4

2008 Annual Report

BSC
Barcelona
Supercomputing
Center
Centro Nacional de Supercomputación

RES
RED ESPAÑOLA DE
SUPERCOMPUTACIÓN

(4)

The 2008 Combined Annual Report
of the Barcelona Supercomputing
Center - Centro Nacional de Super-
computación (BSC-CNS) and the
Spanish Supercomputing Network
(RES) summarises the various support
and research activities for the year
and provides a short description of
the two organisations.

GOBIERNO DE ESPAÑA   MINISTERIO DE CIENCIA E INNOVACIÓN

Generalitat de Catalunya
Departament d'Innovació,
Universitats i Empresa

UPC   UNIVERSITAT POLITÈCNICA DE CATALUNYA

2008 Annual Report

Barcelona
Supercomputing
Center
Centro Nacional de Supercomputación

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Mateo Valero,
Director
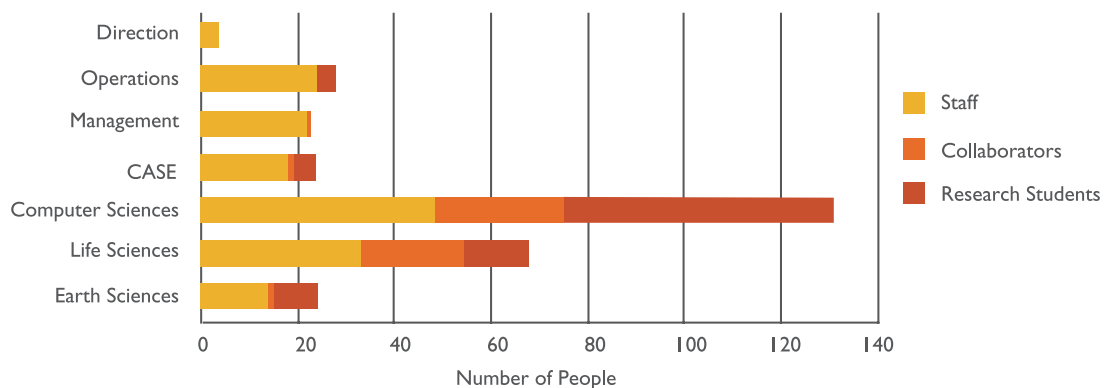
Francesc Subirada,
Associate Director

2008 Review

2008 saw continued strong performance of the BSC-CNS in the key areas of research activity, support services, competitively gained project funding from both public and private funds, and the number of collaborations with scientists from other institutes. The increased efforts to promote technology transfer to the private sector began to bear fruit with the strengthening of existing industry links. At an international level Spain was confirmed as a principal partner in PRACE (the European project that will establish the tier-0 High Performance Computing infrastructure in Europe), with the BSC-CNS as its representative, while at a national level the Spanish Supercomputing Network (RES) which is administered by the BSC-CNS, saw unprecedented demand for computation time from a broad spectrum of scientific disciplines throughout Spain and even from abroad.

Mission
The mission of BSC-CNS is to investigate, develop and manage information technology in order to facilitate scientific progress.

BSC-CNS People 2008

Categories (top to bottom): Direction, Operations, Management, CASE, Computer Sciences, Life Sciences, Earth Sciences

Legend: Staff, Collaborators, Research Students

X-axis: Number of People (0 to 140)

2008 saw the BSC-CNS continue with its strategy to attract the most skilled people from around the world. Despite the limitations of room in the current buildings, during the year some 302 people performed research or provided support at the centre, as compared to 200 in 2007. The dramatic growth in people working at the BSC-CNS is mainly due to a significant increase in the number of students and collaborators working with the key research departments. Over one third of staff are of foreign nationality, with the diversity of nationalities represented growing from 23 in 2007

World Map of Countries of Origin

to 26 in 2008, including: Argentina, Belgium, Brazil, Bulgaria, Canada, Chile, Colombia, Denmark, France, Germany, Hungary, India, Iran, Israel, Italy, Pakistan, Peru, Poland, Portugal, Russia, Serbia, Thailand, Turkey, UK, United States and Spain.

Powerful Computing

The BSC-CNS is the National Supercomputing Facility in Spain and manages Mare-Nostrum, one of the most powerful supercomputers in Europe, located at the Torre Girona chapel. In November 2008, the 32nd edition of the Top500 list ranked the MareNostrum as the 10th most powerful supercomputer in Europe and 40th in the world.

The Spanish Supercomputing Network (RES) which consists of seven nodes, including MareNostrum (Barcelona), Magerit (Madrid), Altamira (Santander), LaPalma (Santa Cruz de la Palma), Picasso (Málaga), Tirant (Valencia) and Caesaraugusta (Zaragoza) supported more than 270 R&D activities in 2008, led by researchers from institutions in over 30 cities in Spain, Europe and overseas, with demand exceeding supply by almost 300%. This is testament not only to the importance of providing access to supercomputing facilities to ensure scientific research in Spain remains competitive, but also to the success of the efforts over the last few years to promote the existence, availability and utility of RES services to scientific communities that have not traditionally been users of supercomputers.

Key support services for the RES continued to be strengthened in 2008, with new administration support and monitoring committees formed, consolidation to a single Access Committee for all access requests, major upgrades of shared memory systems at the BSC-CNS, and the initiation of informative seminars for new users and technical training for operators of RES nodes. Despite all these additional activities, core services were not neglected with the MareNostrum achieving an availability rate of over 80%.

The research departments of the BSC-CNS further grew their international profiles with expanded collaborations, new international projects and increased funding from competitive sources. All departments have focused long-term research programs; Computer Sciences influencing the way computing machines are built, programmed and used; Earth Sciences modelling and understanding the behaviour of the Earth System, in particular atmospheric processes and climate change; Life Sciences understanding the molecular biology and evolution of living organisms using theoretical models and simulation algorithms; CASE developing numerical modelling platforms to provide applied solutions to highly computationally demanding problems.

Broad Access

The powerful resources of the MareNostrum Supercomputer and the RES nodes are accessed by a broad spectrum of Spanish and international scientists. Computing time is allocated by the Access Committee, composed of a Core Team and four Expert Panels of prestigious Spanish scientists external to the BSC-CNS. Additionally, a percentage of computing time is reserved for commercial projects to enable Spanish companies to maintain international competitiveness.

The work carried out by the scientists at BSC-CNS resulted in over 100 journals and book chapter publications and 152 key conference presentations. Additionally, BSC-CNS researchers presented numerous workshops at both national and international levels, and the centre hosted a number of key events.

Support and Research

The BSC-CNS, which provides both Support to other research institutes and as well as undertaking primary Research in its own right, is organised into 6 core departments; Computer Sciences, Life Sciences, Earth Sciences, Operations, Computer Applications in e-Science & Engineering (CASE), and Management.

Computer Sciences
Management
Life Sciences
Executive Commission and Directors
Operations
Computer Applications in e-Science and Engineering
Earth Sciences
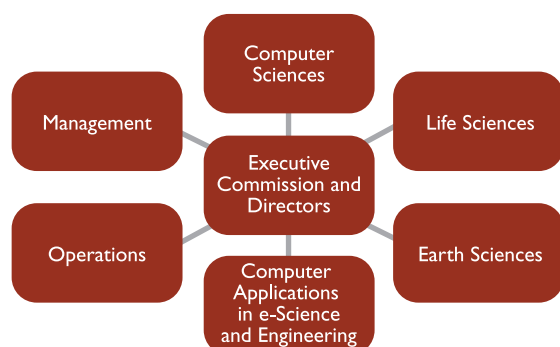
The Support functions provide technical and operational support to internal and external researchers and scientists, collaborators and other institutions and industrial partners. In particular the Operations Department also manages all activities relating to the MareNostrum supercomputer and access to the other nodes of the RES. The various departments have a number of scientific research groups, each headed by a Team Leader, which focus their activities on the study of hardware and system software for the supercomputers of the future and on the application of computer simulation in the fields of genomics, proteomics and dynamic Earth processes.

Strong Governance

Overall governance of the BSC-CNS is provided by the Board of Trustees formed by members of the three institutions that are partners of the BSC-CNS Consortium, and will be further supported by the Scientific and Business Advisory Boards (still in formation).
Strategic direction is provided by the Executive Commission and this devolves to day-to-day management via the Management Board. Reporting to the Management Board are the various scientific and support departments.

Board of Trustees
Scientific Advisory Board
Executive Commission
Business Advisory Board
Management Board
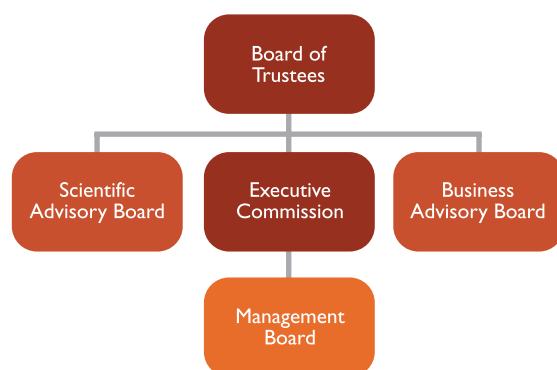
The income of the BSC-CNS in 2008 was 23.9 M. 14.7 M corresponded to the ordinary budget coming from the patrons of the BSC-CNS, the Spanish and Catalan Governments; and 9.2 M from competitive projects. In 2008, the BSC-CNS participated in 23 competitively funded EU projects, 33 collaborative projects with industry and 30 national projects. More importantly than the number of projects, the scope and size of new projects commenced in 2008 are larger than those which completed, resulting in a high growth in R&D activity.

Of special note, Spain was confirmed as a principal partner in PRACE (Partnership for Advanced Computing in Europe) which will see the establishment of five tier-0 world class supercomputers installed in a European grid, with the

Patrons of the BSC-CNS

The BSC-CNS is a legally autonomous, public consortium, with three founding partners, the Spanish Ministry of Science & Innovation (MICINN), the Departament d'Innovació, Universitats i Empresa (DIUE) of the Catalan government and the Universitat Politècnica de Catalunya (UPC).

The voting representation is divided between MICINN (51%), DIUE (37%), and UPC (12%).

BSC-CNS Patronage
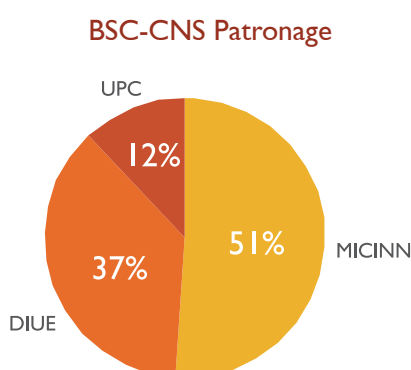
BSC-CNS chosen to be the Spain's representative. A prototype next generation supercomputer has already been installed at the BSC-CNS. Called MariCel, this 14.4 TFLOP/s supercomputer occupies only 2 racks and consumes only 20 kW of power.

The BSC-CNS is very proud to not only provide a world-class supercomputing service, but to also be at the forefront of technology creation; the BSC-CNS both generates new technologies (performance tools, programming models, earth operational systems, computational fluid dynamics application enabling platforms, and protein databanks, amongst others) and also helps other institutes and private companies to create leading technologies via collaborative R&D.

2008 saw the BSC-CNS cement and further expand its close collaboration with key industry leaders, including IBM, Microsoft, Cisco and Sun Microsystems. The IBM-BSC joint research project aims to develop a 10+ PetaFLOP/s supercomputer for 2011/12, while the BSC-Microsoft Research Centre which was inaugurated in April 2008 aims to develop new designs for hardware/software interaction in consumer PCs for the next decade.

Technology transfer to non-computer companies also expanded, with projects ranging in scope from the Kaleidoscope project with Repsol, that aims to produce more reliable and faster (by several orders of magnitude) software tools to aid in sub-sea oil exploration, to air quality monitoring for power companies and improving aerodynamics of airplanes and sailboats.

Collaboration with other institutes was also strengthened, in particular via the formation in 2008 of the Joint Research Program between the BSC-CNS and the IRB (Institute for Research in Biomedicine Barcelona) which has already succeeded in establishing an experimental laboratory to facilitate the validation of models and simulations.

To support the continued growth of the centre a number of key structural actions were initiated in 2008, of particular note funds were approved for the construction of a new building to house the BSC-CNS, including a purpose built chamber for the next generation supercomputer which is already being planned to ensure that the services provided by the BSC-CNS and the RES remain at the highest level and internationally competitive.

The Directors wish to thank all the staff, students, collaborators and visiting researchers who through their dedication, hard work and team spirit contributed to the many successes of 2008 and who can be proud of the reputation they have earned for the BSC-CNS as a key international reference in High Performance Computing and e-Science.

They would also like to give thanks and recognition to the patrons of the BSC-CNS; MICINN, DIUE and UPC for their continued strong support, as well as to the various funding agencies and private companies who sponsor the projects that have enabled the BSC-CNS to grow, compete and perform at the highest international level.

Mateo Valero, Director   Francesc Subirada, Associate Director

Key to the success of the BSC-CNS are the many people of different backgrounds that work and collaborate with the institute. These include contracted staff, visiting academics, students, and collaborators from other institutes and private industry, amongst others.

As at 31st December 2008, the core staff of the BSC-CNS included 83 permanent positions and 89 dedicated to specific projects. These numbers were significantly augmented by additional staff who participated in the BSC-CNS via a number of programs.

Total personnel who worked at the BSC-CNS throughout the year increased from 200 during 2007 to 302 during 2008, mainly through new temporary and shared staff, resident students, and collaborating and visiting researchers. This increase in active personnel was driven by a greatly increased number of research projects.

Annual BSC-CNS Staff and Collaborators
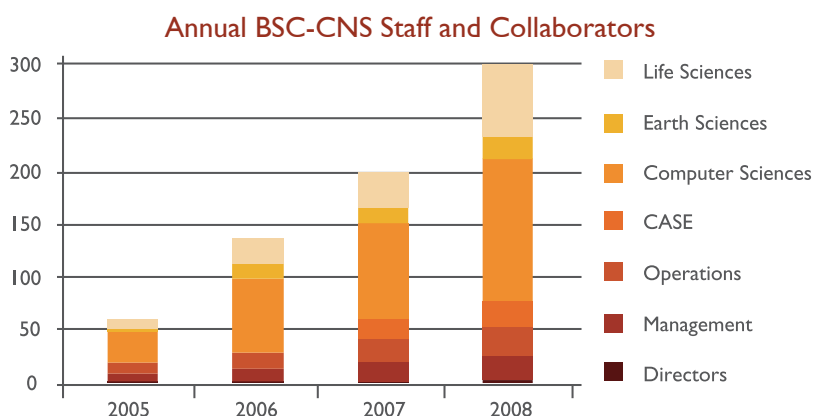
Shared Staff and Human Resource Programs In addition to its own staff, the BSC-CNS hosts shared staff from other public institutions such as the Technical University of Catalonia (UPC), the Institut de Recerca de Barcelona - Parc Scientific de Barcelona - Universitat de Barcelona (IRB-PCB-UB) and the Consejo Superior Investigaciones Cientificas (CSIC).

In 2008 the BSC-CNS also welcomed high level scientific personnel from special human resources public programs such as the Ramón y Cajal Program, the ICREA Program and other personnel training research programs sponsored by various Spanish Ministries.

The BSC-CNS Fellowship Program The BSC-CNS Fellowship program invites applicants from relevant scientific disciplines to participate in several European research projects and collaborations with international industry such as IBM and Microsoft. These fellowships are offered for periods of one year, renewable for the duration of the project. During 2008, the BSC-CNS had 44 student researchers associated to several research projects.

Mobility Programs The BSC-CNS has always supported mobility programs. The objective is to provide access to advanced computing infrastructures to researchers worldwide in order to promote collaborative research involving scientists from different countries and provide training to scientists in high performance computing in order to solve scientific and technological problems. Visitors are also provided with financial support to cover their stay. The BSC-CNS is involved in two major mobility programs:

At the Spanish level, the BSC-CNS participates in a national access program called ICTS, whose objective is to leverage the knowledge in supercomputing and eScience from the BSC-CNS. This program, which holds selection meetings every 4 months, allowed 18 researchers to access the BSC-CNS facilities in 2008; their expenses were covered by the Spanish Ministry of Science and Innovation (MICINN).

At the international level, HPC-Europa is a consortium of six leading High Performance Computing (HPC) infrastructures, including the BSC-CNS. The program 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 HPC facilities in Europe. During 2008 the BSC-CNS hosted 39 such visitors.

