to be resolved in order to accurately describe macroscopic effects resulting from the interaction between the phases. For this purpose our simulations are performed with the aid of a specifically designed immersed boundary method which allows to solve a single set of equations (the Navier-Stokes equations plus an additional volume force term) on a fixed Cartesian grid spanning the entire domain, including the space occupied by the moving particles.

In the simulations it was found that for the chosen parameter range the mean fluid velocity profile tends towards a concave shape, and the turbulence intensity as well as the normal stress anisotropy are strongly increased, mainly due to the wakes. The team has also observed the formation of very large streamwise-elongated fluid structures evolving on a slow time scale. These structures form in the absence of any significant agglomerations of particles, which means that clustering due to wake effects (as previously observed in pure sedimentation flows) is not at the root of the observed phenomenon. In order to further analyze the dynamics of these coherent structures while reducing the constraint due to the limited box size, we have undertaken simulations in an extended computational domain (cf. figure).

It is expected that the results will contribute to the formulation of more realistic engineering models for two-phase flows in the future. These simulations require the largest currently available supercomputers, and, therefore, the use of a system like MareNostrum is vital for the success of our project. The runs involve more than two billion grid nodes and were typically executed on 512 to 1024 processors.



The image shows an instantaneous distribution of particles in thevertical channel. On the right the view is from below, directed in thedirection of the mean fluid motion. The particles are colored according to their instantaneous vertical velocity: red (blue) indicates values higher (lower) than the long-time average, while grey-colored particles move at close to average velocities. The elongated zones where particle velocity fluctuations are correlatedare clearly visible

Publication

M. Uhlmann,"Investigating turbulent particulate channel flow with interface-resolved DNS", in ICMF 2007, M. Sommerfeld, editor, Proc. Int. Conf. Multiphase Flow, Leipzig, Germany, 2007.

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Investigation of the Intrinsic Connectivity of Metal Aquaions and Polyoxoanions in Aqueous Solutions by means of Ab initio MD simulations.

The Theory of Electrolytic Dissociation proposed by Arrhenius established a well defined separation between cations and anions. Their different sign and hydration properties have led to consider separately the formation of metal aquaions and polyoxoanions. The aim of this project is to show how aquaions are not only the most stable form of highly-charged metal cations, but also they can be considered in the origin of their corresponding polyoxo forms. This alternative reactant channel for the formation of polyoxoanions allows an unique view to stabilize ions of different sign in aqueous solutions.

The conversion from aquaions to polyoxoanions can be monitored in the case of S(VI) and Cr(VI) on the basis of ab initio molecular dynamics (AIMD) simulations. The results indicate the possibility of dealing with the formation of XO4(2-) (X being S or Cr) from their aquaions using a model system formed by 1 ion and 80 water molecules. The updating of the wavefunction of the system during the statistical trajectory allows an appropriate flexibility in the quantum mechanical description of the different species involved in the complex hydrolysis process which takes place. Moreover, the fundamental role of water molecules, which dissociate in order to reorganize the strong charge distribution, can be well modeled by AIMD simulations. Despite of being very time consuming, this methodology enables to obtain a detailed microscopic picture of the chemistry of condensed finite temperature systems which can be compared to experimental data and used to investigate theories about reactivity and the origin of polyoxoanions. Furthermore, the feasibility of this hypothesis shed light on new explanations on the appearance of polyoxoanions in interstellar regions.

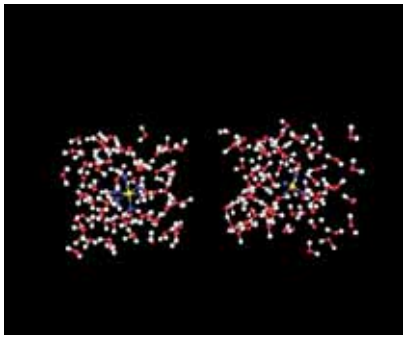

Figure shows the initial (left) and final (right) snapshots of the AIMD simulation of the 1 S(VI) + 80 water molecules where the conversion from the aquaion ([S(H2O)6]6+) to the polyoxoanion ([SO4]2-) species is observed. For the sake of simplicity, oxygens atoms directly bonded to the S(VI) ion are of different color from the other oxygen atoms of the system

Solution Chemistry of Radioactive Po(IV) and Th (IV) ions: insights from ab initio molecular dynamics

Despite of the fact that one of the Marie Curie's pioneering research was the discovery of the polonium metal, the chemistry and properties of this element and its complexes are hardly known, likely due to its rareness and high toxicity. Fundamental aspects of its chemistry in solution such as its coordination number or hydration free energy are far from being fully understood. In this sense, the use of computational chemistry can increase the understanding of this system at no risk. In this work, we have carried out an ab initio molecular dynamics (AIMD) study of the Po(IV) hydration. The analysis of AIMD simulations of Po(IV) in aqueous solutions indicates that this tetravalent ion has a great tendency towards hydrolysis giving rise to hydrolyzed species. These results support previous evidences obtained with semi-continuum models and show the importance of using first principles methods to properly describe multivalent metal cations in solution. Under these simulation conditions (1 ion + 60 water molecules at 298 K), it is not possible to find a unique representative species of Po(IV) in aqueous solutions but an equilibrium of hydrolyzed clusters containing between two and three OH groups in the first hydration shell was

found. The formation of Po=O bonds (typically observed ion the chemistry of tetravalent cations) was not identified along the trajectories. The promising results obtained in this study allow to extent this methodology to gain insight into the chemistry of multivalent metal cations in aqueous solution. This is specially interesting in the case of radioactive species where computational studies can orientate and decrease the number of dangerous experiences in the laboratory.

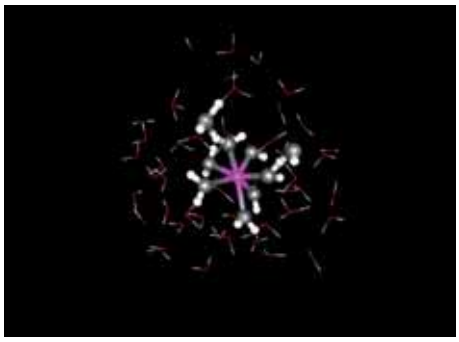

Figure shows an intermediate snapshop of the AIMD simulation of 1 Po(IV) + 60 water molecules. It is seen how two different hydrolysis processes are taking place. Oxygen atoms of the first solvation shell and water molecules involved in the hydrolysis processes are emphasized and of different color from the rest of solvent molecules

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Atomistic simulations of atactic polystyrene in the glassy state

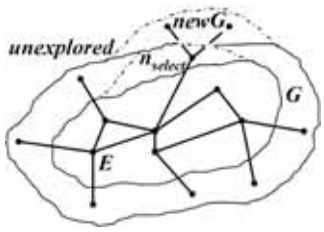
In the area of glasses, considerable progress has been made over the last few years with the help of molecular simulations. Unfortunately, the broad spectrum of time scales for molecular motion present in glassy materials poses severe limitations and challenges for molecular simulation. Any traditional numerical solution of the equations describing the dynamics of a microscopic particulate model is bound by the fastest process present, thereby limiting our ability to track its evolution over the long time scales relevant to laboratory experiments and technological applications of glasses. As a result, "brute force" molecular dynamics simulations are doomed to describing only a very small part of the spectrum of time scales characterizing motion in the system, and therefore can not address questions concerning the long time relaxation processes present in glasses. In our work at BSC we have used the idea of inherent structures, i.e. that the configuration of a glass is trapped for a long time within a basin surrounding a local minimum of its potential energy function, in order to investigate the ageing process of glasses and to perform mechanical deformation experiments at various temperatures. According to this approach, the free energy of the system locked-in in the vicinity of a minimum energy configuration consists of two contributions: (a) the potential energy of the ''underlying'' minimum energy (inherent) structure, about which the system vibrates, and (b) the contribution from vibrational motion about the inherent structure. In terms of the Gibbs energy, a valuable tool for the determination of the vibrational contribution is the quasi-harmonic approximation (QHA).

Within the QHA we have performed a series of constant strain and constant stress uniaxial tension-compression experiments at a series of temperatures in the glassy state of a common polymer glass, atactic polystyrene (a-PS). The constant strain experiments are based on

imposing an extension (or contraction) in one of the dimensions of the periodic simulation box, and minimizing an appropriately defined Gibbs energy (evaluated based on the QHA) with respect to the other two dimensions. The Young's modulus and the Poisson ratio are obtainable as output from such simulations at small strains. Constant stress experiments, on the other hand, impose an external tensile stress and employ perturbations of the box size in all three directions in order to minimize the Gibbs energy.

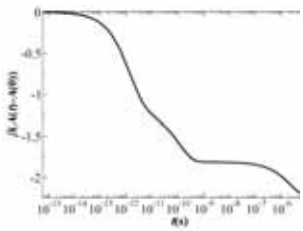
To study dynamics, we have combined the idea of inherent structures, within the harmonic approximation, with a proposed new methodology for tracking the dynamical evolution of Markovian systems, based on the creation of a network of explored states which is progressively augmented according to the distribution of first passage times for reaching its boundaries. Here, each state is a basin in configuration space surrounding an inherent structure.

The proposed methodology constitutes a very general approach to stochastic integration and enables us to track directly the time evolution of the probability distribution. The proposed scheme is designed to sample the new states so as to create an ever expanding network of known states called "explored," see figure 1. The basic ideas are a) to start with the state initially populated and augment the network as time elapses, including more and more states connected to those already considered; b) to track the temporal evolution of the system by direct solution of the master equation for the probabilities of occupancy of the explored states, rather than by Kinetic Monte Carlo; and c) to augment the set of explored states through rigorous criteria based on the theory of mean first passage time, which ensure that states beyond the boundary of the known network (hereafter called "unexplored") have a negligible contribution up to the time of observation.



Schematic of the augmentation of the set of explored states E

The team has applied our approach to the problem of physical ageing in an atomistically represented glassy polymeric material. To do this, we have invoked the dimer method for locating saddle points around a given minimum, constructed transition paths to new minima, and computed rate constants for the paths via multidimensional transition-state theory in the rugged potential energy landscape of the polymer glass.



Instantaneous free energy of ageing atomistic aPS glass for times up to 10-5s

The team has tracked the free energy of the relaxing glass over ten decades in time (shown in figure 2) and have extracted characteristic frequencies for the ageing process that compare favorably with experimental evidence. Thus, the group has shown that our approach is capable of bridging the extremely disparate time scales present in the dynamics of complex systems, such as atomistically represented glassy polymeric materials, over much broader time windows than is possible with other methods.

Publication
Boulougouris, G. C.; Theodorou, D. N. J. Chem. Phys. 2007, 127, 084903

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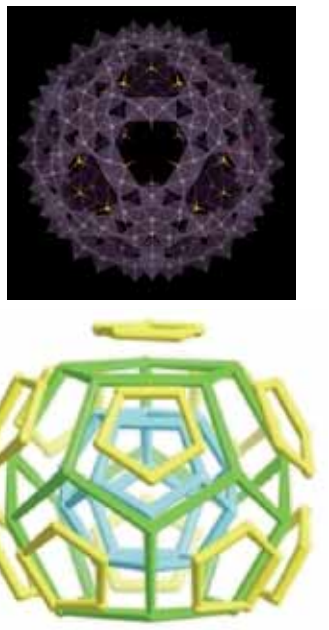
Computational modeling of nanocages: giant polyoxometalates

One of the most significant features of the chemistry of Tungsten and Molybdenum is the formation of molecular clusters known as polyoxometalates (POMs). Nowadays, POMs constitute an immense class of polynuclear metal-oxygen clusters usually formed by Mo, W or V and mixtures of these elements. POMs molecular size span a broad range, from the small Lindqvist anion [M6O19]n- to nano-sized giant balls such as those recently synthesized by Müller containing more than 100 metal atoms and more than 350 oxygen atoms. Such giant metal oxide molecular clusters present big empty cavities that can host other species. POMs have relevant applications in many fields including medicine, catalysis, multifunctional materials, chemical analysis, nanotechnology, etc. Taking profit of MareNostrum capabilities, the team applies classical molecular dynamics simulations to analyze the structure of the counter-ions and water solvent molecules around and inside POMs. In previous activities, Keggin anions [XW12O40]n- (X=P, Si Al, n=3,4,5) and the wheel-shaped compound M21[Mo57O189V6N6H3(H2O)18] (M=Na, Li) has been analyzed. At present, the team is dealing with the giant ball-shaped nanocapsules, such as [{(Mo)Mo5}12{Mo2(ligand)}30]n-, aimed at explaining X-Ray diffraction data and recent neutron scattering experiments on the structure and dynamics of water encapsulated within.

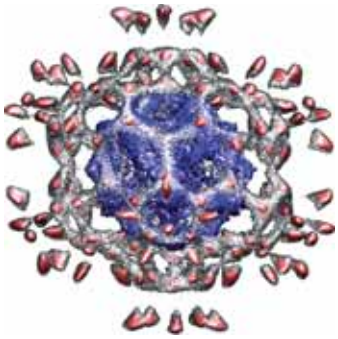
One fascinating phenomenon observed in these nanocapsules relates to the structure of a cluster of 100 confined water molecules. In the case of [({Mo}Mo5O21{H2O}6) 12(Mo2O4SO4)30]72 - displayed in Figure 1, they are organized as two {H2O}20 dodecahedra and a {H2O}60 distorted rhombicosidodecahedron with the radii 3.84-4.04, 6.51-6.83 and 7.56-7.88 Å, respectively (See figure).



Structure of the [({Mo}Mo5O21{H2O}6)12(Mo2O4SO4)30]72- nanocapsule (top) and an schematic view of 'captive water' within the cavity (bottom). It shows the first and second (formal) dodecahedra as light blue and green cage respectively and the rhombicosidodecahedron in yellow, derived from X-Ray data

To gain insight into the nature of these water assemblies, a series of classical molecular dynamics simulations in explicit water solvent were carried out. Our goal was to investigate computationally different configurations of water clusters inside the different capsules, and to prove whether water molecules inside the capsules self-assemble spontaneously or not. Then, the radial (RDF) and spatial (SDF) distribution functions center of the capsule-oxygen water atoms were computed. The computed RDF showed three significant peaks, signaling a three-shell structure, and a shallow inner peak. A remarkable agreement with the experimentally determined distances between the capsule center and of the capsule-water oxygen atoms, and with the number of molecules in each shell was found. The three peaks in the RDF were located at 4.4, 6.7 and 7.4 Å, which integrated to 25, 29 and 43 molecules each. Therefore, in addition to four molecules located in the shallow inner peak, 97 molecules reside in the three main shells. Note

that this is in very good agreement with the experimental values 20:20:60. This result means that although during the simulations water molecules diffuse inside and outside the capsule continuously, some kind of layered structure is formed. This dynamic structure matches experimental data as much in position and in composition.



Isosurfaces of the space distribution function for the oxygen atom of the water molecules inside the model capsule. Two isosurfaces are shown: the red isosurface corresponds to a value one order of magnitude larger than the grey-transparent isosurface. The inner blue isosurface was generated using the same value as for the grey isosurface

When the space distribution function was plotted (as shown in the second figure), it revealed a clear polyhedral type structure. The highest probability regions of finding a water molecule inside the capsule are shown as red isosurfaces. The outer water layer is formed by 72 nodes that correspond to water ligands coordinated to the 12 Mo(Mo)5 moieties and structured as 12 (H2O)(H2O)5 type pentagons. They are clearly identifiable in the second figure (top, bottom). These ligand type water molecules do not diffuse and remain fixed at their locations of maximum probability (red and grey isosurfaces localized around the same area). The third and second shells at 7.4 and 6.7 Å form exactly the same polyhedra as were found crystallographically, i.e. a distorted {H2O}60 rhombicosidodecahedron and a {H2O}20 dodecahedron. In these nodes, the grey isosurface extends towards the edges that connect the vertices of the polyhedra, thus suggesting that water molecules in these shells are rather mobile and can exchange their locations. This exchange seems to occur through the edges and not through the faces of the polyhedra. Visual inspection of the trajectories indicates a stepwise motion with molecules switching shell frequently and in a synchronous way, like a dynamical hydrogen-bonded gear. Thus, our computational results not only reproduce the three shell structure of the (H2O)100 cluster inside the nanocapsule, but revealed a dynamically ordered polyhedral structure, same as seen experimentally. Further studies on related systems are presently under way, focusing both on the structure and on the dynamic properties of encapsulated water.

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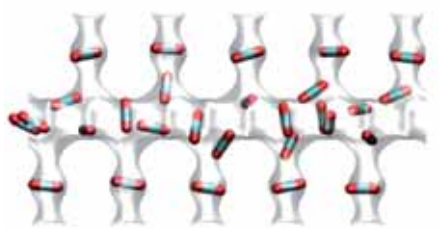
Development of force fields for simulations of substrates and reaction intermediates-photocatalyst-zeolite interactions

The team focus on materials that can, on the one hand, function as a photocatalyst and, on the other hand, act selectively on on e type of molecule or a given target at the nanometer length scale. Photocatalysis has a great pot ential for the activation of a variety of processes by using light, including sunlight. These processes are related to pollution abatement, production of electricity or new fuels, such as H2 and reduced organics, low-cost photovoltaic devices, reduction of meta ls and other substances and even quick and efficient destruction of living cells. The combination of these processes together with some kind of control that provides selectivity at the molecular level will have far reaching implications, both in basic scienc e and in technological applications. One could for example, selectively act on a cell that is expressing a given receptor on its plasmatic membrane, or bind to a given molecu le and oxidize it without affecting other species in a mixture. We plan to work on the combinati on of a photocatalyst with two different materials that will create the selectivity; zeolites and sensors based on metal nanoparticles. The targets on nanostructured photocatalysts in zeolites were 1) the study of the interactions between the zeolites and the hotosensitizers, 2) the investigation of the adsorption/diffusion of substrates and sensitizers in zeolites, 3) the understanding of how the zeolite cages change the photophysical properties of the sensitizers, 4) the understanding how the zeolite influences the photochemistry and 5) to establish a link between this project and available information from experiments. This year activity has been focused on the development of force fields for simulations of substrates or reaction intermediates-photocatalyst-zeolite interactions. The force fields were developed by fitting to available adsorption isotherms, heats of adsorption and Henry constants and validated by computing the diffusion coeffici ents. For the force field development we employed Monte Carlo, Molecular dynamics and Ab initio simulation techniques. As for diffusion the team used Molecular Dynamics simulations and newly developed rare event simulations techniques to those systems for which the diffusion is too slow to be simulated with conventional Molecular Dynamics.



Carbon dioxide adsorbed in MOR type zeolite at 300K and 1000 KPa

Publications

A computational study of CO2, N2, and CH4 adsorption in zeolites. E. García-Pérez, J.B. Parra, C.O. Ania, A. García-Sánchez, J.M. van Baten, R. Krishna, D. Dubbeldam S. Calero. Adsorption, 2007, 13, 469-476.

A Simulation Study of Alkanes in Linde Type A Zeolites: Almudena García Sánchez, Elena García-Pérez, David Dubbeldam, R. Krishna, and Sofía Calero. Adsorption Science and Technology, 2007, 25, 417-427.

A New United Atom Force Field for Adsorption of Alkenes in Zeolites. Bei Liu, Berend Smit, Fernando Rey, Susana Valencia, and Sofía Calero J. Physical Chemistry C (accepted).

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Modeling for NanoElectronics

Activities in the field of Modeling for NanoElectronics Materials by means of ab initio computation have started few years ago. The main objective of the computational project is the advance in the synthesis and processing of nanostructured materials useful for nanoelectronic devices such as gas sensor with improved selectivity and stability in relation to those characteristic of the present technologies. This requires: i) to deepen in the knowledge of the mechanisms involved in the interaction between the gas molecules and the surface of the nanostructures, and ii) to develop suitable technologies for nanomanipulation and fabrication of nanocontacts, for the fabrication of the nanosensor devices on microelectronic based platforms.

This computational project mainly concerns to the study of bottom-up techniques (mainly the growth of Si and metal oxides in CVD). Alternatively the standard top-down approach in the study of nanoparticles, the advances in nanotechnologies and a deeper knowledge of the nanoscaled phenomena allow us an ascending approach or bottom-up in which is feasible the use of structures defined in the nanoscale in an ordered and controlled shape with the objective to induce or dispose the required properties. Nowadays, parameters such as dimension, crystallinity, composition, periodicity and surface area can be controlled, giving new structures with exciting properties such as quantum dots, nanowires, nanotubes, or selfassembled structures in 3D like nanowebs.This scope opens new innovative and promising perspectives in the field of sensors based on new phenomena related with nanoscale. The existence of such new phenomena opens the necessity to carry on studies that allow the whole comprehension for their application as nanosensors.

In this framework, thanks to the use of massive computation, in facilities like MareNostrum, today is possible to attempt the modeling of behavior of nanoparticles aimed for advanced electronics.

The main goals of this work were:

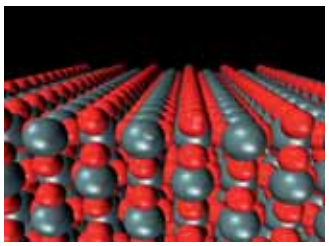
-Modeling of bulk, slab, surfaces, molecules and nanostructures in materials such as SnO2, TiO2, In2O3, ZnO, Wurzite-Si, Diamond-Si.

-Modeling of interaction of surfaces and nanostructures (SnO2, ZnO) with molecules (O2, NO, NO2, SO2) and correlation with TPD experiments and gas sensing devices.

-Modeling of surface vacancies in surfaces (SnO2, ZnO,TiO2) and correlation with.

-Modeling of the thermodynamic stability of nanostructures in metastable phase (Si) and correlation with TEM/HREM observations.

-Modeling of the lattice dynamics in metastable phase (Si) and correlation with Raman spectra.



A SnO2 surface

Publications

Prades JD, Cirera A, Morante JR, et al. Ab initio insights into the visible luminescent properties of ZnO. THIN SOLID FILMS 515 (24): 8670-8673 OCT 15 2007

Prades JD, Arbiol J, Cirera A, et al. Concerning the 506 cm(-1) band in the Raman spectrum of silicon nanowires APPLIED PHYSICS LETTERS 91 (12): Art. No. 123107 SEP 17 2007

Prades JD, Cirera A, Morante JR. First-principles study of NOx and SO2 adsorption onto SnO2(110)JOURNAL OF THE ELECTROCHEMICAL SOCIETY 154 (8): H675-H680 2007

"Quantum Chemical Calculations of Surfaces and Interfaces of Materials", Contributions by C. Pisani, F. Illas, G. Pacchioni, J. Sauer, F. Corà, P. Sautet, N. Rosch, K. Doll, P. Ordejon, J.D.Prades, A. Cirera, J.R. Morante G. Kresse, N. H. De Leeuw and G.Cicero

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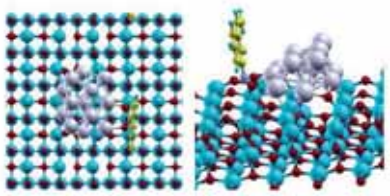
Selective hydrogenation of nitroaromatics catalyzed by gold

To understand the catalytic behaviour of supported Au nanoparticles and improve their activity and selectivity, we studied the mechanism of selective hydrogenation of the nitro group in nitrostyrene, involving the selective activation of the nitro group in the presence of C=C bond, and the dissociacion of molecular H2 into two hydrogen atoms. The team has provided strong theoretical evidence that H2 adsorbs and dissociates with small activation barriers on low-coordinated Au atoms situated in corner positions of different nanoparticles and in edge positions of monoatomic rows without further conditions. The presence of low coordinated Au atoms is also able to slightly activate both the nitro group and the C=C bond in nitrostyrene. However, this could not explain the high selectivity towards nitro hydrogenation experimentally obtained with Au/TiO2 catalysts, and suggests that the metal-oxide support plays a role in activating the nitro group.

Nitrostyrene adsorbs selectively through the nitro group on the TiO2 support, but the interaction is so strong that this adsorbed species seems to be just a spectator. When nitrostyrene adsorbs at the interface between the Au nanoparticle and the support, there is again a strong interaction between the O atoms of the nitro group and the Ti atoms of the support, similar to that previously observed on the clean support, but also a noticeable interaction between the O atoms of the nitro group and two Au atoms at the nanoparticle edge. Interestingly, these are low coordinated Au atoms, such as those that are able to dissociate H2. In this complex the nitro group is strongly activated, while the C=C is almost unaffected. This indicates that, while nitrostyrene is adsorbed and activated through both groups on isolated gold nanoparticles, when the nanoparticles are supported on TiO2 the selective adsorption and proper activation of the nitro group appear to occur naturally, explaining the high chemoselectivity observed experimentally for this catalyst.

The combination of realistic quantum chemical modeling, in situ IR spectroscopy, and kinetic experiments has allowed us to demonstrate that the unique behaviour of the Au/TiO2 catalyst for the chemoselective reduction of substituted nitroaromatics to anilines is due to a cooperative effect between gold and the TiO2 support. This knowledge, at the molecular level, of the interactions between the reactants and the catalyst surface will allow the improvement of existing catalysts and the development of new ones.



Publications

A. Corma, M. Boronat, S. González y F. Illas. "On the activation of molecular hydrogen by gold: A theoretical approximation to the nature of potential active sites" Chemical Communications 2007, 3371- 3373.