BSC-CNS Governing Bodies

Members of the BSC-CNS Board of Trustees as at 31st December 2008

President

José Manuel Fernández de Labastida, General Secretary for Scientific and Technological Policies, MICINN

Vice President

Blanca Palmada, Comissioner for Universities and Research, DIUE

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Juan José Moreno, Director General of Planning and Coordination

Carmen Peláez, Vice President of Organization and Institutional Relations, CSIC

José Ignacio Doncel, Deputy Director General of Promotion, Technological Infrastructure and Large Facilities

Representatives DIUE

Joan Majó, Director General of Universities

Ramon Moreno, Director General of Research

Iolanda Font de Rubinat, Deputy Director General of Research

Representatives UPC

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Josep Casanovas, Vice Rector for University Policy

Sebastià Sallent, Director, Foundation i2CAT

Representatives BSC-CNS

Mateo Valero, Director

Ernest Quingles, Manager

Secretary of the Board

Francesc Subirada, Associate Director, BSC-CNS

Members of the BSC-CNS Executive Committee as at 31st December 2008

President

Juan José Moreno, Director General of Planning and Coordination, MICINN

Vice President

Ramon Moreno, Director General of Research, DIUE

Representative MICINN

José Ignacio Doncel, Deputy Director General of Promotion, Technological Infrastructure and Large Facilities

Representative DIUE

Iolanda Font de Rubinat, Deputy Director General of Research

Representatives UPC

Xavier Gil, Vice Rector for Research and Innovation

Josep Casanovas, Vice Rector for University Policy

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Mateo Valero, Director

Ernest Quingles, Manager

Commission Secretary

Francesc Subirada, Associate Director, BSC-CNS

Management Board

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

Access Committee

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 María Ibáñez, Universidad de Valencia

Assistant: Vicente Caselles, Universidad de Valencia

BSC-CNS Staff and Collaborators during 2008

Direction

Director: **Mateo Valero**

Associate Director: **Francesc Subirada**

Director Assistant: **Lourdes Cortada**

Associate Director Assistant: **Nuria Sirvent**

Computer Sciences Department

Computer Sciences Director: **Jesús Labarta**

Computer Sciences Associate Director: **Eduard Ayguadé**

Autonomic Systems and e-business Platforms

Autonomic Systems and e-business Platforms Group Manager: **Jordi Torres**

Researcher: Kevin Hogan

Researcher: Mario Macias

Researcher: Vicenç Beltran

Associate Researcher: David Carrera

Associate Researcher: Javier Alonso

Associate Researcher: Jordi Guitart

Associate Researcher: Yolanda Becerra

Resident Student: David de Nadal

Resident Student: Ferran Julia

Resident Student: Gemma Reig

Resident Student: Iñigo Goiri

Resident Student: Jorda Polo

Resident Student: Josep Oriol Fito

Computer Architecture for Parallel Paradigms

Computer Arquitecture for Parallel Paradigms Manager: **Adrián Cristal Kestelman**

Computer Arquitecture for Parallel Paradigms Manager: **Osman Unsal**

Researcher: Nehir Sonmez

Resident Student: Alaa Hilal

Resident Student: Amer Jwehan

Resident Student: Azam Seyedi

Resident Student: Chinmay Kulkarny

Resident Student: Cristian Perfumo

Resident Student: Ferad Zyulkyarov

Resident Student: Gokcen Kestor

Resident Student: Gulay Yalcin

Resident Student: Jasmina Tomic

Resident Student: Maximiliano Combina

Resident Student: Milan Pavlovic

Resident Student: Milos Milovanovic

Resident Student: Nebjosa Miletic

Resident Student: Nikola Markovic

Resident Student: Ramzi Younes

Resident Student: Roberto D'Aprile

Resident Student: Sasa Tomic

Resident Student: Srdjan Stipic

Resident Student: Surthitha Sanyal

Resident Student: Vesna Smiljkovic

Resident Student: Vladimir Gajinov

Associate Resident Student: Isidro González

Associate Resident Student: Rubén González

Associate Resident Student: Tanausu Ramírez

Grid Computing and Clusters

Grid Computing Group Manager: **Rosa Maria Badia**

Researcher: Daniele Lezzi

Researcher: Francesc Guim

Researcher: Iván Rodero

Researcher: Jorge Ejarque

Researcher: José María Pérez

Researcher: Marc de Palol

Researcher: Marta Garcia

Researcher: Raül Sirvent

Associate Researcher: Gladys Utrera

Associate Researcher: Julita Corbalán

Resident Student: Enric Tejedor

Resident Student: Isaac Jurado

Resident Student: Judit Planas

Resident Student: Luis Martinell

Resident Student: Maja Etinski

Resident Student: Pieter Bellens

Resident Student: Vladimir Marjanovic

Heterogeneous Architectures

Heterogeneous Architectures Group Manager:
Álex Ramírez Bellido

Researcher: Javier Vera Gómez

Researcher: Miquel Pericás

Researcher: Paul Carpenter

Researcher: Yoav Etsion

Associate Researcher: Carlos Álvarez

Associate Researcher: Carlos Villavieja

Associate Researcher: Daniel Jiménez

Associate Researcher: Esther Salami

Associate Researcher: Friman Sánchez

Resident Student: Antonio Quesada

Resident Student: Augusto Vega

Resident Student: Branimir Dickov

Resident Student: Felipe Cabarcas

Resident Student: Mohammad Shafiq

Resident Student: Vladimir Subotic

Associate Resident Student: Alejandro Rico

Associate Resident Student: Daniel Cabrera

Associate Resident Student: Cecilia González

Network Processors

Network Processors Group Manager:
Mario Nemirovsky

Associate Researcher: Alejandro Pajuelo

Associate Researcher: Javier Verdú

Resident Student: Ruken Zilan

Operating System / Computer Architecture Interface

Operating System / Computer Architectue Interface group Manager: **Francisco Javier Cazorla Almeida**

Researcher: Eduardo Quiñones

Researcher: Roberto Giogiosa

Resident Student: José Carlos Ruiz

Resident Student: Marco Paolieri

Resident Student: Petar Radojkovic

Resident Student: Víctor Javier Jiménez

Resident Student: Vladimir Cakarevic

Associate Resident Student: Carlos Boneti

Associate Resident Student: Carmelo Costa

Associate Resident Student: Kamil Kedzierski

Associate Resident Student: Miquel Moretó

Programming Models

Parallel Programming Models Group Manager:
Xavier Martorell

Researcher: David Ródenas

Researcher: Javier Teruel

Researcher: Jorge Daniel Vaquero

Researcher: Roger Ferrer

Associate Researcher: Alex Duran

Associate Researcher: Juan José Costa

Associate Researcher: Marc González

Associate Researcher: Maria Lluisa Gil

Associate Researcher: Montse Farreras

Associate Researcher: Nacho Navarro

Resident Student: Javier Bueno

Resident Student: Luis Vilanova

Resident Student: Nikola Vujic

Performance Tools

Performance Tools Group Manager: **Judit Giménez**

Researcher: Juan González

Researcher: Eloy Martínez

Researcher: Germán Llort

Researcher: Germán Rodríguez

Researcher: Harald Servat

Researcher: Pedro Antonio González

Researcher: Xavier Aguilar

Researcher: Xavier Pegenaute

Resident Student: Ana Jokanovic

Resident Student: Pau Freixes

Resident Student: Wahedd Iqbal

Associate Resident Student: Marc Casas

Storage Systems

Storage Systems Group Manager: **Antonio Cortés**

Researcher: Ernest Artiaga

Researcher: Jacobo Giralt

Researcher: Jesús Malo Poyatos

Researcher: Jonathan Martí

Researcher: Juan González

Researcher: Ramon Nou

Resident Student: Albert Miranda

Earth Sciences Department

Earth Sciences Director: **José María Baldasano**

Air Quality Group Manager: **Santiago Gassó**

Metereological Modelling Group Manager: **Oriol Jorba**

Mineral Dust Group Manager: **Carlos Pérez**

Senior Reseacher: Pedro Jiménez

Senior Researcher: Arnau Folch

Researcher: Leonor Patricia Güereca

Researcher: Matthias Piot

Resident Student: Ángel Rincón

Resident Student: Juliana Isabel González

Resident Student: Karsten Haustein

Resident Student: Mar Martínez

Resident Student: Maria Teresa Pay

Resident Student: Nathalie Clave

Resident Student: Sara Basart

Resident Student: Simone Marras

Resident Student: Yenny González

PhD Student UPC-BSC: Maria Goncalves

Research Support Engineer: Albert Soret

Research Support Engineer: Eugenio Lopez

Research Support Engineer: Malcom Noshir

Technical Project Support: Laura González

Technical Support: David Carrió

Technical Support: Thomas Loridan

Life Sciences Department

Life Sciences Director: **Modesto Orozco**

Computational Genomics

Computational Genomics Group Manager:

David Torrents

Researcher: Bárbara Montserrat

Researcher: Carlos Quijano

Researcher: Carme Vilamala

Resident Student: Leyden Fernández

Associate Resident Student: Santiago Algilaga

Associate Resident Student: Santiago González

Electronic and Atomic Protein Modelling

Electronic and Atomic Protein Modelling Group Manager:

Victor Guallar

Researcher: Ben Cossins

Researcher: Diego Masone

Researcher: Frank Wallrapp

Researcher: Ken Borrelli

Researcher: Seyed Ali Hoseini

Associate Researcher: Fátima Lucas

Associate Resident Student: Israel Cabeza de Vaca

INB-Computational Node

INB-Computational Node Group Manager: **Josep Lluís Gelpí**

Researcher: Aida Santaolalla

Researcher: Laia Codó

Resident Student: Alexis Torrano

Software engineer: Carles Pons

Software engineer: Jordi Camps

Software engineer: Romina Royo

Software engineer: Dmitry Repchevski

Software engineer: Jesús Maria López

Software engineer: Xavier Pastor

Mollecular Modelling and Bioinformatics

Researcher: Alberto Pérez

Researcher: Agnes Noy

Researcher: Guillem Portella

Researcher: Marco D'Abramo

Researcher: Montserrat Barbany

Researcher: Nadine Utz

Researcher: Oliver Carrillo

Researcher: Rebeca Garcia

Associate Researcher: Agustí Emperador

Associate Researcher: Xavier De la Cruz

Software Engineer: Damjan Cicin-Sain

Technical Support: José Antonio Alcántara

Resident Student: Adam Hospital

Resident Student: Annalisa Arcela

Resident Student: Antonella Paladino

Resident Student: Carles Fenollosa

Resident Student: David Piedra

Resident Student: David Talavera

Resident Student: Ignacio Faustino

Resident Student: Josep Goñi

Resident Student: Laura Orellana

Resident Student: Tim Meyer

Resident Student: Sergio Lois

Associate Research Assistant: Cristina Villanueva

Associate Research Assistant: Margarita Pedro

Protein Interactions and Docking

Protein Interactions and Docking Group Manager:
Juan Fernández- Recio

Researcher: Albert Solernou

Researcher: Solene Grosdidier

Resident Student: Laura Pérez

Structural Bioinformatics & Network Biology

Structural Bioinformatics & Network Biology Associate Group Manager: **Patrick Aloy**

Associate Researcher: Roberto Mosca

Associate Researcher: Andreas Zanzoni

Associate Resident Student: Amelie Stein

Associate Resident Student: Clara Berenguer

Associate Resident Student: Marc Duocastella

Associate Resident Student: Roland Pache

Experimental Bioinformatics Laboratory Platform

Experimental Bioinformatics Laboratory Associate Manager: **Montserrat Soler**

Associate Laboratory Support: Maica López

Associate Laboratory Technician: Mari Luz Ruiz

Associate Laboratory Technician: Ricart Lluis

Associate Resident Student: Özgen Deniz

Associate Research Assistant: Chiara Catellazzi

Computer Applications in Science & Engineering Department

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

High Performance Computational Mechanics Manager Group: **Mariano Vázquez**

Physical and Numerical Modelling Manager Group: **Guillaume Houzeaux**

Researcher: Albert Farrés

Researcher: Alejandro Soba

Researcher: Anne Cecile Lesage

Researcher: Edgar Alejandro Bea

Researcher: Félix Rubio

Researcher: Hadrien Calmet

Researcher: Mauricio Araya

Researcher: Mauricio Hanzich

Researcher: Miquel Català

Researcher: Mohammad Jowkar

Researcher: Pierre Lafortune

Researcher: Raúl de la Cruz

Researcher: Rogeli Grima

Researcher: Romain Aubry

Researcher: Xavier Sáez

Associate Researcher: Carles Serrat

Resident Student: Beatriz Eguzkitza

Resident Student: Cristina Montañola

Resident Student: Jelena Koldan

Resident Student: Margarida Moragues

Resident Student: Ruth Aris

Operations Department

Operations Director: **Sergi Girona**

System Administration

Systems Group Manager: **Javier Bartolomé**

Helpdesk: Antonio Espinar

Helpdesk: Fernando Fernández

Helpdesk: Ferrán Sellés

Network Administrator: Albert Benet

Network Administrator: Carles Kishimoto

Performance technical: Álex Font

Performance technical: Asier Roa

Performance technical: Miquel Ros

Security and Network: Juan Carlos Sánchez

System Administration: Gabriele Carteni

System Administration: Jonathan Evans

System Administration: Jordi Valls

System Administration: Peter Tornyi

System Administration: Sergi Moré

Resident Student: Carles Fenoy

Resident Student: Ivana Teodor

Resident Student: Lucas Rullo

User Support

User Support Group Manager: **David Vicente**

User Support: Jorge A. Naranjo

User Support: Joan Josep Iglesias

Technical Support: Diego Gandia

Technical Support: Xavi Abellán

Resident Student: Christian Simarro

RES Support: David Agudo

Webmaster: Silvina Rusinek

Maintenance Assistant: Albert Riera

Management Department

Management Director: **Ernest Quingles**

Finance and Business Administration

Administration, Finance and Human Resources Group

Manager: **Mercè Calvet**

Administration and Finance Account Officer:

Cristina Calonge

Finance Assistant: Judit Soldevila

General Assistant: Laura Gutiérrez

General Assistant: Neus Jiménez

Human Resources Respons: Sandra Vargas

Human Resources Officer: Ana Martín

Human Resources Officer: Lara Cejudo

Purchasing Officer: Cristina Vargas

Marketing and Communication

Marketing Executive: Renata Giménez

Marketing Communications Officer: Sara Ibáñez

MareNostrum Visitors Manager: Oriol Riu

Project Management

Research Project Manager: Alejandro Pina

Research Project Manager: Gina Alioto

Research Project Manager: Marta Rosselló

Research Project Manager: Nuria Nadal

Projects Project Officer: Anna Monrós

Projects Project Officer: Maria Carreras

PRACE Research Manager: Eugene Griffiths

Academic Programs Coordinator: Ulises Cortés

Technical Support: Valentí Lafuente

Associate Researcher: Fermín Sánchez

The financial accounts for 2008 presented here were drawn up following the accounting principles laid out in the General Plan of Public Accounting.

The operating budget of the BSC-CNS Consortium for the fiscal year 2008 was composed of ordinary income derived from contributions by the administrations and organisations that compose it as well as projects income derived from competitive funding sources and agreements reached with private organisations. This income was then employed to cover expenses, including costs of operations and fulfilment of all financial obligations.

Income 2008

Increased Competitive Funding

In 2008 the BSC-CNS achieved a significant increase in its extraordinary budget thanks to a high success rate in securing competitively funded European projects and collaborative R&D projects with private companies such as Repsol, IBM and Microsoft.

Income

The Consortium income of €23.894.475 recognised for fiscal year 2008 derived from public administration contributions from the Ministry of Science and Innovation (MICINN), Generalitat de Catalunya (GdC) and European Commission (EC), as well as from agreements, contracts or other collaborative agreements with private organisations. Furthermore, the consolidated budget of the BSC-CNS included the assignment of internal resources carried over from the previous year's provisions.

INCOME	AMOUNT €
Ordinary Income	6.700.000
Ministerio de Ciencia e Innovación	4.221.000
Generalitat de Catalunya	2.479.000
Competitive Income	9.195.804
Ministerio de Ciencia e Innovación	1.999.935
Generalitat de Catalunya	6.000
European Commission	3.352.032
Ministerio de Industria	400.000
Ministerio de Medio Ambiente	284.326
Private Companies	3.153.512
Other Income	7.998.653
Strategic Investment	6.622.820
Overheads / Capital Transfers	1.375.833
TOTAL INCOME	**23.894.457**

Ordinary Income refers to the base operating budget provided by the Consortium Partners.

Competitive Income represents the funds derived from competitive project grants from various Ministries, the European Commission and R&D projects sponsored by private companies.
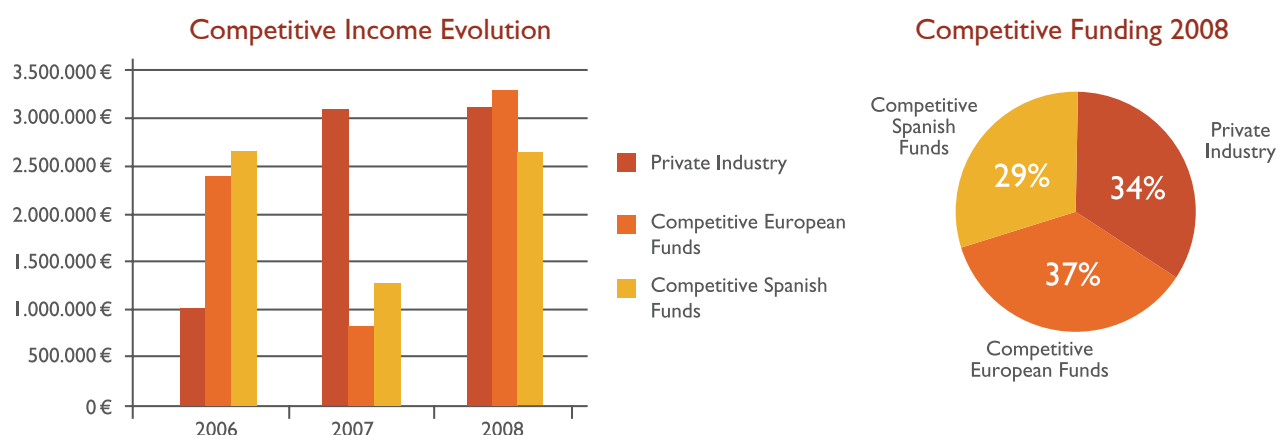
Other Income includes strategic investments, overheads ad capital transfers.