M. Boronat, P. Concepción, A. Corma, S. González, F. Illas y P. Serna. "A molecular mechanism for the chemoselective hydrogenation of substituted nitroaromatics with nanoparticles of Gold on TiO2 catalysts: a cooperative effect between gold and the support" J. Am. Chem. Soc. 2007, 129, 16230 – 16237

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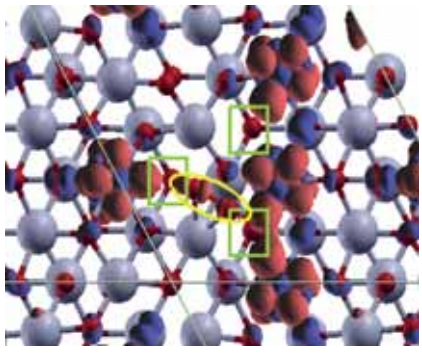
DFT calculation of defects and electron localization at redox-active oxide surfaces

Cerium dioxide is a key component in catalysts for decontamination of automobile exhaust gases, and is being used as well in catalysts for purifying hydrogen from CO in fuel cell applications. Its ease of reduction and reoxidation is an important factor that facilitates these processes. Its reoxidation with molecular oxygen requires that two surface anion vacancies, located in close proximity, accept the two atoms in the molecule after the splitting of the latter; understanding the structure and reactivity of surface anion vacancy clusters is therefore an important issue.

In this work periodic slab models of the cerium dioxide (111) surface (the most stable one) with around 70 atoms per unit cell and containing groups of two or three surface anion vacancies have been built, and the atomic relaxations and electronic structure appearing in them have been elucidated with quantum mechanical studies. A study of the interaction of these surface defects with dioxygen molecules has been subsequently undertaken. The calculations were carried out at the DFT level, including a Hubbard U term to correctly reproduce the localization of excess electrons in the 4f orbitals of the cerium atom. The periodic VASP code, with PAW potentials and a planewave representation of the electronic orbitals, was used.

Accurate evaluation of energies indicated that association of these vacancies to give surface clusters involves a very small enegy balance; thus some literature results from STM measurements, that suggested that such association is favoured, find in these calculations no specific support. However it has been also estimated here, using simplified atomistic potentials, that dispersion (Van der Waals type) interactions, that cannot be modeled with the present DFT methods, could contribute to this balance with energy differences of the order of several tenths of electronvolt per cluster. More developed theory levels are thus needed to model accurately these phenomena. As additional output, it was verified that vacancy clustering is accompanied by jumping of subsurface oxygen atoms to nonlattice positions near the outer atomic plane, probably to compensate partially the accumulated surface electric dipole and to achieve a more even distribution of vacancies in the immediate environment of undercoordinated Ce ions.

Simple dioxygen adsorption on the clusters of two or three anion vacancies leads to the formation of diamagnetic peroxide species coordinated to Ce(4+), even if excess electrons remain on the oxide surface forming localized Ce(3+) centers (see figure); further electron transfer to the adsorbate to achieve splitting of the molecule and replenishing of two vacancies per molecule does not occur spontaneously. Work in progress suggests that strong electron density redistribution resulting in a splitting of the O-O bond may occur, however, upon interaction of the peroxide species with a second oxygen molecule. A study of the energy barrier involved in the dissociation of the O-O bond is under way.



Structure of a cluster of 3 anion vacancies (marked with green squares) at a ceria (111) surface with an adsorbed dioxygen molecule, that becomes a peroxide species (highlighted with a yellow oval). Spin density lobes (blue and red) highlight the 4f electrons of the localized Ce(3+) ions. Ce atoms, grey large spheres; O atoms, smaller red spheres

Publication
J. C. Conesa: "DFT+U studies of oxide vacancy clusters at ceria surfaces", communication presented at the COST D41 Workshop on "Inorganic Oxides: Surfaces and Interfaces", Berlin, October 2007.

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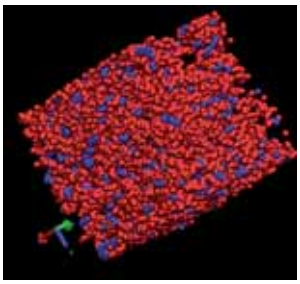
Rheological and crystallization processes of metallocene based polymers by molecular dynamics simulations

Short chain branched (SCB) polyolefins as a model of metallocene ethylene/·-olefin copolymers were simulated by Monte Carlo (MC) and molecular dynamics (MD) methods. Melt density, which was evaluated by MD in the isothermal-isobaric ensemble (NPT-MD), slightly increases with the SCB content. A mix of different MC moves was adopted and connectivity-altering moves, such as end-bridging, were modified in order to incorporate the branches into the simulation. This MC simulation strategy performed very well in equilibrating molten SCB copolymers at all length scales. The chain size and local packing in the melt, as obtained from the MC simulations, are discussed. At given backbone length, chain size, as quantified by the radius of gyration, decreases with the number of branches. On the other hand, the presence of short branches leads to a less effective intermolecular local packing in the melt. Rheological properties of the copolymers are discussed based on a mapping of the Monte Carlo atomistic simulations on the packing length model, and compared with experimental results. In general, good agreement with experimental results is found.

Molecular dynamics simulations have been undertaken with the main objective of studying melt dynamics directly. Thus the team can combine advanced computer MD methodologies to obtain basic polymer features as the entanglement molecular weight, Me, and relaxation time, τe, together with the application of a simplified topological reptation model, has allowed to strictly explain the experimental linear viscoelastic fingerprint of a broad set of linear PE samples avoiding the use of any adjustable parameter. The computer simulations reveal for the first time the experimentally inaccessible characteristic value of Ùe for linear PE, and also an inconsistency between the values of the entanglement features Me and GN0 in the classical Doi-Edwards relationship. The result obtained here points towards a different prefactor value in this relationship, an idea that involves another one step forward in the development of the theoretical reptation models.

The understanding of crystallization and melting processes in polymers is a long standing and crucial issue in polymer science. A new theory of polymer crystallization based on microscopic description is slowly emerging. In this line, computer simulation is a powerful technique to shed light on the early mechanisms involved in the crystallization process of polymers. The team has obtained new results derived from Langevin dynamics simulations of linear and branched polyethylene models concerning the molecular mechanisms involved in the formation of ordered structures during the early stages of crystallization.



Publications

J. Ramos and J. Martínez-Salazar, "Effect of branching on early nucleation stages of polyethylene: A stochastic study". EDM 2007, European Discussion Meetings on Polymer Crystallization, 2007.

J. Ramos, J. Martínez-Salazar, L.D. Peristeras and D.N. Theodorou, "Hierarchical Monte Carlo/Molecular Dynamics simulation of short chain branched polyethylenes in the molten state". EPF 2007, European Polymer Federation Meeting, 2007.

J. Ramos, L.D. Peristeras and D.N. Theodorou, " Monte Carlo simulation of short chain branched polyolefins in the molten state". Macromolecules, 2007, 40, 9040-9050.

J. Ramos, J.F Vega, D.N. Theodorou and J. Martinez-Salazar, "Entanglement relaxation time in polyethylene: simulation versus experimental data". Macromolecules, in Press.

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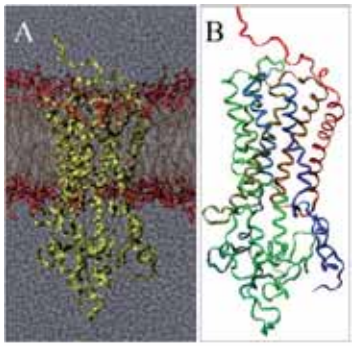
Molecular dynamics simulations of the full-length M1 muscarinic acetylcholine receptor

A full model of the muscarinic M1 receptor was constructed and further subjected to molecular dynamics (MD) simulations in an explicit environment (lipid and water molecules). The results of the simulation were further correlated with the available experimental data, finding a very good agreement between the experiments and the simulations. Hence, a reliable model of this receptor is presented.

The three-dimensional structure of full-length structure of the M1 muscarinic receptor was obtained through the fragmental homology modeling procedure. A 10-ns molecular dynamics (MD) simulation of the protein imbedded in a lipid slab and surrounded by water molecules was further used to relax the model. It was found that the homology model corresponded to the conformation in the ground state, since no significant motions of the backbone of transmembrane domains were observed. Furthermore, the reliability of the model was validated by analyzing key inter-helical contacts, sidechain-sidechain interactions, the formation of stable aromatic microdomains (clusters) and the docking of acetylcholine to its binding site. Moreover, a few conserved interactions observed in the X-ray structure of rhodopsin, such as inter-helical sidechain-sidechain hydrogen bonds were accurately reproduced in the MD simulation. The coupling of ACh to its binding site was found to be dominated by π-cation and salt bridge interactions, while its conformational space was restrained through van der Waals and hydrogen bond interactions. In general, such features were in very good agreement with the available experimental as well as theoretical data. Considering the above, the structural information obtained in this study can be used a starting point to investigate the activation mechanism of the receptor and the ability to develop selective agonists and allosteric modulators which could be used for the treatment of Alzheimer's disease.

Thanks to increasing supercomputing capabilities such as MareNostrum, it was feasible to perform molecular dynamics simulation using an explicit lipid bilayer, water molecules and ions of the full-length 3-D model of the muscarinic M1 receptor. Such simulations are very helpful to gain insight into the structural and dynamical properties of this receptor. The acquirement of such valuable information would not be possible without the tremendous computing capabilities of MareNostrum.



(A) Perspective of the receptor imbedded in the membrane at 10 ns. (B) Side view of the receptor. The structure is colored as follows: N-terminus and TM1, red; TM2, orange; TM3, olive; TM4, dark green; TM5 and IL3, bright green; TM6, blue; TM7 and C-terminus, violet

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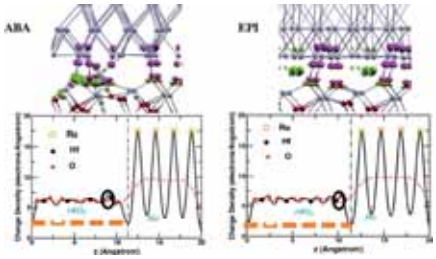
Computational modeling of Ru/HfO2 interface

Because of HfO2's relatively high dielectric constant, wide band gap and sufficient stability on Si, dielectrics based on HfO2 are amongst the most promising high-k candidates for future CMOS technology. Development of processes to fabricate interfaces with desired structures and properties can be aided by an understanding of the interface atomic and electronic structure that controls interface properties. Interfacial structure is determined by process chemistry and subsequent interfacial structural evolution.

In this period the team has analyzed the electronic properties of the Ru/HfO2 interface from first principles DFT calculations. The nature and properties of the metal induced gap states (MIGS) that arise in the interface of two different bilayered Ru films have been considered (atom-by-atom grown, ABA, and epitaxially connected, EPI). Also, the effect of the metal-high-k dielectric interface structure on the effective work function of the metal has been carefully analyzed. The team shows that depending on the structure of Ru deposited on the HfO2 substrate we find a variation of ~0.4 eV in the effective work function of the metal. The interfacial structures determine the extent of charge transfer from metal to the dielectric and hence, affect the nature of the interface dipole. Consequently, variability in interface structure may result in differences in the Schottky barrier height and thus affect the electrode work function.

These extensive simulations have been performed by means of a slab model using a relatively large supercell (~300 atoms), and provide a milestone in materials modeling. Such simulations, which are on the edge of the current supercomputing capabilities, have been possible thanks to the outstanding facilities granted by MareNostrum, BSC-CNS.



Top: electron-density differences at the interface (magenta regions lose electron density whereas blue regions gain electron density upon adsorption of Ru. Ru, O and Hf atoms are represented by green, red and grey spheres, respectively). Bottom: plane-averaged charge-density distribution and plane-averaged total potential. The dotted-dashed vertical line represents the interface

Publications

Atashi B. Mukhopadhyay, Javier Fdez. Sanz and Charles B. Musgrave. Energetics and Electronic Properties of Ru/HfO2 Interfaces, J. Phys. Chem. C 2007, 111, 9203-9210.

Atashi B. Mukhopadhyay, Javier Fdez. Sanz and Charles B. Musgrave. Effect of Interface Structure on the Ru on HfO2 Work Function. J. Chem. Phys. In press.

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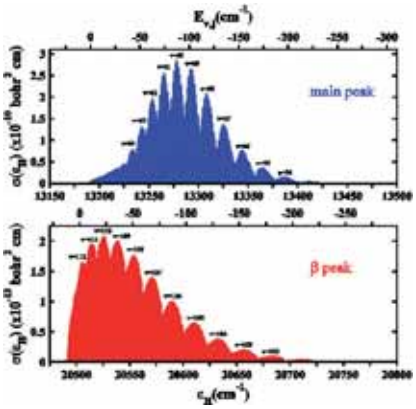
Large scale simulations of solvation effects in the structure and dynamics of weakly bound clusters

Understanding the role of nonadiabatic effects in the photodissociation dynamics of cluster systems is a fundamental issue. One of the most interesting situations arises when manifestations of nonadiabatic effects are induced by intracluster collisions occurring during the photodissociation process. This is the case of the photodissociation of the (HI)2 cluster, for which recent experimental data have been reported. In the present project, a nonadiabatic quantum mechanical model has been developed in order to investigate the nonadiabatic photodissociation dynamics of the (HI)2 cluster. The goal was twofold. On the one side, it was intended to rationalize the available experimental data. On the other side, the purpose of this project was also to throw light on other relevant aspects of the photodissociation process which were not investigated in the experiments carried out so far.

The model developed has proved to be realistic enough to describe the process and to reproduce with good qualitative agreement the available experimental data.

Among our major findings is a very high yield of bound I2 fragments as products of the photodissociation. Such products should be observable in laser-induced fluorescence (LIF) experiments. Another interesting result is that the probability of electronically nonadiabatic transitions increases with increasing excitation energy of the (HI)2 cluster. The implication of this result is that the intensity of the manifestations of nonadiabatic effects would enhance (being more easily observable) as the excitation energy increases. This effect has been explained in terms of the specific nature of the nonadiabatic coupling involved.



Product state distributions of I2 fragments produced after photodissociation with = 266 nm radiation, mediating (upper panel) and without mediating (lower panel) a nonadiabatic transition. The upper Ev,j energy scale of the panels corre- sponds to the I2 rovibrational energy levels, while the lower H energy scale of the panels corresponds to the translational energy of the H atom fragment. Some of the vibrational bands have been labeled in the distributions

Publications

S. López-López, R. Prosmiti, and A. Garcia-Vela, Nonadiabatic Photodissociation Dynamics in (HI)2 Induced by Intra-cluster Collisions, J. Chem. Phys. 126, 161102 (2007).

S. López-López, R. Prosmiti, and A. García-Vela, Modeling the (HI)2 photodissociation dynamics through a nonadiabatic wave packet study of the I*HI complex, J. Chem. Phys. 127, 184307 (2007).

S. López-López, R. Prosmiti, and A. García-Vela, Effect of the excitation energy on the (HI)2 nonadiabatic photodissociation dynamics J. Phys. Chem. A (in press).

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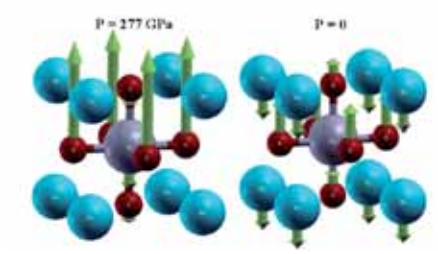
Ab initio simulation of ionic conductors for solid oxide fuel cells

The theoretical study achieved in this group (PhD thesis of Emile Bevillon) aims at improving the understanding of microscopic and elementary processes that occur at the atomic scale in the materials that will probably form the fuel cells of the future. The team uses density-functional calculations, performed with both the ABINIT and SIESTA codes to study various oxides, modified by aliovalent substitution, and their ability to hydrate in the presence of water. The group has especially focused on barium stannate ($BaSnO_3$, perovskite structure) since this compound has been suggested a few years ago to have good hydration and proton conduction properties. The group has first performed an exhaustive study of the structural, dynamical and dielectric properties of this compound, and suggested interesting phenomena under pressure, related to recent developments in the field of ferroelectricity. Then a high content of dopants that reflect that currently used in applications were studied. Various trivalent elements are used to substitute Sn (Ga, In, Y, Sm, Gd, La).

The group has evidenced a nice effect: in most cases, the most stable position for oxygen vacancies and protons is not, as expected, the first-neighbor one but the second-neighbor relative position. The team attributes this phenomenon to two causes: (1) the high content of dopants used leads to an overlap of attractive interactions between the defect and various periodic images of dopant atoms, (2) the dopants used are all (Ga excepted) larger than the atom (Sn) they subsitute, which produced particular distortions when the defect is in second-neighbor position, with hydrogen bonds shorter, and thus stronger, in average.

The team has confirmed that this phenomenon is intrinsically caused by the dopant size only, by performing calculations on large supercells (3 x 3 x 3) within the SIESTA code in the case of La. In this case a similar energy landscape as in the high dopant content case is found. The calculations performed at MareNostrum are necessary for us since the computational power required by such computations is very high.



Eigendisplacements of the lowest-energy TO mode of barium stannate at zero (right) and high (left) pressure

Publications

E. Bevillon, G. Geneste, Phys. Rev. B 75 (2007), 214106. "Unstable polar mode and minimum of the dielectric constant in cubic BaSnO3 under hydrostatic pressure"

E. Bevillon, G. Geneste, Y. Wang, A. Chesnaud, G. Dezanneau, Ionics, submitted. "Ab initio study of La-doped BaSnO3 proton conductor"

E. Bevillon, A. Chesnaud, Y. Wang, G. Dezanneau, G. Geneste, J. Phys.: Cond. Matt, submitted. "Theoretical and experimental study of the structural, dynamical and dielectric properties of perovskite BaSnO3"

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Universidad Politécnica de Valencia

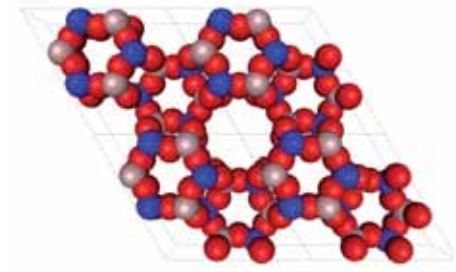
Brønsted acidity of chabasite zeolite

Zeolites are a class of typical solid acids, and their catalytic functions are used in many industrial catalytic processes1 Catalysis in zeolite is caused by the acidic hydroxyl groups; therefore, these properties have been extensively studied experimentally and theoretically by many researchers2,3. Temperature-programmed desorption (TPD) of ammonia has been used for analysis of solid acidity, and the team has proposed a method for quantitative measurement of acid amount and strength (adsorption heat of ammonia, ΔH)4. However, nature of acid sites (Brønsted or Lewis acidity) is not identified from this method, and a understanding of the catalytic activity is complicated by this disadvantage.

Recently, we proposed a method of infrared-mass pectroscopy/temperature programmed-desorption (IRMS-TPD) of ammonia for quantitative measurements of acidity of zeolites. By means of this method, the team can identify the type of acid sites (Brønsted or Lewis); furthermore, the team can analyze exactly the acidic property of each OH group; the amount and strength (adsorption heat of ammonia, ΔH) of each OH group can be measured individually. On the other hand, quantum chemical calculation has been frequently applied for analyzing chemical property of the zeolites, and supporting the experimental findings. For example, deprotonation energy (or proton affinity), adsorption energy of base molecule, frequency of stretching vibration of OH groups have been calculated for understanding the solid acidity.

CHA structure consists of D6Rs (double six-rings) which are connected with tilted 4MRs, and main channel is 8MR. All tetrahedral (T) sites are equivalent; therefore four kinds of nonequivalent oxygen sites exist. Those oxygen sites were labeled as O(1–4) according to literature. Nature of the structurally different four acid sites in CHA-type zeolite has been studied by quantum chemical calculation5-7. However, experimental measurements of solid acidity of CHA-type zeolite have not been carried out sufficiently; thereby no comparison between experimental and theoretical values has been performed. In this study, we will study the Brønsted acidity of high-aluminum H-CHA by means of the ammonia IRMS-TPD method, and compare it with the density functional calculation within periodic boundary conditions.

Brønsted acidity of H-CHA zeolite (Si/Al2=4.2) was investigated by means of ammonia infrared-mass spectrometry/temperature-programmed desorption (IRMS-TPD) method and density functional calculation. Four IR bands were observed at 3644, 3616, 3575 and 3538 cm-1, and they were ascribable to the acidic OH groups on four nonequivalent oxygen sites in the CHA structure. The absorption bands at 3538 cm-1 was attributed to the O(4)H in the 6MR (6 membered-ring), and ammonia adsorption energy (ΔU) of this OH group was the lowest among the 4 kinds of OH groups. The other 3 bands were assigned to the acidic OH groups in 8MR. It was observed that the ΔU in 8 and 6 MR were 131 (± 3) and 101 kJ mol , respectively. On the other hand, the density functional calculation within periodic boundary conditions derived the adsorption energies on these OH groups in 8 and 6 MR to be ca. 130 and 110 kJ mol-1, respectively, in good agreement with the experimentally observed values.



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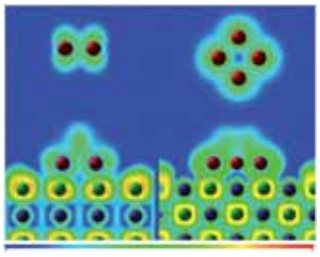
Unraveling the molecular mechanisms of heterogeneous catalysis by combination of computational modeling and controlled experiment in model systems

During the first half of 2007 several catalytic processes have been studied and the molecular mechanism unravelled. It has been shown that the molecular mechanism proposed for ethene epoxidation on Cu(111) and Ag(111), which goes through a common oxametallacycle intermediate, does also hold for Au(111) although with a lower catalytic activity, in agreement with recent experimental findings. Of particular interest are the results concerning propene epoxidation since propylene oxide is produced by tons in the chemical industry. Theoretical studies carried out with the help of marenostrum have permitted to understand while Ag, the industrial catalyst for ethene epoxidation, does not work for propene epoxidation. This is because Ag favours H stripping from the methyl group leading to an allylic species which cannot be transformed into the necessary oxametallacycle intermediate. On Cu, H stripping competes with oxametallacycle formation and we concluded that Cu based catalysts could be useful for propene epoxidation. Indeed, this is in agreement with experiments carried out in the University of Cambridge.

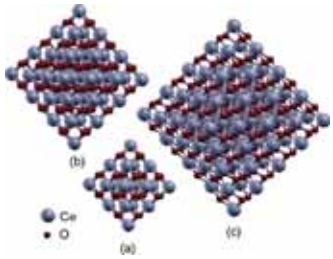
A second part of the project also allowed us to complete a study of the CO oxidation on RhCu bimetallic surfaces. This is a process taking place in the car exhaust although the catalysts used so far contain two expensive transition metals. Calculations carried out at MareNostrum permitted us to conclude that on the bimetallic surface the mechanism is similar to that occurring on Rh(111) although depending on the type of bimetallic site a reduction of the energy barrier is predicted. This may have consequences for the NO reduction by CO reaction taking place at car exhausts. Related to the previous point and of importance for environment is the mechanism of NO dissociation on stepped bimetallic RhCu surfaces which provide more realistic modes of catalysts. Their study also requires large supercells and hence the access to MareNostrum is crucial. Bimetallic PdAg surfaces have also investigates, these are important as fuel cell membranes, another important topic related to alternative energy sources.

The second half of the year has been dedicated to perform a careful analysis of the role of halogens as epoxidation promoter agents, the team has shown the reasons behind this behaviour and provided arguments explaining the better performance of Cl. Another important area of research has focused on the reactivity of transition metal carbides with a complete study of the molecular mechanism of molecular oxygen dissociation on the surface of these compounds. The calculated transition state theory rate constants reveal that TMCs of group IV and V are easy to oxidize whereas this is especially difficult for ‰-MoC. The rate constants trends follow the calculated energy barriers and explain the oxygen preference for carbon on group IV TMCs and ‰-MoC, as well as the preference for metal atoms on group V TMCs. Another important study concerned the reaction mechanism for the water gas shift reaction on TiC; extended surfaces and nanoparticles have been considered. The team found that extended TiC surfaces are better catalyst than nanoparticles, the reason being the too large adsorption energy of reactants and products by the nanoparticles. The reactivity and catalytic activity of Au supported on TiC(001) has been also considered and the calculations provided new and interesting results which have latter been confirmed in a join experimental-theoretical work involving the research group of Prof. Jose. A. Rodriguez of the Brookhaven National Laboratory. The unexpected activity of Au has been attributed to the polarization of the electron density as clearly shown in the figure. Catalytic activity by Au has also been the objective of another project leaded by Prof. Avelino Corma which will be described in the appropriate section of this memory.



Electron Localization Function maps for Au2 and Au4 adsorption on TiC(001). At the top are shown the corresponding results for the isolated Au clusters. The probability of finding one electron varies from 0 (blue color) to 1 (red color)

Still a third relevant activity has been to explore new materials. Accurate electronic structure calculations carried out for two important metal oxides (MgO and ZnO) predict that new low-density nanoporous crystalline phases could be accessible via the coalescence of nanocluster building blocks. A similar approach has been used to model large ceria nanoparticles which provide realistic models for this important catalytic oxide.



Sketches of the studied octahedral (CeO2-x)n nanoparticles of growing size, which are cut by {111} planes from the bulk CeO2: a – Ce19O32 (x = 0.32); b – Ce44O80 (x = 0.18); c – Ce85O160 (x = 0.12).

The study of nanoparticles has also permitted us to understand self assembling processes recently observed by experiment. Again, this involves handling large metallic particles interacting to form nanowires and the accurate treatment of their atomic and electronic structure is only possible thanks to the access to MareNostrum.

The study of the molecular mechanism of the surface catalyzed reactions is a new area demanding powerful computational resources. In particular, search and characterization of transition state structures for chemical reactions taking place at a surface is possible through the Nudged Elastic Band algorithm. This implies minimization of an energy function which requires simultaneous calculation of various structures (images). For the large systems and unit cells in the present project, this is only possible thanks to the use of a large parallel computer such as marenostrum allowing for instance to run simultaneously 8 images in 32 processors each, thus running at least on 256 processors.