Strategic Investments are funds assigned by the Consortium Partners to finance key investments such as the construction of the new building to house the BSC-CNS, increases in supercomputing hardware and the repayment of loans taken out by the Consortium to finance the upgrade of the MareNostrum and the establishment of the RES.

Overheads are incomes derived from ordinary projects, which according to the norms of the BSC/CNS are charged 10% to cover overhead expenses.

Capital Transfers are incomes derived from the yield on the capital accumulated from multiannual reserves for the execution of competitive projects and strategic investments, deposited in different bank accounts.

Breakdown of Competitive Income

Competitive Income Evolution

Private Industry

Competitive European Funds

Competitive Spanish Funds

Competitive Funding 2008

Competitive Spanish Funds — 29%

Private Industry — 34%

Competitive European Funds — 37%

Expenses

The expenses of the BSC-CNS Consortium in the fiscal year 2008 include all costs associated with personnel, running expenses and investments financed either by the ordinary budget or from project funding derived from competitive grants.

EXPENSES	AMOUNT €		
	Ordinary Budget	Projects Budget	Total
Personnel	4.137.741	1.674.552	5.812.293
Investments	1.485.307	1.028.239	2.513.546
Current Expenses	3.523.656	1.739.272	5.262.928
Applied Reserves	5.551.948	4.753.742	10.305.690
TOTAL EXPENSES	**14.698.653**	**9.195.804**	**23.894.457**

Personnel refer to salaries and associated charges directly related to the employment of staff contracted by the BSC-CNS. It does not include salaries and associated charges of visitors or other collaborators who continued to be paid via their originating institution.

Investments include all expenditures on computing and scientific equipment and infrastructure.

Current Expenses include office space rental, furniture, fixtures and fittings, office computer equipment, security services, maintenance and cleaning services, telephones and networking, legal services, marketing, insurances and power.

Expenses 2008

Applied Reserves — 43%

Personnel — 24%

Investments — 11%

Current Expenses — 22%

Applied Reserves are funds not expended in the current year but carried over to future years, and are comprised primarily of two main components; those funds received for strategic investments that have not yet been completed (such as the new BSC-CNS building), and advance competitive project funds secured under various multi-year programs that are progressively applied over the lifetime of each project.
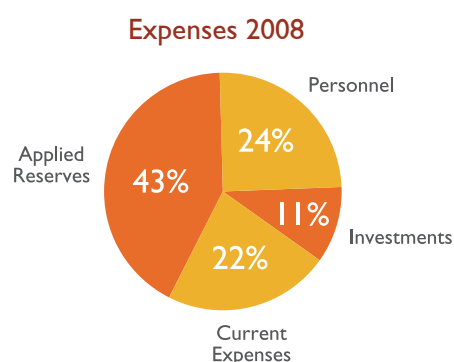
In 2008, the BSC-CNS invited 11 public calls in order to accept 9 supply tenders and 2 services tenders. All of the acquisitions were made following the legal procedures established by the law regulating contracting in public administrations, and all contracts were open to public tenders.

One of the main objectives of BSC-CNS is to pro-actively transfer technology to industry, both as an objective of itself in terms of dissemination of scientific output, and also with the intention to generate industrial returns.

Technology Transfer can occur in many ways, including:

1. Publication of research results in academic as well as industry journals,

2. Licensing of proprietary technology (which is usually protected via patents or copyright) to private industry,

3. Spin-off of technology and knowhow into a start-up company,

4. Joint collaborations with industry in applied research and development of new techniques and products,

5. Training of scientists and technicians who then go on to work for private industry,

6. Direct training of workers via short courses, workshops, etc.

In 2008, the BSC-CNS mainly utilised mechanisms 1, 4 and 5. It is generally very difficult to patent advances in computer coding and chip design and this limits the opportunities to directly license or spinoff new supercomputing technologies.

The Operations Department in 2008 commenced offering training courses for both RES users and operators of RES nodes, and this program will expand further in 2009.

However the key mechanism of technology transfer adopted by the BSC-CNS remains joint collaboration and this is typically undertaken at both the system level, via direct collaborations with industry leaders such as IBM and Microsoft, and at the application level, where a significant research effort is dedicated to providing supercomputing based models for solving engineering problems in industrial sectors such as aerospace, transport, energy, medicine, geology etc.

IBM MareIncognito

An IBM-BSC joint research project towards a 10+ PF supercomputer, MareIncognito is a bilateral project with IBM under the umbrella of a memorandum of understanding, led by Mateo Valero and Jesús Labarta. It encompasses research in several fields related to supercomputing with the aim to define the technical characteristics and the design of components of interest for a new generation of Petascale supercomputers for the year 2011/12, involving all aspects related to that machine: applications, programming models, performance tools, interconnection and processor architecture, etc.

The MareIncognito Project
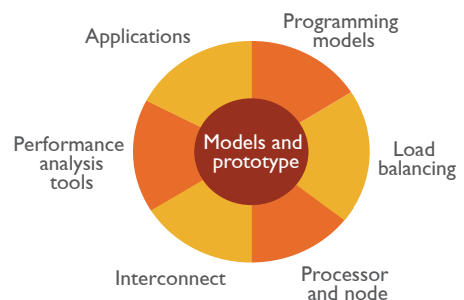
Kaleidoscope (Repsol)

The Kaleidoscope Project led by José María Cela is a "dream team" partnership of top geophysicists, computer scientists and organisations from around the world. It has been initiated by Repsol YPF, a Spanish integrated oil company with large assets in the US Gulf of Mexico, 3DGeo, a leading Houston-based imaging company formed by Stanford University professor and seismic imaging pioneer Biondo Biondi, and the BSC-CNS. The Kaleidoscope Project has privileged access through the BSC-CNS to Cell/BE based systems and technology because the BSC-CNS is one of the few research centres in the world developing libraries and codes for such processors.

The Kaleidoscope Project aims to produce more reliable and faster (by several orders of magnitude) software tools to analyse geo-seismic data and visualise below the thick layers of salt present in the Gulf of Mexico. This will significantly reduce exploration risks and make accessible oil reserves that otherwise would be invisible to the industry.

BSC-Microsoft Research Centre

The BSC-Microsoft Research Centre led by Osman Unsal, was established in April 2008 to focus on the way in which microprocessors and software for the mobile and desktop market segments will be designed and interact over the next 10 years and beyond. The advent of many- and multi-core processor computing architectures will make it possible to deliver enormous computational power on a single chip, with profound implications for the way software is developed. Optimising the design and interaction of hardware and software architectures to take advantage of the new computing power will require tight integration across the industry.

Computer architecture experts at BSC-CNS have teamed up with computer scientists at Microsoft Research Cambridge (MSRC) in the United Kingdom to look for innovative solutions to the challenges and opportunities that massively parallel processing represents. The vision of the centre is of a top-down computer architecture in which software requirements drive the hardware innovation forward rather than letting the hardware design condition software development. In addition to fundamental and applied research in transactional memory, a promising technology that facilitates writing of parallel programs for multi-core processors, hardware support for managed runtimes is being conducted in the initial research projects.

Other Industry Projects and Collaborations

Gas Natural

Goal: to study the impact of natural gas-powered vehicles on the air quality in Barcelona and Madrid.

Airbus

Goal: to improve its eLSA code (fluid dynamics) which was initially developed by ONERA in France and is currently used worldwide by Airbus.

Sun Microsystems

Goal: to propose techniques that allow better exploiting the capabilities of the massive multithreading processors in network servers.

CISCO Systems Inc.

Goal: To model multicore multithreaded architectures in typical network applications and estimate the performance of different architectures.

SGS TECNOS S.L.

Goal: The goal of this collaboration was to perform an impact assessment on the air quality from combined cycle power stations.

PB Power

Goal: to perform air quality modelling.

Gas Natural

Goal: perform air quality modelling.

BCNEcologia

Goal: to perform a simulation for the Air Quality Plan in Catalonia.

AEMET (The State Meteorological Agency)

Goal: to implement, disseminate and validate the operational prediction of the North African dust transport in the Iberian Peninsula as well as to perform modelling, detection, follow-up and characterization studies of atmospheric material.

# PRACE - Partnership for Advanced Computing in Europe

Background

The Partnership for Advanced Computing in Europe, funded in part by the EU's 7th Framework Programme, lays the groundwork for the creation of a persistent pan-European High Performance Computing (HPC) Service, consisting of several tier-0 supercomputing centres. Supercomputers are indispensable tools for solving the most challenging and complex scientific and technological problems through simulations. PRACE will create a top class HPC infrastructure which will be managed as a single European entity connected using grid technologies. Through PRACE, European scientists and technologists will be provided with world-class leadership supercomputers with capabilities equal to or better than those available in the USA and Japan.

Building a world-class pan-European HPC Service is a highly ambitious undertaking that involves governments, funding agencies, centres capable to host and manage the supercomputers, and the scientific and industrial user communities with leading edge applications. In contrast to Research Infrastructures that focus on a single scientific instrument an HPC Infrastructure has two unique characteristics: supercomputers serve all scientific disciplines and tier-0 supercomputers have a three year depreciation cycle as tier-0 implies leading edge services.

PRACE contemplates the collaboration of five Principal Partners, who will host the five Tier 0 supercomputing nodes, the European Union, and a number of General Partners (currently 13) who will contribute financially to the operating costs of the centres and an aggressive upgrade program that will see each centre upgraded on a 3-4 year cycle.
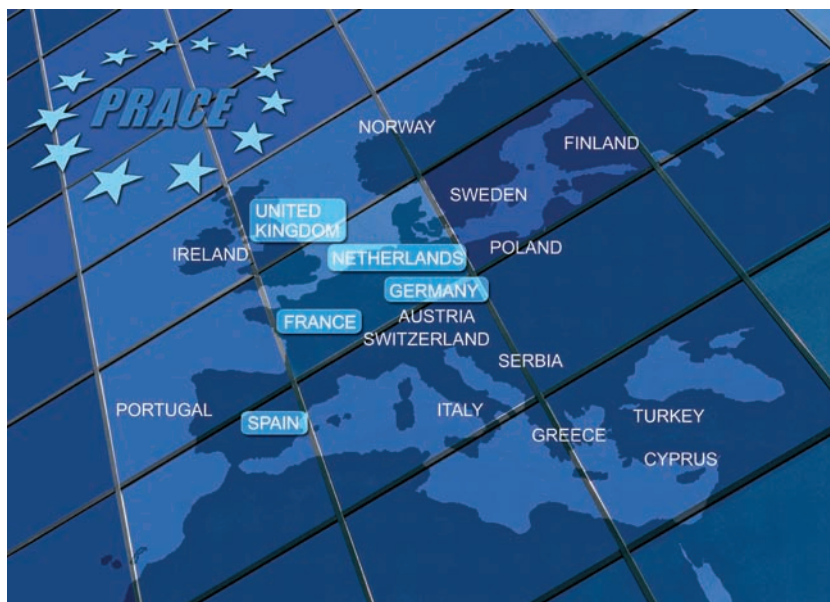
BSC-CNS and PRACE

The BSC-CNS is playing a leading role in the preparatory phase of PRACE which was launched in 2008, not only representing Spain within the consortium but also leading the main work package (Organisational Concept of the Research Infrastructure). The BSC-CNS will host one of the five Tier-0 nodes and is a key contender for the headquarters of the PRACE Infrastructure.

In November 2008, the Management Team organised the third all-hands Annual Meeting of BSC-CNS employees that took place at the Museo de Arte Contemporáneo de Barcelona (MACBA), situated in the city center of Barcelona. Around two hundred staff members participated in the event.

During the Annual Meeting, a number of senior Department and General Directors reviewed the year, presented the latest research results and also outlined the institute's objectives for 2009. The programme also included an external keynote speaker, **Maurici Lucena**, General Director of the "Centro de Desarrollo Tecnológico e Industrial (CDTI)" who spoke about the close relationship between science and industry. Following this an interactive session gave BSC-CNS staff the opportunity to ask questions about the organisation as well as to propose ideas to improve the centre.


The presentations were followed by an interactive information session where researchers detailed many of their activities and results obtained during the year. A poster session highlighting numerous research projects was also incorporated into the coffee break, providing further opportunities for researchers to learn more about the activities of other departments.

In the afternoon, attendees were invited to visit the photographical exhibition "Arxiu universal. La condició del document i la utopia fotogràfica moderna" together with a general visit of the MACBA Contemporary Arts Museum.

In 2008, the BSC-CNS undertook extensive planning for its new home, which will begin construction in 2009 and be completed in 2011.
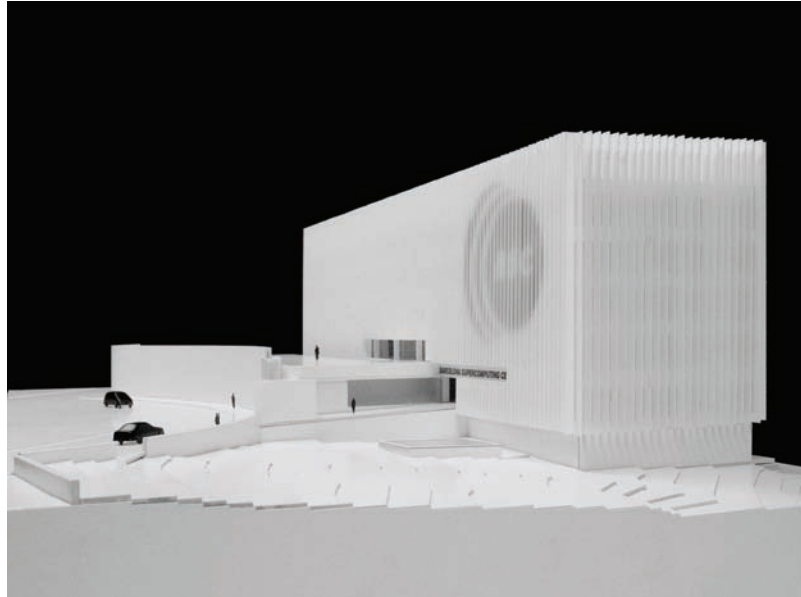
The MareNostrum supercomputer is housed in the Capella Torre Girona in Barcelona, however currently the majority of the management and research staff of the BSC are housed in several separate facilities belonging to the UPC and Consorci de la Zona Franca. A new building has been approved that will enable all the departments of the BSC-CNS to be housed under one roof.

Sectional Plan of the New BSC-CNS Building Showing Functional Areas

The Chapel Girona

The new building, which will commence construction in 2009 and will be located adjacent to the Capella Girona, has a dedicated section to host a future supercomputer even more powerful than the MareNostrum. The Operations Department has been heavily involved in the design of this new facility and will be responsible for its operation once the building is completed in 2011.

Covering 12.965m^2 with 3 levels below ground and 5 levels above ground, the building incorporates advanced features such as water recycling, automatic illumination to maximise use of natural light, and natural cooling to achieve a B-level energy efficiency rating.

The scientific mission of the Computer Sciences department is to influence the way computing machines are built, programmed and used, through demonstration and dissemination of ideas, collaboration with manufacturers and the development of new hardware, systems and applications by bridging computer architecture and application requirements.
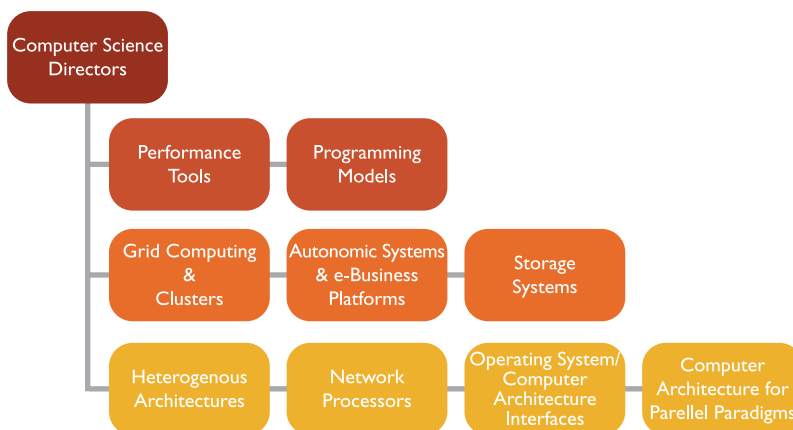

Jesús Labarta and Eduard Ayguadé,
Directors of the Computer Sciences Department

Overview

The Computer Sciences department, led by Jesús Labarta and Eduard Ayguadé is structured in 9 research Groups. Although each Group has its own specialised lines of research and unique projects, the teams often come together to collaborate on larger projects that require vertical integration, such as the MareIncognito project with IBM whose objective is to develop a prototype Petaflop supercomputer. This vertical interaction is considered critical to the quality and success of the research, as feedback between the different Groups enables application programmers to influence the direction of future systems architecture while better knowledge of architectures improves the design and implementation of novel programming models, execution environments and applications.
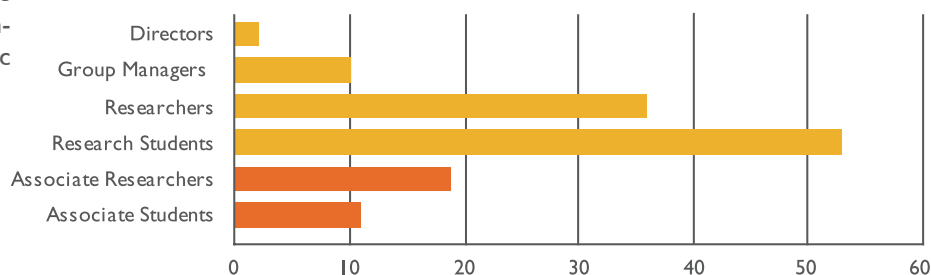
Unique Strength

The combination of broad coverage of all facets of computer systems design and programming along with in depth expertise in each area are somewhat unique amongst supercomputing centres. This unique strength of the BSC-CNS has attracted leading computing companies such as IBM and Microsoft to invest heavily in collaborative systems design R&D projects despite the relative youth of the Centre.