The huge amount of work carried out thanks to access to MareNostrum has resulted in a significant number of publications in the most prestigious international journal.

Publications

"Low oxygen basicity a key in the search for new propylene epoxidation catalysts" D. Torres, N. Lopez, F. Illas and R.M. Lambert, Angew. Chem. Int. Ed., 46 (2007) 2055

"Similarities and differences on the molecular mechanism of CO oxidation on Rh(111) and bimetallic RhCu(111) surfaces", S. González, C.Sousa and F. Illas, Phys. Chem. Chem. Phys., 9 (2007) 2877

"On the Promoting Role of Ag in Selective Hydrogenation Reactions over Pd-Ag Bimetallic Catalysts: A Theoretical Study", S. González, K. M. Neyman, S. Shaikhutdinov, H.-J. Freund and F. Illas, J. Phys. Chem. C, 111 (2007) 6852

"First Principles LDA+U and GGA+U Study of Cerium Oxides: Dependence on the Effective U-Parameter", C. Loschen, J. Carrasco, K. M. Neyman and F. Illas, Phys. Rev. B, 75 (2007) 035115

"Theoretical study of NO dissociation on stepped Rh(221) and RhCu(221) surfaces", S. González, D. Loffreda, P. Sautet and F. Illas, J. Phys. Chem., C, 111 (2007) 11376

"Understanding Ceria Nanoparticles from First-Principles Calculations", C. Loschen, S. Bromley, K. M. Neyman and F. Illas, J. Phys. Chem. C, 111 (2007) 10142

"On the mechanism of formation of metal nanowires by self-assembly", F. Viñes, F. Illas and K. M. Neyman, Angew. Chem. Int. Ed., 46 (2007) 7094-7097

"Viability of ultra-low-density metal oxides constituted from highly stable nanocages", J. Carrasco, F. Illas and S.T. Bromley, Phys. Rev. Lett., 99 (2007) 235502

"Adsorption of gold on TiC(001): Au-C interactions and charge polarization", J.A. Rodriguez, F. Viñes, F. Illas, P. Liu, Y. Takahashi and K. Nakamura, J. Chem. Phys., 127 (2007) 211102

"A systematic density functional study of molecular oxygen adsorption and dissociation on the (001) surface of group IV, V and VI transition metal carbides" by F. Viñes, C. Sousa, F. Illas, P. Liu and J. A. Rodriguez, J. Phys. Chem. C, 111 (2007) 16982

"On the activation of molecular hydrogen by gold: A theoretical approximation to the nature of potential active sites", A. Corma, M. Boronat, S. González and F. Illas, Chem. Comm., (2007) 3371

"A Molecular Mechanism for the Chemoselective Hydrogenation of Substituted Nitroaromatics with Nanoparticles of Gold on TiO2 Catalysts: A Cooperative Effect between Gold and the Support"; M. Boronat, P. Concepción, A. Corma, S. González, F. Illas and P. Serna, J. Am. Chem. Soc., 129 (2007) 16230

"Adsorption of gold on TiC(001): Au-C interactions and charge polarization", J.A. Rodriguez, F. Viñes, F. Illas, P. Liu, Y. Takahashi and K. Nakamura, J. Chem. Phys., 127 (2007) 211102

"Dissociation of SO2 on Au/TiC(001): Effects of Au?C Interactions and Charge Polarization", J. A. Rodriguez, P. Liu, F. Viñes, F. Illas, Y. Takahashi and K. Nakamura, submitted for publication

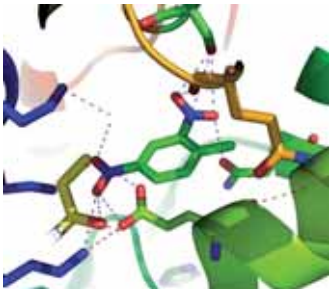
"How halogens promote selectivity in silver-catalyzed ethene epoxidation", D. Torres, R. M. Lambert and F. Illas, submitted for publication

Alfonso Jaramillo
École Polytechnique

Computational design of biosensors for explosives detection

The team has developed a high performance computational biology project to design novel biosensors, based on natural ribose sensors (RBP), for non natural molecules such as commonly used explosives (e.g. RDX and 2,4DNT).

The synthetic receptor will be integrated into Pseudomonas Putida, a non pathogenic saprophytic organism. The biosensors will allow the construction of cheap and efficient land-mine detectors. The methodology uses a high-resolution atomic structure of a protein and combinatorial optimization techniques in order to find the possible sequences stabilizing the corresponding scaffold. Mutant sequences are scored according both to their folding free energy, computed by modeling both an unfolded and folded state at the atomic level using a molecular mechanics force field, and the binding free energy of the complex protein/ligand.



Nuria López
Institut Català d'Investigació Química

Computational high-throughput screening for the selective production of NO on platinum group metal surfaces and alloys

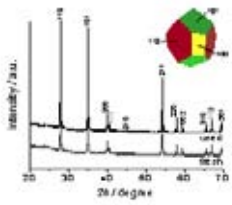
High-Throughput screening of ammonia oxidation. The reduction of expensive noble metals is a must in the search for new active components to reduce the price of commodity chemicals. In particular, HNO3 production is based on the selective burning of ammonia to form NO that is further processed to the desired product. Pt losses are one of the major drawbacks of the present technology because of the high temperatures employed and the high oxidative character of the mixture for this process. The team has performed an extended study for the competitive reactions of N_2 and NO recombination on a set of metals including those employed industrially nowadays: Pt, Rh and others (Ir, Pd, Cu, Au…). The group has been able to complete a database that includes all the binding energies of the key reactants and products to the surface including N, O, NO, N_2O, N_2. Moreover, the team has calculated the barriers for the N_2 and NO formation for all the metals on the list above. Results show the reasons for NO selectivity under given conditions as well as how and why a catalyst not based on Pt can be found. This is of very large interest since the price of Pt is rocketing as a result of its need in developing fuel-cell technologies. The team is working on a detailed mechanistic description of the reaction network, including micro-kinetic modelling, and on the systematization of the results to elaborate a database for N-containing molecules.

The role of copper oxide nanostructures and their self-assembly on the initial stages of Cu oxidation

The second research area has been to study the role of copper oxide nanostructures and their self-assembly on the initial stages of Cu oxidation. The oxidation of metal is fundamental to understand protective coatings but also materials employed as catalyst. The aim of this project has been to analyze the formation of nanostructures and to compare with the detailed studies coming from Scanning Tunnelling Microscopy. The team has found possible way for the initial oxidation process and that can account for the formation of the initial oxide layer.

The Chemistry of RuO2(110) in Selective Oxidations

During 2007 the group started to study the Deacon reaction. The Deacon process consists in the formation of chlorine from HCl. It is a technologically relevant reaction integrated in many chemical plants. The newest catalyst for the reaction is formed by ruthenium oxide grown in a particular support. For this system the group has been able to study the geometric structure, composition under different gas feeds (previous to the reaction and after the reaction) and the reaction mechanism under different conditions. This work constitutes the first atomistic study of the reaction and has laid down the basis for the cooperation with a major chemical company.



Comparison between calculated RuO2 nanoparticles and diffraction experiments

Publications

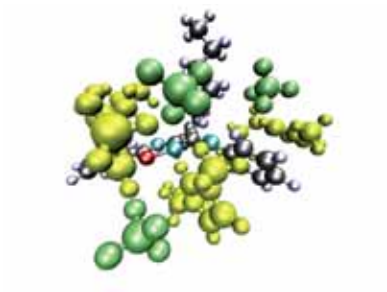
Y. Segura, N. Lopez and J. Perez-Ramirez, J. Catal. 247, 383 (2007)

Feliu Maseras
Institut Català d'Investigació Química

DFT modeling of reactivity in an ionic liquid

Room temperature ionic liquids (RTIL) have generated tremendous enthusiasm in recent years as a new type of solvents. They are viewed as an alternative to the highly contaminant nature of organic solvents often used in the chemical industry. RTIL's possess a very low vapor pressure, and are easier to separate, thus providing a cleaner and more sustainable option. The precise effect of the RTIL environment in chemical reactivity remains largely unexplored from a computational point of view, and it seems difficult to treat with the continuum approaches often applied to more conventional solvents.

The team has applied the powerful computational resources of the Barcelona Supercomputing Center to the problem. In particular, the team has analyzed what would be a reasonable density functional theory (DFT) approach to describe the effect of the presence of the ionic liquid [BMIM][BF4] on the energy barrier for the amine-assisted SN 2 intramolecular rearrangement of the Z-phenylhydrazone of 3-benzoyl-5-phenyl-1,2,4-oxadiazole. The results are of similar quality to those obtained in the reproduction of the barrier in a conventional solvent as water. Analysis of the results furthermore indicates how the ionic solvent lowers the barrier with respect to the value in vacuum. The cation and the anion of the solvent interact strongly with the charge centers that appear in the rate determining transition state, and thus lower its energy with respect to the reactants. The study also suggests that explicit treatment of two ion pairs is a much better solution than use of one, because of the overefficient stabilization associated to the case when a single ion pair is considered. The result of this first investigation of reactivity in an ionic liquid is encouraging and opens the path to apply this same computational approach to study the reactivity of other chemically relevant processes in room temperature ionic liquids.



Explicit introduction of two ion pairs provides a first reasonable estimation of the effect of an ionic liquid on chemical reactivity taking place in this solvent

Publication

F. Bessac, F. Maseras; "DFT modeling of reactivity in an ionic liquid: How many ion pairs?", J. Comput. Chem., in press.

Fernando Martín García
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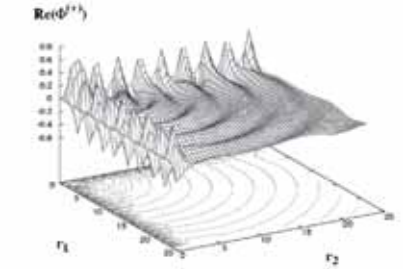
Two-photon double ionization of helium above and below the threshold for sequential ionization

Double ionization of the helium atom by two XUV photons in the range of 40 to 50 eV has recently become the subject of intense theoretical interest as well as the target of new experiments with high harmonic generation sources and experiments underway at the free-electron laser source (FLASH) in Hamburg. Even in the intensity regime where second order perturbation theory is expected to be valid, recent calculated cross sections vary over more than an order of magnitude. We have performed accurate, time-independent calculations of this process well beyond the energy regimes of earlier treatments, using methods which have produced benchmark results for double ionization of atoms. These methods provide grid-based (with B-splines and DVR), numerical solutions of the Schrödinger equation with no appeal to approximate asymptotic forms nor to ansatz wave functions. We have found that, below the threshold for sequential double ionization (54.4 eV), sequential ionization competes with nonsequential ionization. Remarkably, even below 54.4 eV, sequential ionization leaves a clear signature in the magnitude and shape of both the total and energy sharing cross sections -even though at these energies it is only a virtual process. We predict a rapid rise in the total cross section considerably below the threshold for sequential ionization, as well as dramatic changes in the shape of the singly differential cross section caused by this virtual process. These calculations should influence planned experiments on multiphoton ionization with new XUV sources.



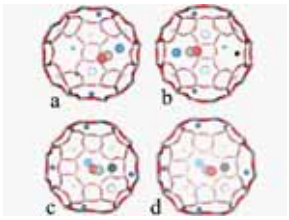
Helium wave function 20 eV above the double ionization threshold

Petr Nachtigall
Institute of Organic Chemistry and Biochemistry. Academy of Science of Czech Republic

Theoretical investigation of metal-exchanged zeolites

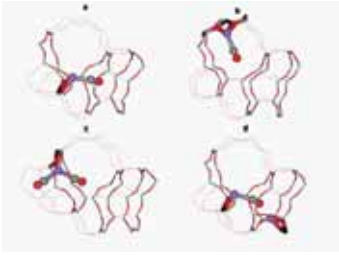
Localization and coordination of extra-framework metal cations in zeolites determine the adsorption and catalytic properties of these systems. Information about the extra-framework metal cations can be correlated with the various physical and chemical properties of metal-exchanged zeolites (M/zeolites) and these properties (as adsorption and catalytic activity) can be understood at the atomic scale level. The systematic investigation of various properties of M/Ferrierite, employing a combination of the periodic DFT model and the experimental investigation gave us a rather complex understanding of this system. While Ferrierite is suitable system for theoretical investigation it has only few applications. Therefore, the goal of this project is to extend our understanding of the details of physical and chemical properties of zeolites on systems that are of much greater interest for experimentalists, such as MFI and LTA.

During the present project this team showed that Infrared spectra of CO adsorbed on the Al-rich Na-A zeolite cannot be interpreted by assigning each IR band to CO interacting with a specific type of single cation site. This concept, which usually works well for high-silica zeolites, should not be uncritically extended to Al-rich zeolites that are crowded with cations in configurations which lead to preferential formation of CO adsorption complexes involving more than one cation site.



Bridged CO adsorption complexes in Na-A zeolite formed on the dual cation sites

Moreover, it often happens that the IR spectra of CO/M-zeolites shows bands (or shoulders) within a frequency range intermediate between the value for free CO and that shown by the blue-shifted M +···CO species (where M+ stands for the alkali metal cation). These features have not hitherto been well understood, and yet they might contain valuable information about the zeolite cation sites. The team studied the adsorption of CO molecule in Na-MFI zeolite using periodic DFT calculation. It has been shown that besides M +···CO (monocarbonyl) and M+···OC (isocarbonyl) species, bridged M +···CO···M+ complexes are also formed in M/MFI zeolite.



CO/Na-MFI complexes: a) and b) Mono-carbonyl complexes, c) Di-carbonyl complex and d) CO molecule bridged on a Na+ dual site

Thanks to the increasing supercomputing capabilities such as MareNostrum, it is feasible to do projects where large periodic system, as zeolites, are studied using periodic DFT and take into account the interaction of absorbed molecules with large part of zeolite framework that has been shown to be crucial for obtaining reliable calculations of vibrational frequencies of weakly absorbed molecules.

Publications

C. Otero Areán, M. Rodriguez Delgado, C. López Bauca, L. Vrbka, and P. Nachtigall, "Carbon monoxide adsorption on low-silica zeolites - from single to dual and multiple cation sites", Phys. Chem. Chem. Phys., 9 (2007) 4657.

C. Otero Areán, M. Rodríguez Delgado, K. Frolich, R. Bulánek, A. Pulido, G. Fiol Bibiloni, and P. Nachtigall, "Computational and FTIR spectroscopic studies on CO adsorption on the zeolites Na-ZSM-5 and K-ZSM-5: evidence of dual-cation sites", J. Phys. Chem. C, in press.

Juan J. Novoa
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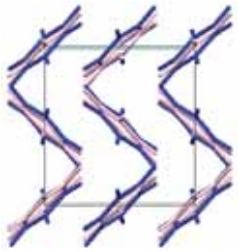
Accurate methods for the theoretical prediction of polymorphic crystalline materials of technological interest

This project is part of a long term research line devoted to the accurate prediction of the polymorphic forms of crystals of technological interest (that is, having conducting, superconducting, magnetic, or pharmacological properties) using a new molecule-molecule pixel-based potentials. The interest in this proposal is to continue with the validation tests of the program with a database of 35 experimentally known crystals representative of the type of crystal packings found in the literature. The team has properly developed a parallel code capable of polymorph prediction studies using PIXEL molecule-molecule potentials. The code has been shown to properly reproduce the experimental structure of a wide variety of known polymorphs. It has also been used to study the polymorphism of benzene with results that reproduce the experimental data.

The results obtained have been presented in a series of invited talks in various universities, and at a recent international workshop on polymorphism. A full paper with these results is almost finished. The main reason to use MareNostrum is its architecture. Clearly, PIXEL potentials are too computationally demanding for scalar machines, and only the use of a very efficient parallel computer can allow to reach our results in a reasonable ammount of time. Thus, MareNostrum has been a key piece in the development and testing of our code. Even if the team is entering into the polymorph studies of real molecules of pharmaceutical or technological interest, it should be even more important (given the size of these molecules, and the complex properties of their molecular crystals).



Optimum structure of the benzene crystal computed using the PIXEL potentials, overlapped to the experimental one. The two are similar, with a small difference in distances and angles

Gianfranco Pacchioni
Dipartimento di Scienza dei Materiali,
Università di Milano

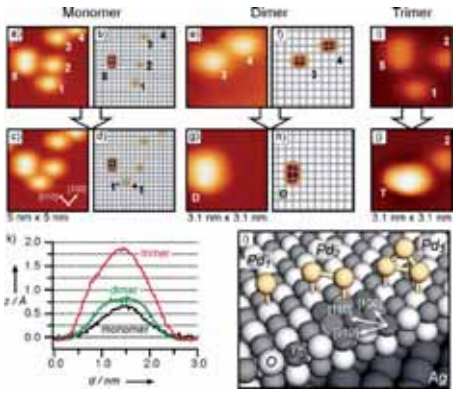
Metal clusters on oxide ultra-thin films: the way towards new materials with unprecedented properties

Objective of this research activity is the identification of the mechanisms of nucleation, growth, and reactivity of metal nanoclusters supported on oxides surfaces and thin films. A special attention is dedicated to ultra-thin oxide films grown epitaxially on metal substrates: they represent a new class of materials with unprecedented properties. To this end first principle DFT calculations with relatively large supercells have been performed. The activity has been done in close collaboration with experimental groups.

In one study the team has considered the evidences of the formation of anionic Au atoms on ultra-thin MgO films. The formation of anions on the surface remains difficult to prove experimentally. Also theoretically, the discrimination between neutral or charged adsorbed species is not straightforward. The team has performed an accurate analysis of the observable consequences of the formation of Au anions on an oxide surface. To this end the team has considered the following properties: spin distribution, density of states, Bader charges, substrate relaxation, simulated scanning tunneling microscopy (STM) images, work function changes, CO vibrational frequency, electric field effects, core level shifts. Most of these properties are also accessible experimentally. Taken together, these measurements provide a solid proof of the charge nature of the gold adsorbate.

In a second study the team has considered the geometry, adsorption sites, and electronic states of small Pd particles (Pd_1, Pd_2, Pd_3) on regular surface sites of MgO thin films. These particles have been generated using STM-based manipulation at very low temperature and complementing the experimental information with results from DFT. This allows to identify (1) the best position and orientation of the Pd nanoclusters and their electronic structure, combining single molecule spectroscopy with

electronic states determined by theory. The study has shown for the first time the possibility to manipulate and create ultra-small clusters by means of an STM instrument.



a-d) Detailed view of Pd atoms before (a,b) and after (c,d) applying a voltage pulse. Pd atom (1) moved to the new position (1*). e-h) Formation of a dimer (D) out of two monomers (3,4). i-j) Formation of a trimer (T) out of a dimer (5) and a monomer (1). k) Comparison of line profiles taken from STM images of Pd1, Pd2, and Pd3. l) Schematic representation of the structure of Pd1, Pd2, and Pd3 on the surface of an Ag(001)-supported, 2 ML thin MgO(001) film as obtained from DFT calculations

Publications

L. Giordano, U. Martinez, S. Sicolo, G. Pacchioni, "Observable consequences of formation of Au anions from deposition of Au atoms on ultra-thin oxide films", J. of Chemical Physics, 127, 144713/1-9 (2007).

M. Sterrer, T. Risse, L. Giordano, M. Heyde, N. Nilius, H.-P. Rust, G. Pacchioni, H.-J- Freund, "Pd monomers, dimers, and trimers on the MgO(001) surface viewed individually", Angewandte Chemie Int. Ed., 46, 8703-8706 (2007).

Silvia Picozzi
CNR-INFM (Italy)

Ferroelectricity and magnetism in RMnO3 : Coupling mechanisms from ab-initio studies

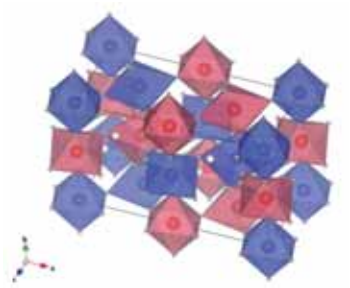
Multiferroic materials, which show at the same time long-range magnetic order and ferroelectric polarization, represent an important class of multifunctional materials in the field of spintronics, offering both potentially high technological applications as well as fascinating fundamental physical properties. Within this context, we focused on distorted orthorhombic rare-earth manganites (such as $HoMnO_3$), showing the unconventional E-type antiferromagnetic spin configuration.

As a follow-up of the activity in the previous year - in which the team suggested the first ab-initio example of a magnetically-driven mechanism for the rising of ferroelectricity in manganites – the team has payed the attention focused on the E-type antiferromagnetic spin configuration of $HoMnO_3$, where ferromagnetic zigzag spin-chains in the MnO_2 planes are coupled antiferromagnetically (see figure). Using ab-initio density functional approaches and performing a careful analysis based on Wannier functions, we have revealed that the 'asymmetric electron hopping' of orbitally-polarized Mn-eg states is the key ingredient for the rising of polarization (see figure). Furthermore, a systematic analysis of the link which combines ferroelectricity with spin, orbital and lattice degrees of freedom in the entire ortho-$RMnO_3$ series has revealed clear chemical trends, showing for example that the exchange coupling between Mn sites is determined by the Mn-O-Mn angle and that the Mn-eg contribution to the polarization dramatically increases with the Mn-O-Mn angle.The team should stress that this result is obtained by means of ab-initio studies which do not rely on any model assumptions. In addition, the group shed light on a plausible mechanism which can cause a high ferroelectric polarization by purely quantum mechanical effects.

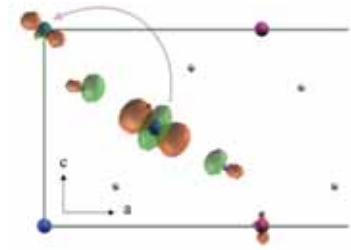
Ramón Reigada Sanz
Universidad de Barcelona

1. Molecular dynamics simulations for the study of mitochondria Cardiolipin membrane properties

2. Effects of Cholesterol and headgroup charges on the structural properties of cell membranes



Atomic structure of ortho-RMnO3 in AFM-E phase. Blue and red spheres denote Mn with up and down spins, whereas white (small) spheres denote O atoms. The Mn-O6 octahedrons are highlighted



Wannier function of Mn-eg state in top-view of MnO2 plane in AFM-E ortho-HoMnO3. The pink arrow shows the adjacent Mn site with same spin, where the 'asymmetric hopping' occurs

Publications

"Magnetically-induced ferroelectricity in orthorhombic manganites: microscopic origin and chemical trends", K. Yamauchi, F. Freimuth, S. Bluegel and S. Picozzi, submitted to Phys. Rev. B.

"Microscopic mechanisms for improper ferroelectricity in multiferroic perovskites: a theoretical review", S. Picozzi, K. Yamauchi, I. A. Sergienko, C. Sen, E. Dagotto, J. Phys. C: Cond. Matter (submitted)

In the frame of high computer performance Molecular Dynamics Simulation in Biosystems, three different projects were performed in 2007. All of them tackle the Biological membranes. Biological membranes are highly complex mixtures of many lipid species belonging to 3 major classes. These are glycerol based lipids, sphingolipids, and sterols. A typical biological membrane is composed of a hundred or more lipid species and its composition is regulated by cellular mechanisms to ensure a proper environment for membrane proteins. Specifically, bilayer systems with only a limited number of lipid components were simulated, since the study of the whole complexity of cell membranes is unavailable by any simulation technique. The proposed projects want to investigate the role of some of the membrane constituents to determine membrane properties and their capacity to interact with other components or to add some extra functionality.

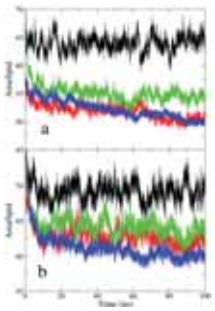
In the first project, the team has studied the Cardiolipins(CL). These lipids moieties are really interesting because they are highly charged (-2e) and also because are very common in mitochondrial membranes as well as in heart tissue. It's well established the connection of these lipid species with cell energy production and its distribution, although the specific role in these processes is still unknown. The team performed two groups of simulations with different initial disposition of the CL, and one without CL used as reference. From the two groups of simulations containing CL, in the first group the CL molecules were randomly distributed among the bilayer and in the second case the CL molecules were located forming a single cluster. There is some controversy about whether the CL molecules are disposed in the bilayer forming clusters or they are placed far away to each other to avoid electrostatic

interaction. Even our 100ns simulations are not long enough to simulate complete diffusion, the group observes the fracture of CL clusters, and the formation of smaller and more dispersed aggregates. This result reveals that the idea of CL molecules randomly distributed is closer to the equilibrium state than the clusterized one. This result is consistent for the two lipid mixtures (Phosphatidilcholine (PC) and Phosphatidilethanolamine (PE) used to form the lipid bilayers.

From the initial analysis of the dynamics with initial random CL configuration we can point out the following results. The team observes that presence of CL in simulated lipid bilayers leads to a stabilization of membrane properties. The group observed small membrane condensation which results in small increase of membrane order and thickness. Such changes are known to improve membrane mechanical properties. At the level of water-membrane interface we observed a decrease of headgroup mobility, increase of the lifetime of lipid-lipid interactions such as H bonds and charge pairs and an increase of the number of these interactions. Most of these effects are related to the high stability of cardiolipine-phosphatidylcholine charge pairs comparing to PC-PC and PC-PE charge pairs and higher stability of CL-PE H bonds comparing to PE-PE and PE-PC hbonds. The higher stability of the interactions come from a better accessibility of CL phosphate groups to these interactions due to their external location in the interface without steric obstacles (choline or ethanolamine group), the low mobility (due to their big size), and the charged nature of CL. Stabilization of the interface as well as small membrane condensation can be mechanisms which decrease membrane permeability as observed experimentally for similar systems.