Organisational Structure

The Department has around 60 staff members with a similar number of collaborating researchers and students, organised in 9 research Groups; four focused on Computer Architecture (Parallel Paradigms, Network Processors, Operating System/Computer Architecture Interfaces and Heterogeneous Architectures), two focussed on improving productivity when developing parallel applications on large scale parallel systems (Programming Models and Performance Tools) and three focused on programming models and resource management middleware for distributed cluster and GRID architectures, including file systems (Storage Systems, Grid Computing and Clusters, and Autonomic Systems and e-Business Platforms).

Computer Science Directors

Performance Tools

Programming Models

Grid Computing & Clusters

Autonomic Systems & e-Business Platforms

Storage Systems

Heterogenous Architectures

Network Processors

Operating System/ Computer Architecture Interfaces

Computer Architecture for Parellel Paradigms

Computer Science Deptartment Staff & Collaborators 2008

|	
Directors	
Group Managers	
Researchers	
Research Students	
Associate Researchers	
Associate Students	

0   10   20   30   40   50   60

Key Projects & Networks

During 2008, the Computer Sciences Department participated in:

▶ 6 ongoing IST FP6 projects (ACOTES, BEinGRID, BREIN, SARC, SORMA and XtreemOS);

▶ 3 networks of excellence (HiPEAC, CoreGRID and HPC-Europa);

▶ The DEISA2 (Distributed European Infrastructure for Supercomputing Applications) consortium;

▶ Several research contracts with companies (IBM, Microsoft and Sun Microsystems);

▶ 2 new IST FP7 projects (MERASA and Velox) were initiated;

▶ Coordination of the Basic Research in Supercomputing section of the Spanish Consolider program "Supercomputing and eScience";

▶ The inauguration of the BSC-Microsoft Research Centre (www.bscmsrc.eu) in January 2008.

Computer Science Projects 2008
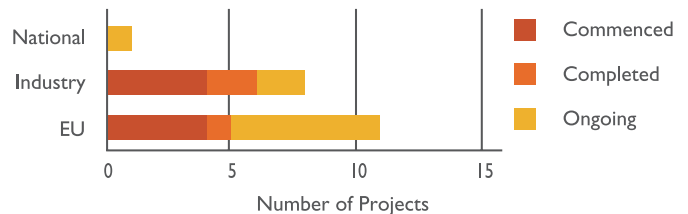
Scientific Output

Impacting the Future of Computing

In collaboration with market leaders such as IBM, Microsoft, Sun and Cisco Systems, as well as other international computing centres, the researchers of the Computer Sciences Department are involved in a range of projects covering the full spectrum of next generation computer design, from novel processor architectures, advanced video codecs, network scheduling, transactional memory, through to grid architectures and programming models. The results of their work are constantly being integrated into new specifications, systems and products.

The research results of the Department have been published in the proceedings of high quality conferences in the area, including International Symposium on Computer Architecture (ISCA), International Conference on Parallel Architectures and Compilation Techniques (PACT), International Conference on Supercomputing (ICS), International Conference on Parallel Processing (ICPP), Supercomputing (SC), International Parallel & Distributed Processing Symposium (IPDPS), International Symposium on High Performance Distributed Computing (HPDC) and International Conference on Cluster Computing (Cluster). All these are conferences ranked within the A+ and A tiers in the CORE (COmputing Research Education) conference classification and with high EIC (Estimated Impact of Conference) in the Computer Sciences Conference Ranking. In addition, other more consolidated research results have been published in prestigious journals in the area.

Communication & Dissemination 2008	
Publishing	
Journal Articles	13
Book Chapters	10
Books	0
Conference Presentations	
International	71
National	6
Workshops	
Workshops	25
Education	
Theses Read	9

Autonomic Systems and eBusiness Platforms Led by Jordi Torres, this Group performs high-level research in eBusiness applications and platforms executing on high-productivity multiprocessor architectures as well as distributed environments and new architectural proposals. Current trends in service computing are moving towards the creation of virtualized execution environments to run all kind of business applications. The goal is to create large pools of resources where users can run their computing tasks, independently of their nature. These kind of generic computing clusters are known as computing clouds. During 2008 the Group continued efforts to build a self-adaptive execution environment for cloud environments, participating in a number of EU projects (SORMA, Brein, CoreGRID and Xtree-mOS) and several areas of collaboration with IBM Watson.

Performance Tools Led by Judit Giménez, this Group is working on the design of tools to instrument, analyse and predict the behaviour of parallel applications on parallel systems. The main goal of the Group is to provide technology to understand the issues that determine the actual performance of a parallel application or that contribute to its bottlenecks. This is extremely important both in novel homogeneous and heterogeneous multicore architectures as well as in highly scalable cluster systems. The activities of the Group have focused in developing new features in the Paraver trace analysis tool (automatic analysis and sampling of traces) and tools integration (including multiscale simulation that mixes coarse-grain system simulation with instruction-level simulation). In November 2008 the Group started its collaboration on the DEISA2 project.

Programming Models Led by Xavier Martorell, this Group is researching new programming models and their efficient implementation for future architectures, ranging from multicore architectures (homogeneous and heterogeneous) to future exascale systems. The implementation for these programming models requires the development of compiler prototypes as well as intelligent adaptive runtime systems. The team explores the usability of these programming models in different application scenarios, proposing extensions to the standards to accommodate the requirements of novel applications for supercomputer systems. In 2008 the Group influenced the evolution of the OpenMP standard with the ideas behind proof-of-concept implementations (StarSs and NANOS) in direct collaboration with IBM (OpenMP for Cell and XL production compiler) in the framework of the MareIncognito project, and continued the development of programming models for distributed memory architectures, specifically in two directions; NanosDSM and PGAS (with IBM Watson). In addition, the Group is participating in the ACOTES and SARC European projects and coordinating the programming models cluster and applications taskforce in the HiPEAC network of excellence.

Grid Computing & Clusters Led by Rosa Mª Badia, this Group is researching new programming and execution models and resource management infrastructures for computational Grids. The team explores solutions in order to simplify application development, enable dynamic exploitation of parallelism at runtime and perform combined scheduling decisions at different levels. The efforts of the Group are focussed mainly in two projects, GRID superscalar and eNANOS. In addition, the Group is participating in a number of EU projects (CoreGRID, BEinGRID, Brein, OGF-Europe and XtreemOS) and international projects (LAGrid).

Storage Systems Led by Toni Cortés, this Group explores appropriate solutions to the scalability of parallel file systems in large installations (in which very large volumes of data need to be generated and accessed) and file systems for the grid that solve the problems currently found (data location, replication and striping) and that will make these environments more efficient. In 2008 the Group focussed on two areas; file system scalability and Input/Output for Grid systems. Within these, key efforts were the development of AdaptiveZ for heterogeneous storage systems, the application of COFS for composite file systems, and a number of improvements in the XtreemOS project, in particular related to its file system XtreemFS.

Heterogeneous Architectures Led by Àlex Ramírez, this Group, in close interaction with the Programming Models Group, aims to design and evaluate next generation multicore architectures composed of heterogeneous components with a dual purpose: to focus the developments on the actual needs of the applications and the runtime system, and to anticipate the needs of the runtime system for future architectures so that software can be ready when research trends become products. During 2008 the Group has continued its participation in a number of projects (SARC, MareIncognito, ACOTES) with key efforts in developing TaskSim for simulating large heterogeneous multiprocessor systems, parallelisation of video and bioscience algorithms, CellBE processor design and compiler technologies for heterogeneous architectures.

Computer Architecture for Parallel Paradigms Led by Adrián Cristal and Osman Unsal, this Group does research on architectural support to novel programming models and execution environments for novel multicore architectures. During 2008, the Group focused on development of complex transactional memory applications and the research and development of novel proposals for transactional memory (software and hardware). The Group constitutes the core of the BSC-Microsoft Research Centre which has mainly focused on lowering the programmability wall raised by new multicore architectures. In addition the Group has participated in and coordinated the European VELOX project.

Operating System / Computer Architecture Interface Led by Francisco Cazorla, this Group focuses on three main areas; Kernel/architecture interaction towards load balancing in high-performance computing applications, scheduling of network applications in massive multithreading processor architectures and multicore hard-real time systems. In 2008 the Group continued its work in the european MERASA project and HiPEAC network of excellence, and in the collaborations in topics related with massively multithreaded architectures with Sun (scheduling of tasks in network applications) and IBM (hardware thread priorities and power consumption).

Network Processors Led by Mario Nemirovsky, this Group is conducting research on the massive multithreaded architectures focused on L4-L7 network applications. The Group also analyses the exploitation of parallelism within network processing by improving current parallel programming models and workload management. During 2008 the Group prepared a major research collaboration with Cisco Systems (to commence in 2009) to investigate analytical models to overcome the problems of simulating different realistic network processing scenarios. The Group also participated in the HiPEAC network of excellence.

José María Baldasano, Director of the Earth Sciences Department

The Earth Sciences Department of the BSC-CNS has the aim of modelling and understanding the behaviour of the Earth System, focusing its research activities on atmospheric processes and climate change modelling.
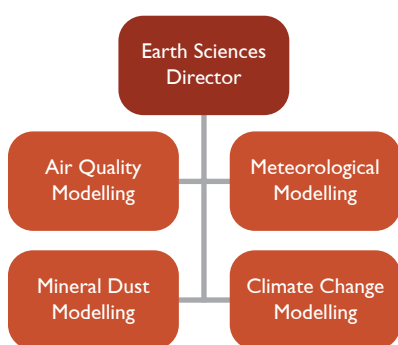
Overview

The high performance capabilities of MareNostrum enables the Earth Sciences Department to increase the spatial and temporal resolution of earth systems, in order to improve knowledge of dynamic patterns of air pollutants in complex terrains and interactions and feedbacks of physico-chemical processes occurring in the atmosphere. Also possible are analyses with high-resolution global circulation models (2°x2.5° to 1°x1°) and downscaling to regional models. This coupling of global and regional climate models will contribute to a detailed description of the impacts of climate change in complex regions.

The main topics of research are: 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 Spain (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 (www.bsc.es/projects/earthscience/DREAM).

The Department also collaborates with the World Meteorological Organization (WMO) and the Spanish Meteorological Agency (AEMet) in the creation of the Regional Center for Sand and Dust Storm Warning System (SDS-WAS) covering Europe, northern Africa and the Middle-East. Other research activities involve the diagnosis of the behaviour of Earth System Modelling (ESFM) codes in a supercomputer framework and the improvement of parallel versions of atmospheric models to increase their horizontal and temporal resolution.

Organisational Structure

Earth Sciences Director
- Air Quality Modelling
- Meteorological Modelling
- Mineral Dust Modelling
- Climate Change Modelling

Earth Sciences Deptartment Staff & Collaborators 2008

| Role	Count
Director	1
Group Managers	3
Senior Researchers	2
Researchers	2
Research Students	9
Technicians	3
Research Support Engineers	3
Associate Students	1
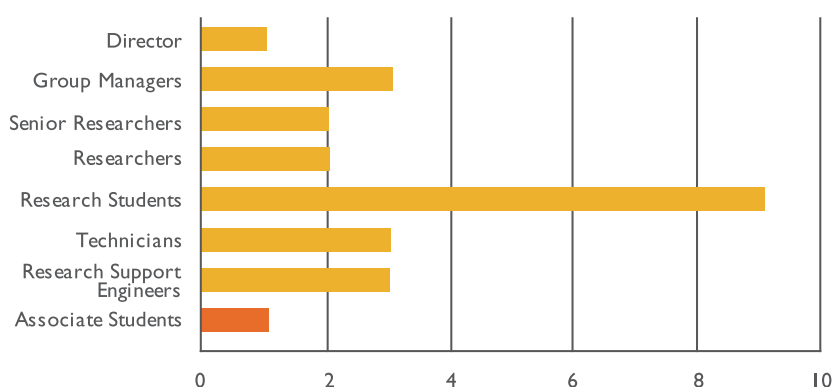
The Department is structured in four Groups that represent the main topics of Earth Sciences research: air quality modelling, mineral dust modelling, meteorological modelling and global and regional climate modelling. These Groups are interrelated and work in a cooperative form. They are led by a senior scientist and composed of a researcher, post-doctoral fellows and doctoral students. The technical support staff is shared by all the research Groups. During 2008 some 25 staff and collaborators worked with the Department.

Key Projects

▶ Completed and satisfactorily closed the diagnostic phase of the CALIOPE project, funded by the Spanish Ministry of the Environment, within the framework of the National Plan of I+D+i 2004-2007;

Earth Sciences Projects 2008

Legend: Commenced, Completed, Ongoing. Number of Projects.

▶ Coordinated the new forecast phase of the CALIOPE project, supported by the Spanish Ministry of the Environment, Rural and Marine within the framework of the National Plan of Scientific Research, Development and Technological Innovation 2008-2011;

▶ Extended the CALIOPE project to the Canary Islands, funded by Government of the Canary Islands;

▶ Led the Earth Science work package in the Consolider Program coordinated by the BSC;

▶ Supported by the Environmental Department of Catalonia Government (Spain), analysed the effects on air quality of introducing a speed limit of 80 km/h in the road network of Barcelona Metropolitan area;

▶ Initiated a new CICYT project: Coupling of a Fully Online Chemical Mechanism within the Atmospheric Global-Regional UMO Model funded by MICINN;

▶ Participated in the European Climate Change project: EC-Earth;

▶ Participated in the European Network for Earth System Modelling (ENES);

▶ Participated in the European Aerosol Research Lidar Network: EARLINET. The dataset generated is used to validate and improve models that predict the future state of the atmosphere and its dependence on different scenarios;

▶ Participated in AERONET (AErosol RObotic NETwork), an optical ground based aerosol monitoring network and data archive supported by NASA's Earth Observing System and expanded by federation with many non-NASA institutions;

▶ Actively contributed as a member of the Spanish network RETEMCA (Red Temática de Modelización de la Contaminación Atmosférica);

▶ Implicated in several projects of technology transfer, such as the participation in four EIAs for Modelling Air Quality of thermal power plants and incinerators.
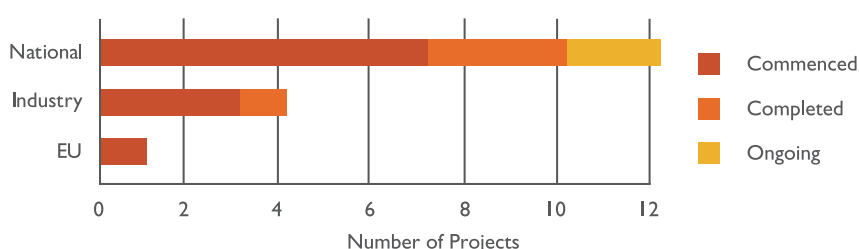
Scientific Output

The diffusion of research results obtained by the Earth Sciences Department has been noteworthy. These results have been presented in a numerous ISI-JCR journals, European and international congresses and symposia organised during 2008, such as the International Technical Meeting on Air Pollution and its Application supported by NATO, Harmonisation within Atmospheric Dispersion Modelling for Regulatory Purposes; American Union Geophysical, European Geosciences Union General Assembly Meeting and other congresses organized by the European Meteorology Society (EMS). The number of papers published increased from 51 in 2007 to 59 in 2009, and considerable augmentation of the number of ISI-JCR publications (from 3 in 2007 to 14 in 2008). The JCR publications have an average quality of 2,1 (average ISI Impact Factor) and were distributed over six subject categories, mainly in Geosciences (31%), Environmental Sciences (25%) and Meteorological & Atmospheric Science (19%).