The second and third projects analyze the effect of different lipid headgroups on the bilayer properties, and particularly their interaction with an extremely important membrane lipid: cholesterol. To do so the team has simulated four common membrane phospholipids moieties: Phosphatidylcholine (DPPC), Phosphatidylethanolamine (DPPE), Phosphatidylserine (DPPS) and Phosphatidylglycerol (DPPG). The simulations were performed slightly above the main phase transition temperature, T=343K. Even thought, the team can see that DPPS and DPPE pure bilayers udergo a phase transition to the gel phase (see figure). This was not expected and probably is due some problems with the coupling to temperature and pressure baths that effectively make these simulations to be performed 10K below the expected temperature. This problem is being analyzed now, and can be relevant for the development of GROMACS molecular dynamics package. Additionally, the group has found an interesting result. The simulations of bilayers containing 25% of cholesterol do not undergo phase transition to the gel phase (see figure). This reveals that the used forcefield is able to reproduce quite accurately this extremely important cholesterol property. Cholesterol influence in lipid bilayers allows many phospholipids to be used in membranes at body temperature avoiding the gel phase, which will result in a rigid solid-like membrane and fatal fragility. These results obtained from some preanalysis make the results are very promising. Even though, the complete analysis has just started and will take as usually in the Molecular dynamic simulation on biological systems at least 3months more.

Thanks to the supercomputing capabilities in MareNostrum, it has been possible to perform projects like the proposed. They involve atomistic level simulations of membranes with a large number of atoms by molecular dynamics, reaching significant biological time scales in a reasonable run time that can only be done with this high-level supercomputer facility.



Evolution of the superficial Area per Phospholipid molecule along the simulation for a) Pure systems; b) sytems containing 25% of cholesterol. DPPC (black) , DPPE (Red), DPPG (Green) and DPPS (blue). The continuous drop down in some curves reflex the phase transition to the gel phase

Octavio Roncero
Instituto de Matemáticas y Física Fundamental (C.S.I.C.)

Quantum non-adiabatic reactiondynamics

During 2007 the group had one period of 4 months to develop a parallel version of the wave packet method to treat non-adiabatic reactive processes in small molecular systems. The team started such a work and also obtained a visiting grant by Estela Carmona Novillo at BSC.

However, the parallelization was not finished at this period but later, thanks to a seconf 4monts computation grant at CESVIMA and thanks to the use of the own opteron cluster at IMAFF.

The team would also like to stress, that in the third computation grant for the third 4 months of 2007 the team planned to exploit our code at CESVIMA but it was not possible because of a) many technical problems at CESVIMA, b) too few technical support from them due to lack of available specialized persons and c) low priority computational grant.

Apart from finishing the parallelization of the code, that will be pursuit at FINISTERRE CESGA thank to their support, the team has been carrying out calculations on the ion/molecule reaction H^+ + D_2, difficult to treat with wave packets because of the insertion mechanism it presents. Thus some approximate WP calculations have been performed giving rise to a of publication in collaboration of several groups, one of them experimental.

Publications

"Transition state spectroscopy of open shell systems: angle-resolved photodetachment spectra for the adiabatic singlet states of OHF" by S. Gomez-Carrasco, A. Aguado, M. Paniagua and O. Roncero in Journal of Photochmistry and photobiology A: Chemisty 190 (2007) 145

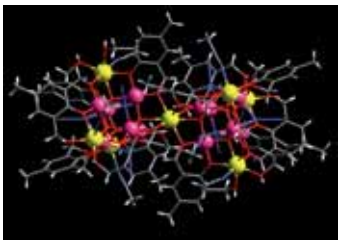
Eliseo Ruíz
Universitat de Barcelona

Magnetic Properties of Large Single Molecule Magnets

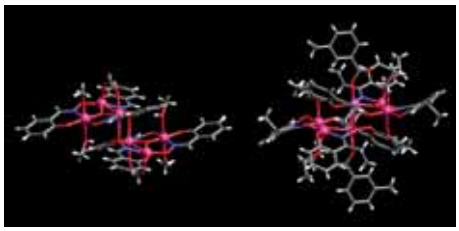
Some polynuclear transition metal complexes, usually known as single molecule magnets (SMM), show a slow relaxation of the magnetization and, as a result, each individual molecule behaves as a magnet. For that reason, such molecules have been proposed either as potential materials for information storage at the molecular level or as qubits in quantum computers, due to their quantum-controlled spin flip. The first known SMM was discovered in 1993, a Mn12 compound. During the last years several transition metal complexes have been synthesized, mainly having iron and manganese as paramagnetic centers, that present a similar magnetic behavior. In this field, the holly grail is the existence of an SMM with a high enough spin inversion barrier to avoid both the thermal spin flip and quantum tunneling effects. Thus, many experimental groups are working in the synthesis of new polynuclear complexes in search for large energy barriers that should be reached increasing the total spin and the magnetic anisotropy of the molecule. However, due to the difficulty of the prediction of these magnetic properties the experimental search is basically a serendipitous process. The two magnitudes play a crucial role and both can be determined using theoretical methods based on Density Functional Theory. The calculation of such magnitudes allows to use the theoretical methods not only to compare the results with known complexes also to predict values for not-yet-synthesized systems and to understand to dependence of these two magnitudes with the structure of the complexes, helping for a rational search of improved SMMs. Due to the complexity of the electronic structure and the presence of a large number of atoms, this kind of studies require large computational facilities as those provided by BSC with MareNostrum.

The mixed-valence MnII-MnIII polynuclear complex, Mn19 (see figure), is so far the world record for molecular spin, with S = 83/2, significantly surpassing the previous highest S = 51/2 and 61/2 values for Mn25 complexes. A full characterization of the exchange interactions that determine such high spin state is not directly obtainable from experimental techniques, such as

the temperature dependence of the magnetic susceptibility. The presence of many exchange coupling constants in this kind of systems results in the existence of multiple sets of exchange constants that perfectly fits the experimental data being impossible to determine the right set of values. Hence, the direct calculation of the exchange coupling constants using NWChem and Siesta codes should provide us with valuable information for the future design of new molecular systems with still higher spin.



As mentioned above, the magnetic anisotropy is the second magnitude together the total spin of a SMM determine its critical temperature. The magnetic anisotropy is usually represented by the zero-field splitting parameter D, which can be determined by Density Functional Theory calculations including spin-orbit effects using the NRLMOL code. Such theoretical methods could be employed to estimate the D values in simple model complexes to provide a good understanding of the factors that affect its sign and magnitude, finally facilitating a rational design of new systems with large magnetic anisotropy.



Recently, we have studied the magnetic anisotropy of some Mn6 complexes (see figure) that are the SMMs with largest known spin barrier and, showing the influence of the total spin in the magnetic anisotropy, that up to now were considered as independent properties and we propose new strategies of how to increase the energy barrier.

Publications

J. Cano, R. Costa, S. Alvarez, E. Ruiz. "Theoretical Study of the Mgnetic Properties of an Mn12 Single-Molecule Magnet with a Loop Structure: The Role of the Next-nearest Neighbor Interactions". J. Chem. Theor. Comput., 3, 782-788 (2007).

E. C. Sañudo, T. Cauchy, E. Ruiz, O. Roubeau, S. J. Teat, G. Aromí. "Molecules of Weakly Magnetically Coupled [MnIII4] Clusters as Models for Magnetic Quantum Gates". Inorg. Chem. 46, 9045 – 9047 (2007).

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CPMD Study of Planar Metal Complexes of Pd(II) and Pt(II) in Solution

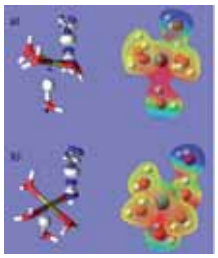
There is only scarce information available for hydration of Pd(II) and Pt(II) from experiment and theory. Their aqua ions are both well known to form square-planar tetrahydrates, which introduces a strong asymmetry in their hydration patterns. As a result, the concentric shell model' of Frank and Evans is no longer valid and thus cannot be used to understand the solvation structure in the non-equatorial regions. In this sense, although overall consensus between different experimental and theoretical investigations is achieved on the gross square-planar structure of these aqua ions, describing the axial regions above and below the metal-oxygen plane remains controversial. The delicate balance among ion-solvent and solvent-solvent interactions in the axial and equatorial regions is a key-point to understand the different chemical and pharmacological activity of Pd(II) and Pt(II) complexes, as far as hydrolysis and aquation are present in the chemical processes joined to the activity of several antitumoral products derived from Pt(II) amino-complexes, such as cis-platin, carboplatin or oxaliplatin.

During previous activity periods at MareNostrum the team have performed Car-Parrinello Molecular Dynamics (CPMD) simulations for Pd(II) and Pt(II) in aqueous solutions. Beyond the well-defined square-planar first solvation shell encompassing four tightly bonded water molecules as predicted by ligand field theory, a second coordination shell containing about 10 water molecules is found, which can be described as a dense and rigid crown-like equatorial region enclosing the aqua ion core complex.

Additional solvation in the axial regions is observed for both metals which is demonstrated to be induced by the condensed phase. Only for Pt(II), however, this water molecule is bonded with one of its hydrogen atoms towards the cation, thus establishing a typical anionic solvation pattern, which is traced back to the electronic structure of Pt(II) versus Pd(II) cations, in particular to the anisotropic polarizability of their tetrahydrates.

Furthermore, transient protolysis of water molecules in the first shell is observed for both divalent transition metal cations being more pronounced for Pt(II) versus Pd(II). These solvation features agree qualitatively with the different acidity of Pt(II) and Pd(II) aqua ions in water and their different water ligand exchange rates.

Once the behaviour of Pd(II) and Pt(II) water solutions have been characterized, in the continuation of our activity, the problem of an organometallic compound of platinum has been undertaken: the structure and related properties of Oxaliplatin (cis-[(1R,2R)-1,2-cyclohexanediamine-N,N']-oxalatoplatinum(II), a third generation anticancer platinum drug) in water solution. Due to the bulky cyclohexane substituent, CPMD simulations have been performed on the closely related complex, ethyldiamine-oxaliplatiunum(II). Pt-O and Pt-H RDFs show wide and diffuse peaks, suggesting the solvation pattern around metal cation to be scarce and not well defined. This difference with respect to the hydration pattern previously found for the Pt(II) aquaion is to be expected given the markedly different chemical character and bulkiness of the amine and oxo ligands compared to water. However, a small shoulder around 2.5 A in the Pt-H (H coming from water) RDF, integrating up to 0.3 H atoms, suggests the possibility of anionic hydration taking place in the axial region of the complex.



Electronic structure analysis of the anionic hydration of the solvated Pt(II) tetrahydrate compared to a proper hydrogen bond between a first--shell and a second--shell water molecule. Representative snapshot is shown in two orientations revealing the axial (a) and equatorial (b) interactions. Left: Electronic (valence) density difference shown by isosurfaces at +0.005 |e| (white lobe) and -0.005 |e| (blue lobe). Right: Electronic (valence) density surface (isosurface at +0.02 |e|) onto which the change in electrostatic potential is mapped ranging from -0.02 a.u. (red) via yellow and green to +0.02 a.u. (blue)

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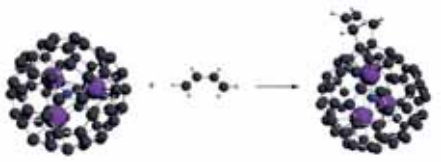
Chemical reactivity of D3h-C78 (Metallo) Fullerenes: Regioselectivity Changes Induced by Sc3N and Y3N encapsulation

Endohedral fullerenes are formed when a metal atom is encapsulated inside the cage. However, the most studied metallofullerenes are the so-called TNT as they can be produced in high yields. This new type of fullerenes contains metal nitrides inside the fullerene, i.e. $M_3N@C_x$, which results in a formal electronic transfer of six electrons from the M_3N unit to the fullerene structure ($M_3N^{6+}:C_x^{6-}$). This electron transfer modifies the physical properties and has an enormous influence on the reactivity of these compounds.

Functionalization of these TNT endohedral metallofullerenes is important to obtain nanomaterials with unique properties that can be potentially used in a variety of fields ranging from molecular electronics to biomedical applications.

Although the chemistry of fullerenes is nowadays well-established and understood, less is known about the reactivity of endohedral metallofullerenes. Such species are currently becoming one of the most studied classes of compounds within the field of fullerenes. In fact, there is a lack of comprehension of how the encapsulated species affects the exohedral reactivity of endohedral metallofullerenes when compared to free fullerenes.

The team is interested in investigating the change on the exohedral reactivity of free fullerene C_{78} when a metal cluster is encapsulated inside the cage. In particular, we analyze both the thermodynamics and the kinetics of the cycloaddition Diels-Alder reaction of 1,3-butadiene over all different bonds of C_{78} and the endohedral derivatives: D_{3h}-$Sc_3N@C_{78}$ and D_{3h}-$Y_3N@C_{78}$. The complexity and the cost of the ab initio calculations carried out in the proposed activity make this project only possible in a supercomputer like MareNostrum. Hence, this project provides a detailed description of a concrete reaction, whose results can serve as reference for future studies. In this way, a new step will be done to understand fullerene properties and reactivity, which could probably be useful for future medical and biological applications.