Journal Publications by Subject
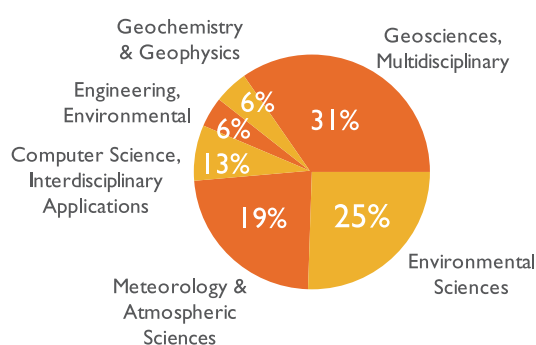
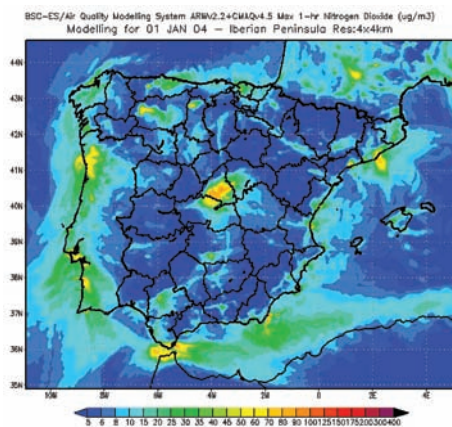| Communication & Dissemination 2008	
Publishing	
Journal Articles	18
Book Chapters	7
Books	0
Conference Presentations	
International	34
National	22
Workshops	
Workshops	9
Education	
Theses Read	1

Air Quality

Figure 1 - Air quality modelling system (WRF/HERMES/CMAQ/DREAM)

The Air Quality Group seeks to understand the dynamics of air pollution with the aim of obtaining a precise estimation of the air quality through high-resolution modelling, especially the relation between emissions, atmospheric transport, chemistry and deposition.

In order to understand the physico-chemical processes in the atmosphere that contribute to a decrease of air quality, an air quality modelling system with high spatial and temporal resolution (1–4km and 1 hour) that will take into account emissions of anthropogenic and natural pollutants, meteorology and chemistry is under development, implementation and validation. The system will provide end-users with an air quality forecasting and assessment service for Spain and Europe with higher detail for some hot spot areas (http://www.bsc.es/caliope). In 2008 the performance evaluation in a diagnostic phase was completed, and a forecast operational evaluation phase was then initiated.

Air quality models (WRF-ARW/HERMES/CMAQ) were improved (Figure 1) and were also used to assess the effects of hypothetical mitigation measures planned by the regional administration to ameliorate air quality conditions in urban areas, including the effects of introducing a speed limit of 80 km/h in the Barcelona Metropolitan area and comparing emission scenarios based on vehicle fleet composition of Barcelona and Madrid, differentiating by category (weight, age, fuel) and activity (taxis, public transport vehicles, etc).

Technology transfer activities were also undertaken with several companies and institutions (Inypsa, PB-Power, SGS, RESA, BCN-Ecología, Fundació CREAL, Gobierno de Canarias, DMAH, Puertos del Estado, Centro Regional-AEMET), strategies were developed for managing air pollution in large cities (Madrid and Barcelona) and the environmental impact of new industrial stack installations were analysed.

Climate Modelling

The Climate Modelling Group develops and tests regional climate downscaling models for the generation of high-resolution regional climate information from coarse-resolution global circulation models simulations.

In 2008 the activities were mainly related to the EC-Earth project, which aims to bring down the frontiers between weather and climate following a seamless prediction paradigm. EC-Earth is a joint initiative of several member state representatives (National Weather Services) of the European Centre for Medium-Range Weather Forecast (ECMWF). EC-Earth project aims to develop a global Earth System model consisting of a state-of-the-art atmospheric general circulation model, a state-of-the-art ocean general circulation model, a sea-ice model, a land model, and an atmospheric-chemistry model. Key activities in 2008 were porting code to MareNostrum, diagnosing the performance of the system in MareNostrum, and testing the model in high resolution (1x1 degrees). A 10-year preliminary simulation was run, of which some of the outputs can be observed in Figure 2.
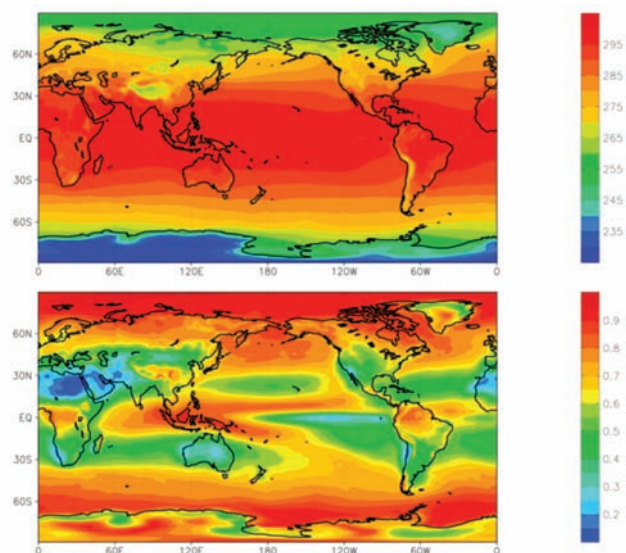

Figure 2 - Geopotential (up) and 2-m Temperature (down) Obtained by the Application of the T159L91 Experiment in MareNostrum

Meteorological Modelling

The Meteorological Modelling Group takes advantage of the computing performance of MareNostrum to study mesoscale phenomena, focusing on the improvement of the skills scores of numerical meteorological codes.

In the CALIOPE project, the WRF-ARW model was used to provide meteorological inputs for air quality modelling in the Barcelona area (1km resolution), Canary Islands (2km), Iberian Peninsula (4km) and Europe (12km). Additionally, the Group performed and evaluated high-resolution meteorological simulations for a selected year (2004) using European and national observations networks.

Together with the CASE Department, the Group continued development of new atmospheric codes capable of exploiting massively parallel architectures. First results are encouraging for the next steps towards the development of a new dynamical core for atmospheric modelling.

Figure 3 - Surface Incoming Shortwave Radiation (W/m2) at 12 UTC in Spain Obtained by the Application of the WRF Model on Marenostrum

Research in clean energy resources is also carried on. A solar irradiance forecasting system for Spain by means of numerical weather prediction is under development. The new system aims to provide useful short-term forecasts of solar irradiance for energy production from photovoltaic solar plants, and for improving the management of electrical grid networks.

At the end of the year, the Group started the development of a new on-line global/regional chemical weather prediction module in strong collaboration with the Mineral Dust Modelling Group. The system is based on a new multi-scale atmospheric model developed at National Centers for Enviromental Prediction (NCEP).
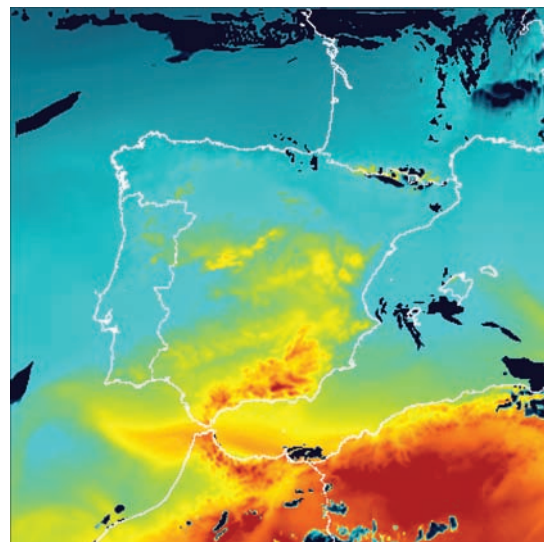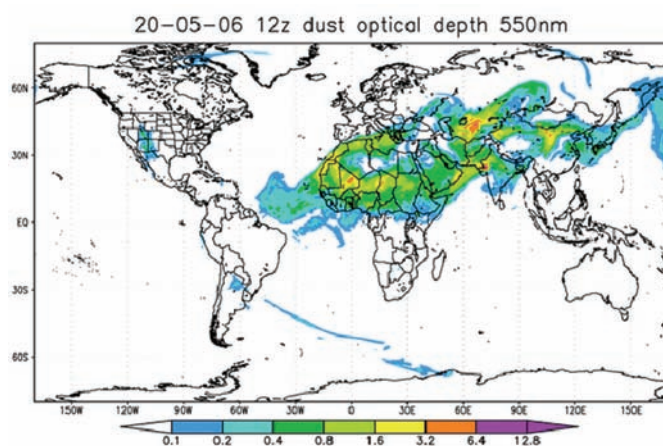
Mineral Dust Modelling

Figure 4 - First Simulations With the NMM/BSC-Dust Dust Modeling System on Marenostrum

The Mineral Dust Group provides daily operational forecasts of mineral dust for North Africa, Middle East, Europe and East Asia based on the Dust Regional Atmospheric Model (DREAM). In 2008 the Group developed a new generation atmospheric mineral dust model (BSC-Dust) coupled on-line to the new generation unified atmospheric model NMMb of the National Centers for Environmental Prediction (NCEP).

The new modelling system is intended to be a powerful tool for research and to provide efficient global and regional chemical weather forecasts at sub-synoptic and mesoscale resolutions on MareNostrum supercomputer (Figure 4) including a physically-based dust emission scheme taking into account the effects of saltation and sandblasting, soil moisture and viscous diffusion close to the ground.

The World Meteorological Organization (WMO) has launched the Sand and Dust Storm Warning and Assessment System (SDS WAS) that bridges the technological gap between research and operational services. Regional activities related to modelling, observations and applications are coordinated through the Asia/Central Pacific Regional Centre for SDS WAS at the China Meteorological Agency in Beijing, China. The Regional Centre for Northern Africa, Middle East and Europe is based at the BSC and the AEMet (Spanish Weather Service) in partnership with other operational and research organisations (e.g. ECMWF, MeteoFrance, LISA, LSCE, IFT, EUMETSAT, CNR, AERONET/PHOTONS).

Modesto Orozco,
Director of the
Life Sciences
Department

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

Overview

The Department benefits greatly from its unique situation in a major Supercomputer Centre, and also exists within a large and active environment of research in experimental biology. Its research program is tightly integrated in a collaborative effort with the Institute of Research in Biomedicine IRB-PCB-UB (Joint IRB-BSC Research Program on Computational Biology) and also has strong collaborations with ICREA and the National Institute of Bioinformatics (INB).

Major areas of research include Molecular Modelling, Structural Bioinformatics, Computational Genomics, Network Medicine, Subatomic Study of Protein Functions, and Protein-Protein Docking.

Joint IRB-BSC Program on Computational Biology

The agreement in 2008 for the creation of the Joint Research Program was a milestone in the development of computational biology in Barcelona. One of the major outcomes of the program was the establishment of an experimental laboratory (already employing 9 scientists) which facilitates the validation of models and simulations. Because the two departments are now tightly integrated, this report describes the combined effort of the Joint IRB-BSC program.

Organisational Structure

Life Sciences Director

- Molecular Modelling/ Bioinformatics Group
- Protein-Protein Interactions Group
- Electronic & Atomic Protein Modelling Group
- Computational Genomics Group
- Algorithmic Support for Computational Biology Platform
- Structural Bioinformatics/ Network Biology Group
- Experimental Bioinformatic Laboratory Platform

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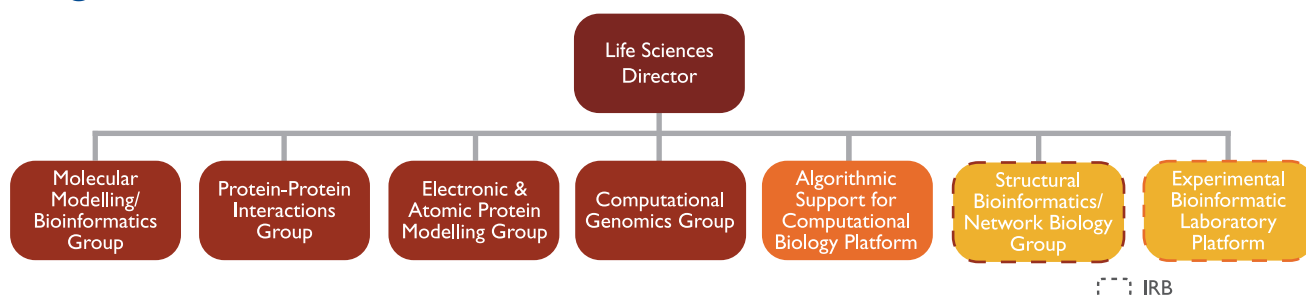
The structure of the Department and the technology platforms in its research program enables coverage of the entire field of Computational Biology, from atomistic detail to holistic views of the entire ecosystem. The Groups integrate different independent researchers led by senior scientists who work in different aspects of computational biology. The Department continues to grow strongly, from 37 staff and collaborators in 2006, to 53 in 2007, to 64 in 2008.

Life Sciences Department Staff & Collaborators 2008

Category	Value
Director	1
Group Managers	4
Researchers	20
Research Students	14
Software Engineers	7
Technical support	1
Associate Group Manager	2
Associate Laboratory	3
Associate Students	8
Associate Researchers	8
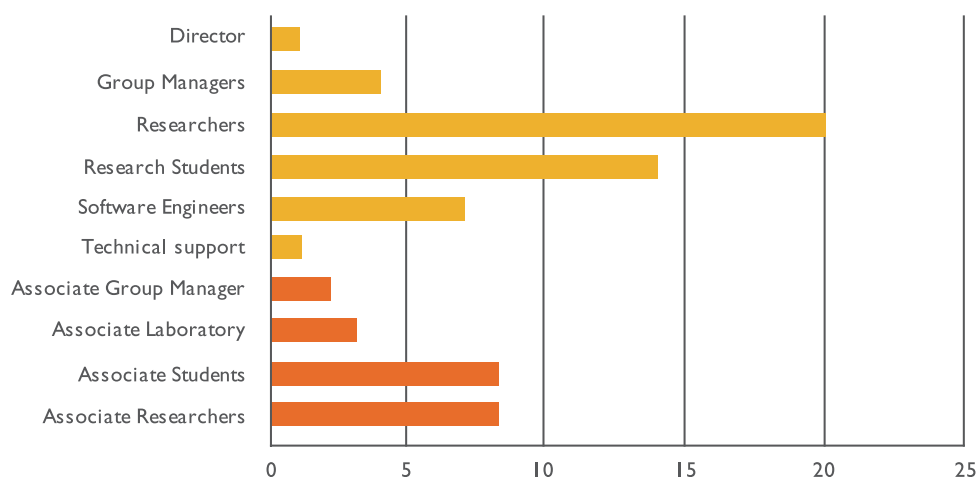
EU & National Projects

- Continued collaboration with the DEISA project,
- Successfully passed a 3-year-evaluation by Genoma España of the BSC-nodes at the INB,
- Assumed responsibility for the "feasibility package" of the ELXIR project, which will define the EU bioinformatics road-map for the next decade,

Life Sciences Projects 2008

- Leadership of the Bioinformatics package in the Consolider Program coordinated by the BSC,
- Participated in the Computational Biomedicine Research Network funded by the Instituto de Salud Carlos III.
- Assumed responsibility for collecting and processing data in the IMID-KIT project where the BSC collaborates with the National Genotyping Facility (CEGEN), various Hospitals and the INB in determining the genetic roots of rheumatoid arthritis,
- Leadership of the Bioinformatic package in the Consolider Program coordinated by the BSC,
- Supported the Metagenomics of the Human Intestinal Tract (MetaHIT) EU project led by EBI-EMBL for the characterisation of peroxysomal metabolome.
- Involved in a number of other key projects, funded by the EU and MICINN on a new network-based approach to treat diabetes, obesity and ageing-related pathologies.
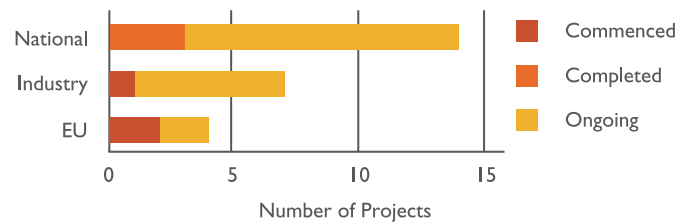
Internationally Active
During 2008, the Department hosted 10 prestigious international scientists for periods greater than 1 month. Over 20 international collaborations resulted in publications.

Internationally Competitive
Less than 14% of BSC-IRB staff are paid by core funds. All Group Leaders are fully funded by competitive grants and groups have won committed competitive grants exceeding 4.6 million.

Scientific Output

The research results of the Department have been presented in a large number of scientific publications, presentations to congresses and conference lectures. The number of papers published increased from 38 in 2007 to 53 in 2008, while maintaining the average quality, measured as an average ISI Impact Factor of 5,4.

ISI Impact Factor of Published Articles 2008
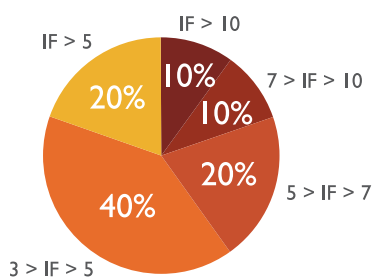
Communication & Dissemination 2008	
Publishing	
Journal Articles	53
Book Chapters	0
Books	0
Conference Presentations	
International	0
National	0
Workshops	
Workshops	2
Education	
Theses Read	5

Molecular Modelling and Bioinformatics Group

Led by Modesto Orozco, the long term objective of this Group 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. The research effort is focused in three major areas: i) study of small model systems, ii) analysis of stressed or unusual nucleic acids and iii) dynamics of proteins.