The Diels-Alder reaction involving 1,3-butadiene and the endohedral fullerenes M3N@C78 (M=Sc, Y)

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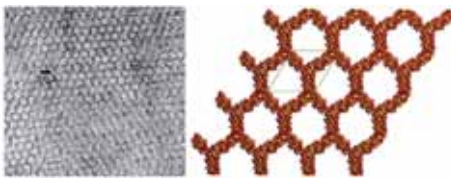
Ab initio simulation of amorphous silica surface and its interaction with biological molecules

Mesoporous ordered materials are attractive supports for the adsorption or immobilization of biologically relevant molecules in confined spaces, since they are characterized by high surface areas and pore volumes. Moreover, due to their regular pore distribution, these materials have been proposed and analyzed as drug delivery systems. This was evidenced for the first time by the confinement of ibuprofen in MCM-41 matrices, a rather complex material. Its peculiarity resides in the large pores that cross the material, the average diameter being around 20-30 Angstroms, and in its silica walls, of around 10 Angstroms thick, which are amorphous in nature. One important factor that determines the adsorption and subsequent release of a drug is its interaction with the pore wall, which contains large amounts of silanol groups. Thus, in order to get information at a molecular level of these drug delivery systems, a detailed an accurate model of an amorphous silica surface is required. However, no realistic models of amorphous silica surfaces have ever been reported

During 2007 periods, BSC resources were used to simulate a variety of amorphous silica surfaces with different degrees of hydroxylation since this is the key factor that fixes the adsorption features of the surface, and can be controlled experimentally by thermal treatment of the silica sample. Calculations were done using a fully ab-initio B3LYP periodic treatment based with the massive parallel version of the CRYSTAL06 code (http://www.crystal.unito.it), kindly provided by the Theoretical Chemistry Group at the Torino University. Results show that the H-bonding pattern between surface SiOH groups is strongly dependent on the OH density. For the 4.5 OH/nm2 case (the closest to represent an experimental silica sample pre-treated at 150 °C) H-bond contacts were found to be of moderate strength and only pair of OH groups were involved in H-bonds, so that the surface remains rich in OH groups free to interact with adsorbed molecules. In contrast, for fully hydroxylated surfaces optimizations resulted in stronger and longer H-bond chains and, as a consequence, in a much smaller number of OH groups available for adsorption.

In addition, thanks to MareNostrum the team has been able to generate and optimize for the first time a realistic model of a fully hydroxylated MCM-41. This optimization required a large amount of computational resources since the number of atoms in the unit cell is 579 and the number of Gaussian based atomic orbitals is 7756. Analysis of the results indicates that the H-bond interactions between OH groups leave a sensible number of terminal OH which will be responsible of the interaction with adsorbed molecules. In the figure the team reflects the comparisons between the experimental transmission electron micrograph of MCM-41 obtained with a JEOL 200CX operating at 200 kV with our B3LYP/6-31G(d,p) optimized structure. Clearly the general structural features are in remarkable agreement to each other, supporting this model as a realistic one to mimic the real MCM-41 material.



Left: transmission electron micrograph of MCM-41 [2]. Right: van der Waals representation of the B3LYP/6-31G(d,p) optimized model of MCM-41

Publication
Advanced Material as a communication (P. Ugliengo, M. Sodupe, F. Musso, I. Bush, R. Orlando and R. Dovesi, "Large scale periodic B3LYP modelling of realistic models of hydroxylated amorphous silica surfaces and MCM-41 mesoporous material", in preparation).

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Parallel scaling of the Amsterdam Density Functional (ADF) program

The ADF program

The Amsterdam Density Functional (ADF) package is software for first-principles electronic structure calculations. ADF is used by academic and industrial researchers in such diverse fields as pharmacochemistry and materials science. It is particularly popular in the research areas of homogeneous and heterogeneous catalysis, inorganic chemistry, heavy element chemistry, various types of spectroscopy, and biochemistry.

The underlying theory of the ADF package is the Kohn-Sham approach to the Density-Functional Theory (DFT). Kohn-Sham DFT is an important first-principles computational method to predict chemical properties accurately and to analyze and interpret these in convenient and simple chemical terms. The method implies a one-electron picture of the many-electron systems but yields in principle the exact electron density (and related properties) and the total energy. The exact exchange-correlation (XC) functional is unknown, but the currently available XC functionals provide in most cases already a 'chemical' accuracy of a few kcal/mol for binding energies. Moreover, the computed orbitals are suitable for the typical MO-theoretical analyses and interpretations.

Kohn-Sham DFT is a relatively efficient computational method, and its fundamental scaling properties do not deteriorate when methodological precision is increased, in particular, when a more accurate XC functional is applied. Recent research paves the way to implementations that scale only linearly with the system size. This brings within reach the treatment by fundamental quantum chemical methods of systems with hundreds, maybe even thousands of atoms.

The QUILD program

A recent extension of the ADF program package is the "QUantum-regions Interconnected by Local Descriptions" (QUILD) program, as developed by M. Swart and F.M. Bickelhaupt. It serves as wrapper around the ADF program and enables QM/QM, QM/MM and QM calculations. The QUILD program contains an improved geometry optimization setup using adapted delocalized coordinates (Int. J. Quant. Chem. 2006, 106, 2536-2544), which is especially beneficial for systems containing weak coordinates. Recent benchmark studies revealed a reduction of the number of geometry steps needed to fully optimize a set of weakly bound systems (to a gradient maximum of 1.0·10-5 a.u.) by a factor of 4.

Additional features are: optimization using numerical gradients (for use with excited states, Meta-GGA/hybrid functionals, or Spin-Orbit relativistic calculations), spin contamination corrected (i.e. pure spin-state) geometry optimizations, decoupling of geometric and electronic symmetry (i.e. one can use S4 symmetry for the geometry and C2v for the electronic symmetry), and an improved model Hessian. The latter is especially useful for Transition-State searches as it automatically generates the correct Hessian curvature (i.e. one and only one negative Hessian eigenvalue), thereby obviating the need to do a full Hessian calculation at the start of the calculation. Note that because QUILD serves as wrapper around ADF, any feature within ADF (different XC functionals, Scalar or Spin-Orbit (ZORA) Relativistic corrections, COSMO solvent model) is automatically possible within the QUILD program.

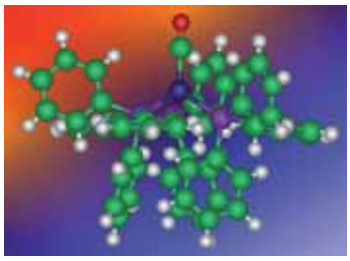
Parallellization of ADF

The ADF program is maintained by a spin-off company (Scientific Computing and Modelling, SCM) of the VU University of Amsterdam, which split of from the Baerends group in 1995. The program has already been developed in the Baerends group (in collaboration with the Ziegler group in Canada, and other scientific developers) since the beginning of the 1970's. SCM cooperates with most major hardware vendors to optimize performance of the ADF software for all popular computer platforms. This includes fine-tuning of the code for different compilers and hardware configurations. These efforts include various types of Linux clusters.

Most parts of ADF have been efficiently parallelized for both shared-memory and

distributed memory systems, such as multi-core multi-CPU machines or simple Linux clusters; the parallellization of the program has been supported in the past through the Europort2 project (ESPRIT-III). For most standard types of calculation, including NMR, analytical Hessian, and TDDFT calculations, ADF approaches perfect parallel scaling fairly well, even for a significant number of CPU's. On MareNostrum, the team installed the development version of ADF using OpenMPI (version 1.2.5) with support for GM_Myrinet for the parallel communication.

Below the team shows the timings of a typical example (*Ptcomp_METECC*, see figure). This example deals with one geometry step of a $Pt(P(Ph)_3)_3CO$ system containing 105 atoms, which was studied using the BP86 functional, and has been used before in benchmark tests



This report represents the timings using two different basis sets, the first consists of a triple-ς valence plus polarization (TZP) on Pt, combined with a double-ς valence plus polarization (DZP) on the rest. The second (larger) one uses the TZP basis for all atoms.

Nr. of nodes[a]	Wall-time (s) DZP(rest)	reduction[b] (s)TZP(Pt)-	Wall-time	reduction TZP(all)
1(4)	3165	-	-	-
2(8)	1717	0.54	8681	-
4(16)	932	0.54	4395	0.51
8(32)	580	0.62	2515	0.57
16(64)	372	0.74	1512	0.60
32(128)	300	0.86	998	0.66

a) in parentheses the number of processors (tasks); b) ideally, the reduction in time would be 0.5 when doubling the number of tasks

For the job with the smaller basis set, a reduction in elapsed (wall) time is still being achieved up to 128 tasks, but the amount of work actually to be done is reduced to that extent that the communication between the different tasks is starting to dominate the timing results with a larger number of tasks (from 64 and higher). Therefore, the team examined the same $Pt(P(Ph)_3)_3CO$ system but now with the TZP basis on all atoms. This improves the parallel scaling significantly, and a substantial reduction is still achieved in going from 64 to 128 tasks.

After this initial test of the parallel scaling of the ADF program, the combination of QUILD and ADF has been successfully used in scientific projects on the chemical reactivity of (metallo)fullerenes.

Publication

"QUILD: QUantum-regions Interconnected by Local Descriptions", M. Swart and F.M. Bickelhaupt, J. Comput. Chem. 2008, 29, online, DOI 10.1002/jcc.20834.

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Quantum Chemical Study of Self Assembled Monolayers of Mixed Thiols on Noble Metal and Metal Oxide Surfaces

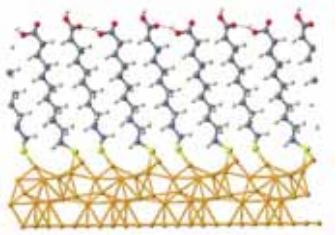
Immersion of a gold surface in thiolate solution leads to a spontaneous adsorption of thiols1. These types of layers have attracted much attention because they may constitute ideal platforms for further binding or reactivity. Thiolate rapidly adsorb to form a quasi saturated layer in a few minutes to one hour; this preliminary adsorption step is followed by an ordering of the thiolate chains leading to a crystalline-like layer depending on time and conditions of immersion.

Our objective is to characterize and understand the behavior of mixed SAMs that contain a mixture of thiolates. Previous XPS systematic study helped us to define conditions where the surface composition is very close to that in solution2 and corresponding to complex, but rather homogenous AFM images2. This prompted us to use and combine other techniques to better characterize the layer structure of these SAMs at a molecular level.

Characterization of mixed SAM layers through a combination of experimental techniques and first principle calculations enables to obtain fundamental insights on the organization of the thiol chains on a macroscopic level. Mixtures of different types of undecanethiol SAMs tend to organize in domains on the surface. Controlling the dispersion of SAM domains enables to control the dispersion of e.g. biological systems to be attached on the SAM. The investigation of the substitution of the tail group (COOH/OH/NH2/CONH2) will enable to shed some light on the dispersion mechanism within the mixed SAM.

In this project the adsorption of mercapto alkanethiol derivates was studied from pure and mixed solutions on Au nanostructured films. In other words the geometry and the chemical properties of different SAM systems were studied, using state of the art periodic DFT calculations, in combination with our in-house PM-IRRAS, XPS, AFM and other experimental techniques done by our colleagues. The characterization of these undecanethiols is a logic continuation of our earlier works on the designing of biosensors2,3 and characterization of SAMs4.

Based on the above, the present project used a quantum chemical approach (Periodic DFT) to characterize the SAMs geometry/energetics and investigate their reactivity towards organic/biologic molecules. The thorough investigation of the local geometry via energy minimization DFT calculations and the calculation of phase diagrams (global geometry) for different SAM mixtures is the first step in our project. The second step is the prediction of the SAMs reactivity and comparison/interpretation of the experimental data obtained in our laboratory. In a former study some first steps were made into the investigation of the adsorption of mixed alkanethiol SAMs on noble metal surfaces5. However, some major questions stay unanswered. Such as: what is the effect of the chain length, end group, degree of mixing between two types of end group substituted alkanethiols on the geometry, energetics and reactivity. Very few studies were done on these systems (mixed SAMs), until now only one type of SAM was considered in the model and this mainly for short chain thiols. In this project we want to investigate the effect of mixtures between different thiols (having longer alkyl chains and complex end groups) at different covering concentrations. For this particular systems require a considerable computation power, which is not possible from a price/quality point of view on the machines available at the Université Pierre et Marie Curie. Moreover, since the adsorption geometry is not only dependent on type of thiol but also on the coverage concentration, the calculation of larger unit cells is needed.



Optimized adsorption geometry of carboxylic acid terminated acidundecanethiol Self Assembled Monolayer (SAM) on Au(111) surface, showing the hydrogen bond stabilization between pairs of chains, and the reconstruction of the surface

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