Protein Interaction and Docking Group

Led by Juan Fernández-Recio, this Group aims to study the mechanism and function of proteins in living organisms, with a special focus on the biomolecular interactions at atomic and residue level. Proteins interact to form highly specific complexes that are fundamental for the majority of cellular processes. The prediction and characterization of such complexes has enormous interest, both at academic level and from a practical point of view. The ultimate scientific goals are: to understand the mechanism of protein-protein association, and to design molecules capable of targeting protein interactions of biomedical interest. The major research areas are: i) development and optimization of protein docking tools, ii) development of new tools for protein structure and function predictions and iii) modelling protein interactions of biological and therapeutical interest.

Electronic and Protein Modelling Group

Led by Victor 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. During 2008 the Group continued its research in two key areas: i) Classical simulations using approximate analytical potentials to describe the nuclear energy landscape and ii) Quantum chemistry simulations of electron transfer processes in proteins.

Computational Genomics Group

Led by David Torrents, the ultimate goal of the research in this Group is the identification and understanding of the molecular and evolutionary processes that determine the biology of genomes, and also the biomedical implications that derive from its malfunction. Increasingly, together with the generation of new genomic sequences, there is a massive and automatic production of functional data associated with these sequences. Based on these datasets and also on detailed experimental data, the Group applies computational approaches to identify, classify and analyse functional genomic regions and regulatory associations between the components of defined biological systems. The key research lines of the Group are: i) function prediction of regulatory regions in vertebrates, ii) identification of regulatory modules of transcription binding sites conserved in cancer genes.; and iii) computational modelling of human complex diseases: diabetes and obesity.

Structural Bioinformatics and Network Biology Group

Led by Patrick Aloy, IRB, the main scientific interests of this Group are in the field of structural bioinformatics. In particular, on the use of protein sequences and high-resolution 3D structures to reveal the molecular bases of how macromolecular complexes and cell networks operate. Special emphasis is made on the molecular characterisation of pathological pathways. The main projects carried out for the Group during 2008 have been: i) incorporating high-throughput proteomics experiments into structural biology pipelines, ii) the analysis of contextual specificity in peptide-mediated protein interactions, iii) exploiting gene deletion fitness effects to understand the modular architecture of protein complexes under different growth conditions and iv) towards a molecular characterization of Alzheimer disease network.

Algorithmic Support for Computational Biology Platform (ASU-INB Computational Node)

Led by Josep Lluis Gelpi, the platform´s main purpose is to facilitate access to biological databases and programs by the bioinformatics community and to support the research Groups in the program. One of the main activities of the node is to coordinate the computational node of the Instituto Nacional de Bioinformática (INB-GN6). The internal structure of the node consists in two subteams: i) external projects support engineers which are assigned to the INB supported projects and help in the implementation and optimization of users' applications in the supercomputing environment, and ii) the Web Services and Database development subteam, which is in charge of building web services and web interfaces and create and manage biological databases. During 2008 the ASU has provided external support to the Bioinformatics community in areas such as molecular dynamics simulations, protein-protein interactions and computational genomics. Especially relevant in this area is the collaboration into the IMIDKIT project, where the unit is in charge of creating and managing the epidemiology database.

Experimental Bioinformatics Laboratory Platform

Led by Montse Soler, this platform was established in January 2008 as part of the IRB-BSC collaboration. The platform is dedicated to implementing advanced experimental approaches that provide computational biologists in the program the opportunity to integrate experimental measurements into their predictions. The most important activity during 2008 was the set-up of the experimental laboratory, which is now fully equipped enabling more than 10 people at a time to work in the areas of systems biology (protein-protein interaction networks) and genome regulation.

José Maria Cela, Director of the CASE Department

The aim of the Computer Applications in Science & Engineering (CASE) Department is to identify, engage and support user communities in science and engineering that are potential users of High Performance Computing, boosted by its own research lines in High Performance Computational Mechanics.

Overview

The applications developed by the CASE department are truly multidisciplinary, requiring depth of expertise in many fields. In order to successfully develop these applications, the skills of the CASE team in numerical methods and parallel programming must be complemented by experts in appropriate areas. The Department therefore develops collaborations with other scientific groups, especially those with expertise in areas which the BSC-CNS Groups do not have extensive experience. Examples include CIEMAT, CSIC, IAC, ICFO and different universities.

Major research areas are ab-initio DFT and TDDFT molecular dynamics, plasma core and edge transport, plasma wall interaction, biomechanics, geophysics, atmospheric flows and CFD.

Organisational Structure

CASE Director

Physical & Numerical Modelling

High Performance Computational Mechanics
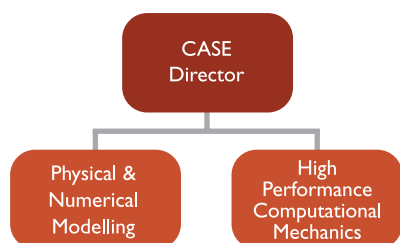
CASE Department Staff & Collaborators 2008
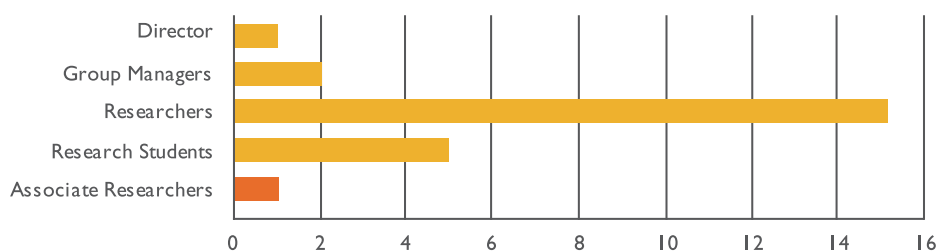
The CASE Department is led by José María Cela, and although there is high interactivity amongst all the scientists in the Department, the research lines fall naturally in two main Groups; Physical & Numerical Modelling (PNM) and High Performance Computational Mechanics (HPCM).

Each Group consists of 8-10 people at any given time, comprising several senior scientists, post and pre-doctoral students and visiting scientists. PNM research lines are horizontal and HPCM lines are vertical, in the sense that the PNM Group is in charge of developing the core components which are then assembled and modified as required by the HPCM Group into applications tailor-made to meet specific project needs.

Key Projects

In 2008, the CASE Department carried out work under the scope of the following projects:

EU funded projects

▶ EUFORIA: Generating a software infrastructure for support of the ITER design community. In 2008 several codes were tuned: BIT1, EIRENE, GENE, ELMFIRE.

▶ ETSF: Generating a software infrastructure for support of the spectroscopy community, in particular work was undertaken on the scalability of OCTOPUS.

▶ W2PLASTIC: Magnetic Sorting and Ultrasound Sensor Technologies for Production of High Purity Secondary Polyolefins from Waste. The physical problem to be simulated was modelled.

▶ DEISA: Continued collaboration, leading work packages 5 and 9.

▶ PRACE: Several codes (ALYA, BSIT, CPMD, EUTERPE) were analysed and tuned for PRACE prototypes.

Enterprise funded projects:

▶ Kaleidoscope (REPSOL): With the goal of developing the most powerful seismic imaging tools, an RTM application 10 times faster than any other implementation was developed.

▶ MareIncognito (IBM): Leading work package 1 for applications porting, some codes (such as SIESTA) were scaled for the MareIncognito architecture.

Nationally funded projects:

▶ Supercomputación y e-Ciencia (CONSOLIDER): Coordination of the project, whose aim is to develop a set of scientific Grand Challenges for Petaflop supercomputers and design the architecture of those machines. Some of the applications were also developed with the collaboration of CASE researchers.

▶ OPTIDIS (Plan Nacional): This project was completed in 2008 with a software prototype for optimal design of building ventilation using CFD tools.

▶ CDTEAM (CENIT): Designing a cardiac simulator. The cardiac electrical model was completed and the development of the mechanical model was initiated.

The CASE department also develops two international collaboration projects in the area of biomechanics:

▶ Airflow in the Human Nasal Cavity: In collaboration with both the Aeronautics and Bioengineering Departments at Imperial College London. A complete simulation of the Human Nasal cavity airflow was obtained with a speed-up of 500 compared with commercial codes.

▶ Cerebral Hemodynamics Model: In collaboration with the CFDLab George Mason University, USA, the Krasnow Institute for Advanced Studies, George Mason University, USA, the Inova Fairfax Hospital, Virginia, USA, the National Center for Computational Biology, UCLA, USA and the Brain Research Institute, Melbourne, Australia. A deflated preconditioner with conjugate gradient solver was used to accelerate the pressure solver in this simulation. A speed-up of 10 with respect the original solver was obtained.

Scientific Output

Although a large part of the Department's work is private and in/confidence and therefore cannot be published, some important research results of the Department have been presented in congresses and conference lectures well as a number of scientific publications, including: WCCM8 and ECCOMAS 2008 in Venice, SEG International Exposition and 78th Annual Meeting in Las Vegas, International Conference on Mathematics and Continuum mechanics in Porto, Architecture ISCA2008 - WCSA2008 in Beijing, as well as the Grand Challenges in Computational Biology - Joint BSC-IRB Barcelona Conference in Barcelona.

CASE Projects 2008

Number of Projects
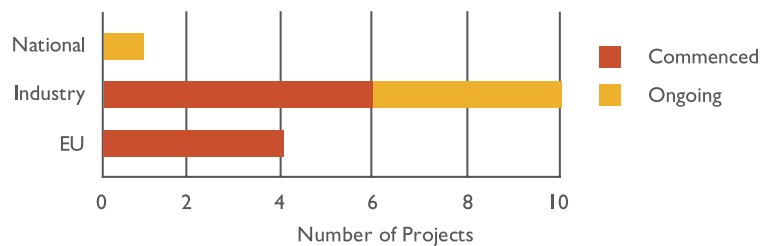
Communication & Dissemination 2008	
Publishing	
Journal Articles	2
Book Chapters	0
Books	0
Conference Presentations	
International	15
National	4
Workshops	
Workshops	0
Education	
Theses Read	0

Physical and Numerical Modelling (PNM)

The PNM Group researches basic themes, such as numerical modelling of physical phenomena, stabilisation techniques, algorithms and solution strategies, parallelisation strategies, coupled problems with domain decomposition methods, optimisation algorithms and error estimation techniques. In addition, PNM researchers investigate pre-process, post-process, data management and visualisation topics.

The research lines within PNM cover the full range of techniques required to simulate a physical problem, usually governed by partial or ordinary differential equations. The main areas of investigation are:

Car Engine Intake

▶ Mathematical modelling of a given physical process;

▶ Numerical modelling of the mathematical equations - space and time discretisation: high order time integration schemes; variational multi-scale; finite element; domain decomposition (Chimera, non-overlapping meshes); turbulence models; PIC methods; Spectral methods.

▶ Numerical algorithms to solve the discrete equations 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 parallelisation with MPI/OpenMP, code optimisation; architecture dependent implementation (VMX, Cell);

▶ Code performance analysis and optimisation.
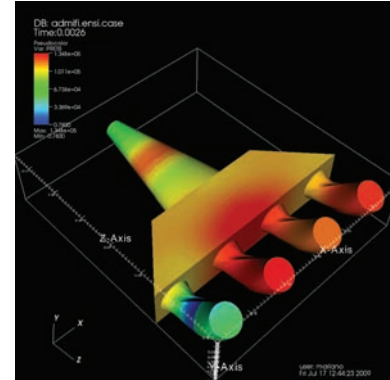
Within these areas, in 2008 the PNM Group developed:

▶ A parallel deflated preconditioner for incompressible fluid problems.

▶ Linelets pressure preconditioner for atmospheric flows.

▶ Low Mach preconditioner for compressible flows.

▶ Orthomin(1) iterative solver for the pressure Schur complement problem.

▶ Automatic mesh generation facilities for different problems: Atmospheric flows with real topography, supersonic flows, etc.

▶ Automatic surface remeshing.

▶ Anisotropic semi-structured volume mesh generation.

Wind Streamlines Over Sant Antoni Quarter, Barcelona

▶ Adaptive Cartesian mesh generation.

▶ Edge base formulation for compressible flows.

▶ A domain decomposition Chimera scheme for different fluid problems.

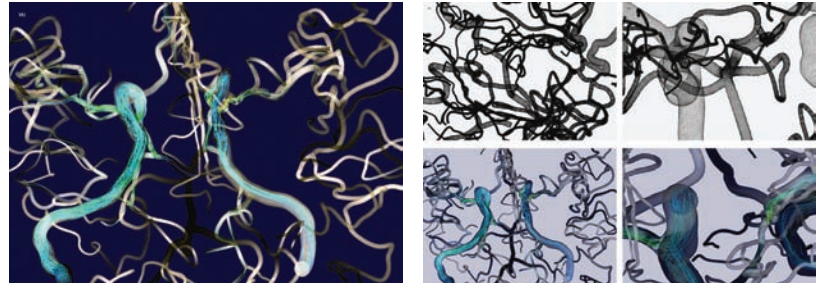▶ Variational multiscale scheme for compressible fluids.

High Performance Computational Mechanics (HPCM)

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

The activities of the HPCM Group are driven by direct interaction with users and industry. Usually the core problem requires modelling of physical processes which then must be solved by intensive numerical calculation. The principal application fields that have been developed to date are:

Brain Hemodynamics

▶ Bio-mechanics: Hemodynamics, respiratory system air low, cardiac simulation

▶ Geophysics: seismic imaging and oil reservoir simulations.

▶ Plasma Physics

▶ Atmospheric flows

▶ Energetically Efficient Building Design

▶ Ab-inito DFT and TDDFT molecular dynamic simulations

▶ CFD: subsonic and supersonic flows, free surface problems, coupled problems

Within these fields, in 2008, the HPCM Group developed:

▶ An anisotropic cardiac activation potential propagation simulation.

▶ An arterial brain hemodynamics simulation.

▶ A superior human airways simulation.

▶ An RTM seismic imaging facility on Cell processors.

▶ A hybrid openMP-MPI PIC code for plasma simulations.

▶ A dynamic atmospheric mesoscale parallel code.

▶ A parallel version of SIESTA code with better load balancing and sparse iterative eigensolvers.

▶ Free surface parallel solver for sailing boats.
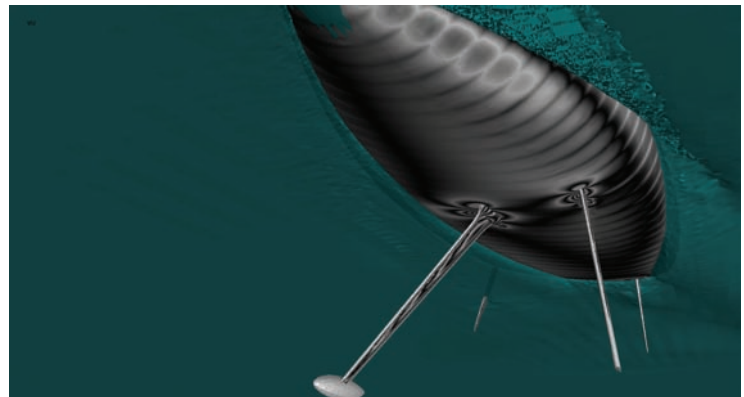
Sailing Yacht Hydrodynamic

The key mission of the Operations Department is to ensure the continued availability and accessibility of RES systems 24 hours a day, 7 days a week and to provide support to all the users of the RES.

Further core objectives are to manage upgrades to the MareNostrum and other RES nodes; facilitate access to RES facilities, including online electronic applications, remote access, and porting of code; manage the environmental aspect of the BSC-CNS installations; manage the technical aspects of integration of the MareNostrum in the DEISA and European HPC network grids; and ensure that RES staff receive appropriate training and skills development in order to be able to professionally carry out their duties in an environment of constant technological change and advancement.

Sergi Girona, Operations Department Director

Overview

The Operations Department led by Sergi Girona, ensures the continued daily functioning of the RES supercomputers and remote access by users both within Spain and internationally. In addition to all the routine maintenance and operations tasks, the Department's staff is also heavily involved in planning and design of new systems and support facilities. Additionally, the entire Department participates in European projects such as DEISA2, PRACE and HPC-Europa.

The constant upgrading and utilisation of cutting edge technology implies that staff within the Department, liaison staff at the RES nodes and scientific users all face continuous change in systems and procedures. The management of these changes and their dissemination to all who may be affected by them are also regular activities of the Department.

Organisational Structure

```
          Operations
           Director
              |
      ┌───────┴───────┐
   User            System
  Support       Administration
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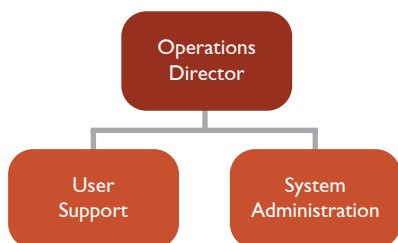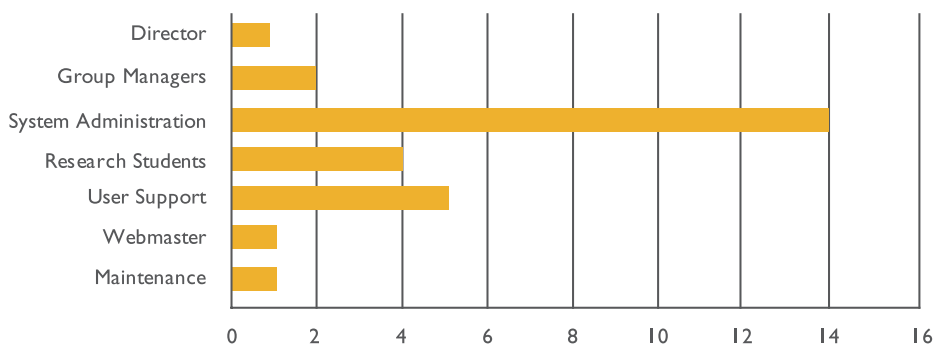
The Operations Department is structured in two divisions, System Management and User Support.

Systems Management supervises the daily operations of two key resources, the MareNostrum Supercomputer and the Spanish Supercomputing Network (RES), bearing responsibility for system administration, security, resource management, networking and helpdesk. This Group also takes care of running all the other IT equipment installed at the BSC-CNS and related facilities.

User Support is responsible for direct user support providing detailed knowledge of programming models, libraries, tools and applications, and also is responsible for management of the BSC website, including the electronic management of access applications.

Operations Department Staff & Collaborators 2008

| Category	Value
Director	1
Group Managers	2
System Administration	14
Research Students	4
User Support	5
Webmaster	1
Maintenance	1

System Administration

The System Administration Group is responsible for general operation, upgrades and maintenance of the MareNostrum and other BSC-CNS systems, as well as providing technical support to the operators of the other RES nodes. The Group also undertakes numerous special projects for continuous improvement of BSC-CNS systems and services and provides technical support to key research projects.

MareNostrum Performance 2008

Weekly Use of the MareNostrum in 2008
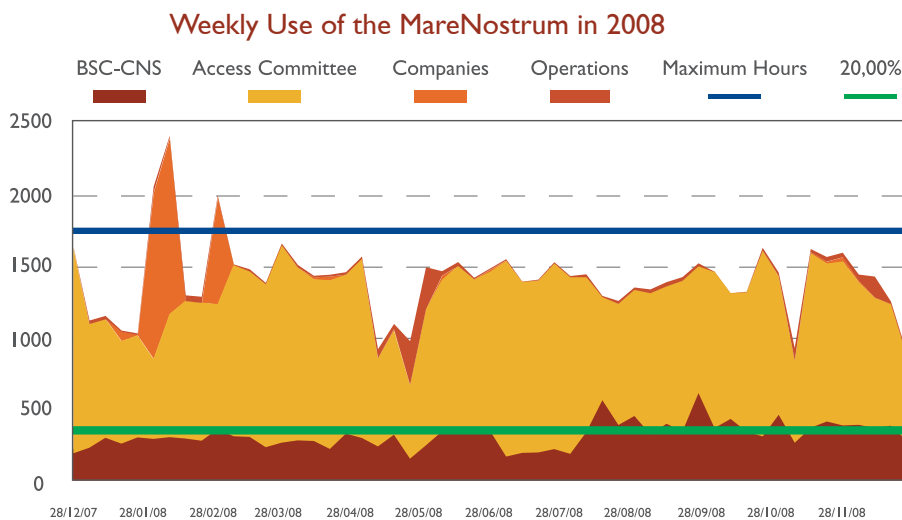
MareNostrum has been in production the whole year, except for the scheduled maintenance periods.

Using the remaining part of the year as the basis for calculations, the observed system utilisation is approximately 80%.

Utilisation is defined by the formula:

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

Training and Seminars

The Operations Department organises two kinds of seminars for the RES – technical and scientific. In the technical seminars engineers share knowledge and experience, for example with manufacturing companies in order to inform attendees about their products, technical processes etc. During 2008 RES organised the following technical seminars:

RES Seminar, 2009

▶ User Support Workshop for RES Administrators
(16, 17 January 2008)

▶ Moab Workshop - Cluster Resources & BSC
(11, 12 March 2008)

▶ RES User Training - optimization and debugging
(21, 22 April 2008)

▶ MareNostrum supercomputer and ITC installation
(20 – 22 October 2008

The objective of the scientific seminars is to inform the scientific community about the advantages of supercomputing using studies and calculations. In 2008, one such seminar was organised in Barcelona with more than 70 participants from different scientific backgrounds.

Key Projects and Upgrades 2008

Myrinet protocol change in MareNostrum The Myrinet (high speed, low latency and non-blocking) network in MareNostrum connects all 2560 JS21 blades and it is responsible for the MPI communications of the applications that are running in MareNostrum. The software and driver for the myrinet network was fully changed from GM to MX in MareNostrum during 2008. The GM and MX systems provide protected user-level access to the Myrinet (secure in multi-user, multiprogramming environments); reliable, ordered delivery of messages; network mapping and route computation; and other features that support robust and error-free communication.

Installation and setup of a new RES node The Instituto Tecnológico de Canarias (ITC) acquired in 2008 a cluster composed of 84 JS21 blade nodes from IBM. This cluster was installed and physically integrated into the RES network by the Systems management team.

In parallel with the installation of the cluster a technical seminar was developed for Canarias staff to demonstrate the day to day operational tasks of the supercomputer as well as all the tools necessary for the integration of the new supercomputer node into the RES infrastructure.

The new ITC node

Installation and setup of the MariCel - PRACE Prototype The BSC-CNS, as a principal partner of PRACE, hosts one of the six prototypes for petaflops systems. The experimental machine, which has been named MariCel, was installed during the second half of 2008. The prototype specification is based on QS22 blades from IBM, for a peak performance of 15.6 Teraflops and a power consumption of 20kW.

Upgrade of the Altix shared memory system In 2007, BSC installed an SGI Altix 4700 shared memory system, allowing researchers to perform specific pre and post-processing analysis that require large shared memory systems. The system was upgraded twice in 2008, doubling its computational capacity, and increasing by 5 its memory capacity, enabling researchers to perform more complex analysis and work with larger data sets.

Installation of a new centralised authentication / authorisation system A new Network Access Control (NAC) and a custom user database for management of the system were installed at the BSC-CNS during 2008. This NAC provides a unique technology to access BSC-CNS resources from internal and external networks with high security.

Schematic of the new NAC
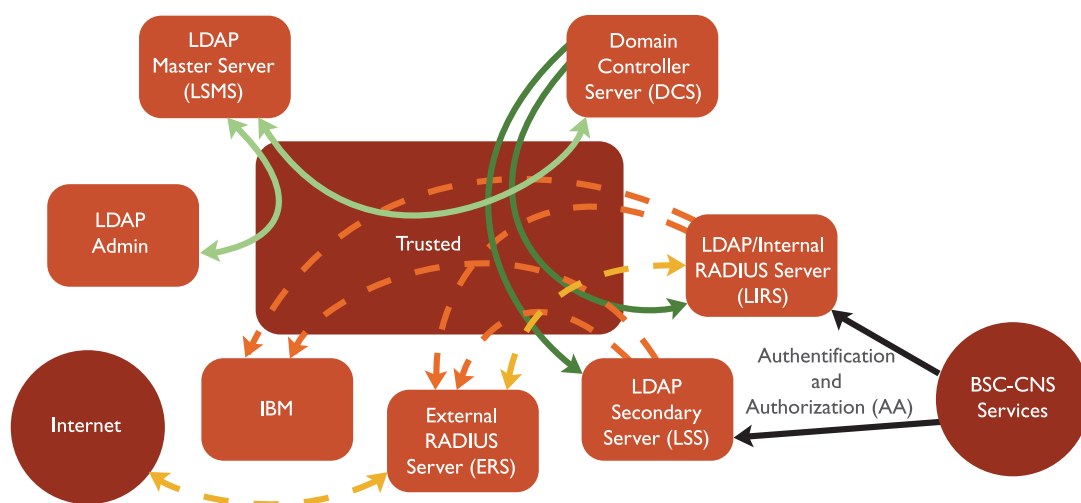
Upgrade of the Samba Data and BBDD storage platform The Samba platform of storage servers was upgraded to the latest version. This upgrade allows clients with the latest Samba version to take advantage of new Samba features, such as password encryption and the use of new transport protocols.
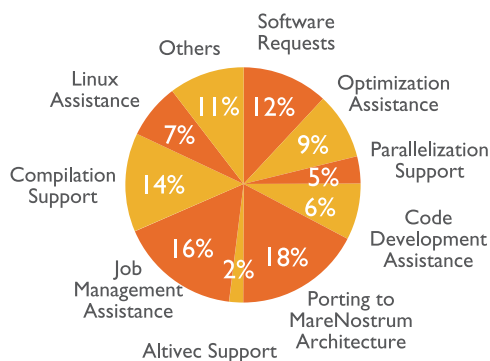
User Support

The User Support Group provides assistance with all aspects of scientific computing, this assistance includes general user support, code optimization, parallel model building support and porting serial and parallel codes for supercomputers such Mare-Nostrum. 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.
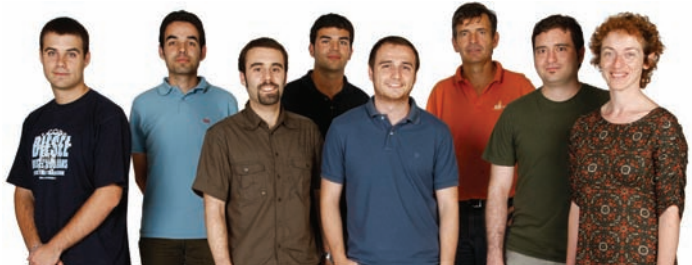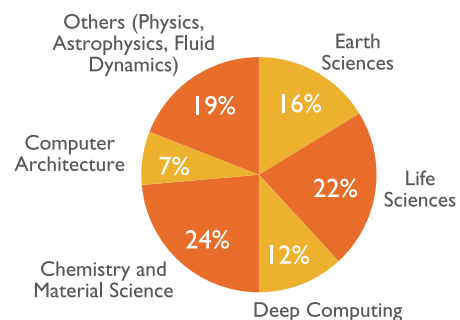
Support Requests in 2008

The number of support requests received in 2008 was 5007 and these are presented in the figures below split by support request topic and by scientific area.

User Support Requested by Topic 2008

Software Requests — 12%
Optimization Assistance — 9%
Parallelization Support — 5%
Code Development Assistance — 6%
Porting to MareNostrum Architecture — 18%
Altivec Support — 2%
Job Management Assistance — 16%
Compilation Support — 14%
Linux Assistance — 7%
Others — 11%

User Support Requested by Scientific Area 2008

Others (Physics, Astrophysics, Fluid Dynamics) — 19%
Earth Sciences — 16%
Life Sciences — 22%
Deep Computing — 12%
Chemistry and Material Science — 24%
Computer Architecture — 7%

Establishment of the BSC-CNS Intranet

In 2008 the support Group established a new intranet for the BSC-CNS, providing a standard way of disseminating internal information to employees and collaborators locally and in remote offices worldwide. Examples of such information include employee handbooks, technical documentation, technical announcements, corporate policies and medical insurance instructions. The number services provided through the intranet are very heterogeneous and a continuous improvement program is planned.

The key mission of the Management Department is to optimise coordination of the activities of the BSC-CNS and provide consolidated planning and management of support services to better meet the future challenges facing the centre.

Ernest Quingles, Management Department Director

Other core objectives include reliable and timely financial reporting, human resources management, and building awareness of the BSC-CNS, its mission, activities and its services. The department also assists other departments in identifying, applying and managing competitive projects, initiating and developing systems and processes to increase the efficiency and effectiveness of staff and the quality of work, and developing electronic management tools.

Overview

The Management Department, led by Ernest Quingles and supported by Mercè Calvet, was formed in 2007 as part of the internal reorganisation of the management structure of the BSC-CNS. During 2008 this structure was further consolidated and roles and processes were more clearly defined.

The constant changes at the BSC-CNS arising from its rapid growth, ever-expanding project portfolio, the temporary nature of working facilities pending the dedicated BSC building and the changes in technology and systems that accompany each upgrade cycle, make for a very dynamic environment with often intense and urgent requirements. The Department therefore aims to maintain a certain degree of flexibility and multi-skilling amongst its staff and encourages them to work closely with each other and their key points of contact in other departments.

Organisational Structure

Management Director

Finance & Business Administration

Project Management

Marketing & Communication
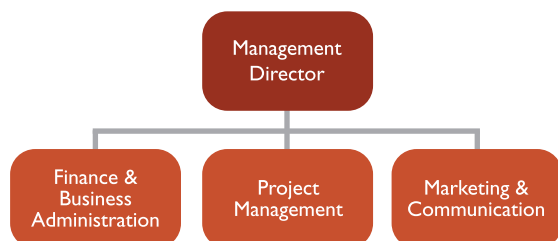
The Management Department is structured in three units; Finance & Business Administration provides three key services: Human Resources, Finance and Accounting, and General Administration Support, the Project Management unit is responsible for managing projects and technologies, identifying opportunities, initiating and managing project proposals

Management Department Staff & Collaborators 2008

Unit	Count
Director	1
Group Managers	1
Projects & Tech. Transfer	6
Marketing & Communication	3
General Administration	2
Direction Secretarial	2
Finance & Accounting	3
Human Resources	2

funded by public scientific calls as well as by industry sponsored research contracts, the Marketing & Communication unit is responsible for all activities related to the corporate image such as communication (media), events management, public visits to the MareNostrum supercomputer, dissemination of activities and results to academia and industry and promoting science in society.
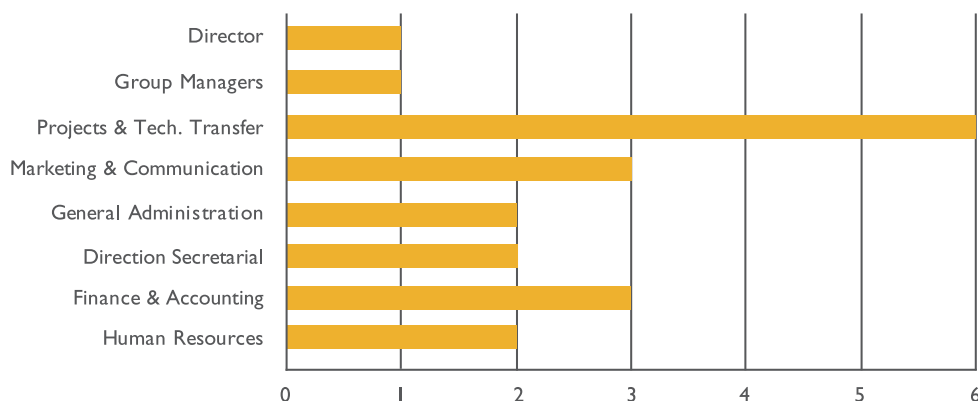
Finance and Business Administration

In 2008 the key focus of the Finance & Business Administration unit was on improving internal management and reporting systems to better support the rapid growth in research projects and to facilitate the integration of new staff and visitors from local universities, and national and international mobility programs.

Finance & Accounting

The Finance & Accounting service is responsible for the financial resources management of the BSC-CNS (expenses, budgets, audits, bank relations, suppliers, receiving payments and budget deviations). The Group also prepares the financial reporting for project audits, working closely with the Project Management Group, and the Marketing & Communication team in preparing budgets. In 2008 planning commenced for a series of new budgeting tools and resources to provide more comprehensive support, including the implementation of the SAP B1 tool.

Human Resources

The Human Resources service is responsible for managing selection processes, hiring and training, job descriptions, labour relations and collective bargaining, planning careers and internal promotion, and preventing work-related accidents. In 2008 a number of improvements were made in the areas of recruitment, mobility programs and induction processes. A working group was also established to implement a career plan for future individualised professional development programs for all BSC-CNS staff.
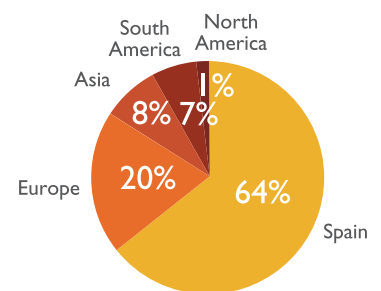
2008 Personnel by Function

Managerial Support 10%
Technical Support 18%
R&D 72%
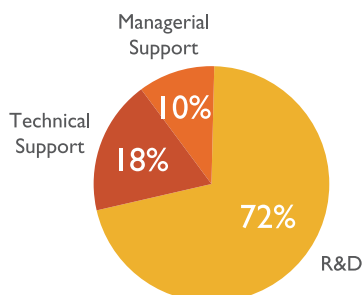
2008 Personnel by Gender

Female 24%
Male 76%
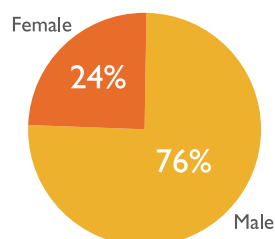
2008 Personnel by Region of Origin

South America 8%
North America 1%
Asia 7%
Europe 20%
Spain 64%

General Administration Support

The General Administration service is responsible for activities such as organisation of official meetings including those of the Access Committee, the Executive Commission, the Board of Trustees and other events. The Group manages travel services, space allocation, supply orders and execution of public tender processes as well as providing general administrative support and reception services such as receiving visiting researchers, official representatives and invited speakers.

Project Management

The team responsible for Project Management is responsible for the management of proposals and projects funded by public calls as well as by sponsored research contracts.

In 2008, the BSC-CNS participated in over 90 projects, funded by national agencies, the European Commission and private industry.

In addition to administering active projects, the Project Management Group assisted BSC-CNS researchers to submit a large number of new project proposals during 2008 which will likely see a further strong increase in the number of active projects next year.

BSC-CNS Projects 2008

Commenced
Completed
Ongoing

Number of Projects
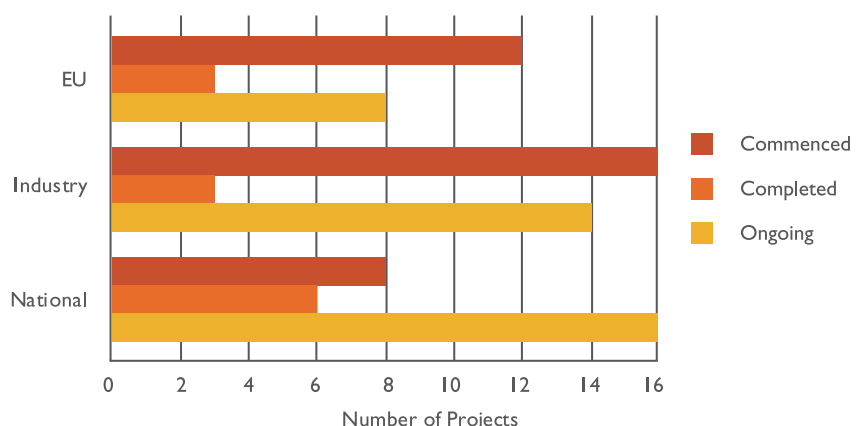
Marketing & Communication

The Marketing and Communication Group is in charge of increasing awareness of the centre, disseminating information about research activities both to the scientific and industrial communities as well as to society in general.

Visitors

In the course of 2008, the BSC-CNS received a total of 5872 visitors from national and international centres, including universities, research centres, industry and non-profit organisations.

Visitors to the MareNostrum are given a tour of the supercomputer and view a specially prepared video describing the technology utilised in the centre and the applications to which supercomputing research results are being applied.

BSC-CNS in the Media

Media coverage of the BSC-CNS increased considerably in 2008. Including national and international newspapers and magazines, BSC was mentioned 313 times, as compared to 136 times in 2007. In total, BSC issued 13 press releases in Spanish, Catalan and English that are included online http://www.bsc.es/plantillaA.php?cat_id=44. The BSC-CNS received most coverage in print media, followed by TV, radio and finally wires and online press.

Events Organised by the BSC-CNS

In 2008, BSC-CNS organised the following key events:

▶ Grand Challenges in Computational Biology, Joint BSC - IRB Barcelona Conference HiPEAC Computing Systems Week, 2nd – 6th June 2008

▶ BMW08: Barcelona Multicore Workshop, June 5-6, 2008

▶ The 23rd Open Grid Forum - OGF23, Barcelo Sants Hotel, June 2-6, 2008

In addition, many BSC-CNS researchers and representatives actively participated in a large number of international conferences, seminars and workshops.

Visits to the MareNostrum 2008
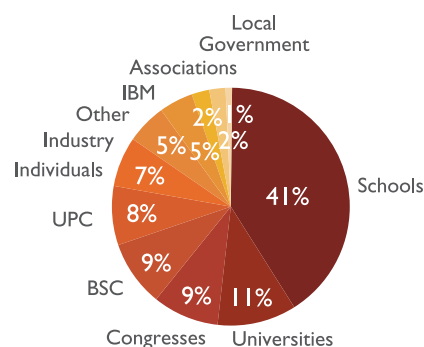
Computer Sciences 2008 Publications

Journals

» Felix Hupfeld, Toni Cortes, Björn Kolbeck, Jan Stender, Erich Focht, Matthias Hess, Jesus Malo, Jonathan Marti, Eugenio Cesario . The XtreemFS architecture—a case for object-based file systems in Grids. CONCURRENCY AND COMPUTATION: PRACTICE AND EXPERIENCE, Vol 20, No. 17, December 2008.

» R. Nou, S. Kounev and J. Torres. Autonomic QoS control in enterprise Grid environments using online simulation. Journal of Systems and Software . ISSN: 0164-1212. 2008. (83). November 2008.

» Nicolas Poggi, Toni Moreno, Josep Lluis Berral, Ricard Gavaldà, Jordi Torres. Self-Adaptive Utility-Based Web Session Management.. Computer Networks Journal, 2008, November 2008.

» M. Macías, O. Rana, G. Smith, J. Guitart, and J. Torres. Maximizing Revenue in Grid Markets using an Economically Enhanced Resource Manager. Concurrency and Computation: Practice and Experience, ISSN: 1532-0634, September 2008.

» Kyle J. Nesbit, Miquel Moreto, Francisco J. Cazorla, Alex Ramirez, Mateo Valero, and Jim E. Smith . Virtual Private Machines: Hardware/Software Interactions in the Multicore Era. IEEE Micro, special issue on Interaction of Computer Architecture and Operating System in the Manycore Era, vol. 38, no. 3, June 2008.

» Miloš Milovanovic , Roger Ferrer, Vladimir Gajinov, Osman S. Unsal, Adrian Cristal, Eduard Ayguadé and Mateo Valero. Nebelung: Execution Environment for Transactional OpenMP. International Journal of Parallel Programming. Vol 36, number 3, May 2008.

» Rosa M. Badia, Dennis Gannon, Craig Lee. Special section: Selected papers from the 7th IEEE/ACM international conference on grid computing (Grid2006). Future Generation Computer Systems, May 2008. Vol: 24, Issue: 5, pags: 402-403

» J. Guitart, D. Carrera, V. Beltran, J. Torres, and E. Ayguadé. Dynamic CPU Provisioning for Self-Managed Secure Web Applications in SMP Hosting Platforms. Computer Networks, Vol. 52 (7), pp. 1390-1409, ISSN: 1389-1286, May 2008.

» Miquel Moreto, Francisco J. Cazorla, Alex Ramirez and Mateo Valero. Dynamic Cache Partitioning based on the MLP of Cache Misses. Transactions on High Performance Embedded Architectures and Compilers. vol. 3, no. 1, March 2008.

» Jesus Labarta, Germán Rodriguez, and Rosa M. Badia. An Evaluation of Marenostrum Performance. International Journal of High Performance Computing Applications (IJHPCA), Special Issue on Performance Characterization of the World's Most Powerful Supercomputers, Vol. 22, No. 1, pages 81-96, February 2008.

» M. Valero and J. Labarta. "Supercomputing for the Future, Supercomputer for the Past". Keynote Lecture. HiPEAC 2008 Conference. High Performance Embedded Architecture Embedded Architectures and Compilers. LNCS 4917, pp. 3-5. Göteborg, Sweden, January 2008.

» M. Pericás, E. Ayguadé, J. Zalamea, J. Llosa and M. Valero. "Power-efficient VLIW design using clustering and widening". IJES, International Journal on Embedded Systems, Vol. 3, No 3, pp. 141-149, 2008.

» M. Pericás, A. Cristal, R. González and M. Valero. "Decoupled State-Execute Architecture". LNCS-4759, pp.68-78. Paper from ISHPC-2005. International Symposium on High Performance Computers. Nara, Japan. September 7-9, 2005. January 2008.

Book Chapters

» M. Ejdys, U. Herman-Izycka, N. Lal, T. Kielmann, E. Tejedor and R.M. Badia. Integrating Application and System Components with the Grid Component Model. From Grids to Service and Pervasive Computing, August 2008.

» Rosa M. Badia, Gargi Dasgupta, Onyeka Ezenwoye, Liana Fong, Howard Ho, Sawsan Khuri, Yanbin Liu, Steve Luis, Anthony Praino, Jean-Pierre Prost, Ahmed Radwan, Seyed Masoud Sadjadi, Shivkumar Shivaji, Balaji Viswanathan, Patrick Welsh, and Akmal Younis. Innovative Grid Technologies Applied to Bioinformatics and Hurricane Mitigation. High Performance Computing and Grids in Action, March 2008. IOS Press

» Carlos Boneti, Francisco J. Cazorla, Roberto Gioiosa and Mateo Valero. Scheduling Real-Time Systems With Explicit Resource Allocation Processors . Dresden, Germany, Lecture Notes in Computer Science. Volume 4934/2008, February 2008. International Conference on Architecture of Computing Systems (ARCS)

» E. Tejedor, R. Badia, T. Kielmann and V. Getov. A Component-Based Integrated Toolkit. Making Grids Work, CoreGRID series, Vol 7, pp 139-152. M. Danelutto, P. Fragopoulou and V. Getov, Eds. Springer., January 2008.

» I. Rodero, F. Guim, J. Corbalan, J. Labarta, A. Oleksiak, K. Kurowski, J. Nabrzyski. Integration of the eNANOS execution framework with GRMS for GRID purposes. Achievements in European Research on Grid Systems, Pages 25-39, January 2008.

» Rosa Badia, Raül Sirvent, Marian Bubak, Wlodzimierz Funika and Piotr Machner. Performance monitoring of GRID superscalar with OCM-G/G-PM: Integration Issues. Achievements in European Research on Grid Systems, Pages 193-205, January 2008.

» El bieta Kr pska, Thilo Kielmann, Raül Sirvent and Rosa Badia. A Service for Reliable Execution of Grid Applications. Achievements in European Research on Grid Systems, Pages 179-192, January 2008.

» Raül Sirvent, Rosa Badia, Natalia Currle-Linde, Michael Resch. GRID superscalar and GriCoL: Integrating Different Programming Approaches. Achievements in European Research on Grid Systems, Pages 139-150, January 2008.

» Ani Anciaux-Sedrakian, Rosa M. Badia, Raul Sirvent, Josep M. Perez, Thilo Kielmann, Andre Merzky. GRID superscalar and Job Mapping on the Reliable Grid Resources. Making Grids Work, CoreGRID series, January 2008.

» Rosa M. Badia, Raul Sirvent, Marian Bubak, Wlodzimierz Funika, Piotr Machner. Performance Monitoring of Grid Superscalar with OCM-G/G-PM: Tuning and Improvements. Making Grids Work, CoreGRID series, January 2008.

International Conferences

» J. Ejarque, M. de Palol, I. Goiri, F. Julià, J. Guitart, R. Badia, and J. Torres. SLA-Driven Semantically-Enhanced Dynamic Resource Allocator for Virtualized Service Providers. 4th IEEE International Conference on e-Science (e-Science 2008), Indianapolis, Indiana, USA, December 2008.

» Vicenç Beltran, Jordi Torres and Eduard Ayguadé. Improving Web Server Performance Through Main Memory Compression. The 14th IEEE International Conference on Parallel and Distributed Systems (ICPADS'08) Melbourne, Victoria, AUSTRALIA. 8th-10th December, 2008., December 2008.

» David Carrera, Malgorzata Steinder, Ian Whalley, Jordi Torres and Eduard Ayguadé. Enabling resource sharing between transactional and batch workloads using dynamic application placement. ACM/IFIP/USENIX 9th International Middleware Conference (Middleware 2008)ACM/IFIP/USENIX 9th International Middleware Conference (Middleware 2008), Leuven, Belgium, December 2008.

» I. González, M. Galluzzi, A. Veidenbaum, M. A. Ramírez, A. Cristal and M. Valero. " A Distributed Processor State Management Architecture for Large-Window Processors". Micro-41, IEEE-ACM "International Symposium on Microarchitecture". Lake Como, Italy, November 8-12, 2008.

» J. Verdu, M. Nemirovsky and M. Valero. "MultiLayer Processing: An Execution Model for Parallel Stateful Packet Processing". ANCS08, ACM-IEEE Symposium on Architectures for Networking and Communications Systems. San Jose, California, November 6-7, 2008.

» J. Alastruey, T. Monreal, F.J. Cazorla, V.Viñals and M.Valero "Selection of the Register File Size and the Resource Allocation Policy on SMT Processors". Proceedings of the 20th International Symposium on Computer Architecture and High Performance Computing (SBAC-PAD), Campo Grande, Brasil, 29 Oct- 1 Nov. 2008. IEEE Computer Society, p. 63-70, ISBN 978-0-7695-3423-7

» P. Radojkovic, V. Cakarevic, J. Verdú, A. Pajuelo, F. J. Cazorla, R. Gioiosa, M. Nemirosvky and M.Valero. "Measuring Operating Syastem Overhead on CMT Processors". IEEE SBAC-PAD, Campo Grande, Brasil, October 29 to November 1, 2008.

» José Luis González and Toni Cortes. Distributing Orthogonal Redundancy on Adaptive Disk Arrays. International Conference on Grid computing, high-performAnce and Distributed Applications (GADA'08), Monterrey, Mexico, November 2008.

» Carlos Boneti, Roberto Gioiosa, Francisco J. Cazorla and Mateo Valero. A Dynamic Scheduler for Balancing HPC Applications, International Conference for High Performance Computing, Networking, Storage and Analysis (SC). Austin, USA, November 2008.

» Alejandro Duran, Julita Corbalán, Eduard Ayguadé. An Adaptive Cut-off for Task Parallelism . Proceedings of the Supercomputing Conference (SC08), November 2008. Austin, TX, USA

» "Barcelona Supercomputing Center". M.Valero. Invited Talk. Information and Brokerage Conference on Information and Communication Technologies in the EU's 7th Framework Programme. Moscow, 21-23 October 2008.

» "Overcoming the Memory Wall: Kilo-Instruction, Runahead and SMT Processors". M.Valero. Invited lecture.VIPSI Conference. Lake Bled, Slovenia, October 3th. 2008.

» "On the Future of Supercomputers". M.Valero. Invited Lecture.VIPSI Conference. Lake Bled, Slovenia, October 3th. 2008.

» "Xavier Teruel, Priya Unnikrishnan, Xavier Martorell, Eduard Ayguade, Raul Silvera, Guansong Zhang, and Ettore Tiotto . OpenMP Tasks in IBM XL Compilers . Proceedings of CASCON 2008, October 2008. IBM Toronto Lab, Toronto, Canada"

» Marc Gonzalez, Nikola Vujic, Xavier Martorell, Eduard Ayguade, Alexandre E. Eichenberger, Tong Chen, Zehra Sura, Tao Zhang, Kevin O'Brien, and Kathryn O'Brien . Hybrid Access-Specific Software Cache Techniques for the Cell BE Architecture . Proceedings of the 17th International Conference on Parallel Architectures and Compilation Techniques (PACT'08), pp. 292-302, October 2008. Toronto, Canada

» Josep L. Berral, Nicolas Poggi, Javier Alonso, Ricard Gavaldà, Jordi Torres and Manish Parashar. Adaptive Distributed Mechanism Against Flooding Network Attacks Based on Machine Learning. Procs. The First ACM Workshop on AISec, Alexandria, VA, USA. October 27, 2008., October 2008.

» "On the Future of Supercomputers". M.Valero. Invited Lecture. University of Belgrade, Serbia. September 12th, 2008.

» "Will the First Exascale Machine be a Commodity Cluster, or Something Else?" J. Labarta Panel session. IEEE Cluster 2008, Tsukuba, Japan, September 2008.

» Josep M. Perez, Rosa M. Badia, and Jesus Labarta. A dependency-aware task-based programming environment for multi-core architectures. Proceedings of the 2008 IEEE International Conference on Cluster Computing, pp. 142ï¿½151, September 2008.

» Pilar Gonález-Férez, Juan Piernas, and Toni Cortes. Evaluating the Effectiveness of REDCAP to Recover the Locality Missed by Today's Linux Systems. 16th Annual Meeting of the IEEE International Symposium on Modeling, Analysis, and Simulation of Computer and Telecommunication Systems (MASCOTS) (poster), Baltimore, MD, September 2008.

» C. Acosta, F.J. Cazorla, A. Ramírez and M.Valero. MFLUSH: Handling Long-latency loads in SMT On-Chip Multiprocessors. 37th International Conference on Parallel Processing (ICPP 2008), pp. 173 - 181. Portland, USA . ISBN 978-0-7695-3374-2, September 2008.

» Marc Casas, Rosa M. Badia, Jesus Labarta. Prediction of Behavior of MPI Applications. IEEE Cluster 2008, September 2008.

» Rosa M. Badia, Du Du, Eduardo Huedo, Antonis Kokossis, Ignacio Martín Llorente, Rubén S. Montero, Marc de Palol, Raúl Sirvent and Constantino Vázquez. Integration of GRID superscalar and GridWay Metascheduler with the DRMAA OGF Standard. Proceedings of the Euro-Par Conference 2008, August 2008.

» "Supercomputing for the Future, Supercomputing from the Past". M.Valero. Invited Lecture. Onasssis Foundation Summer School. Lectures on Computer Science. Heraklion, Crete, July 25th, 2008.

» "Overcoming the Memory Wall: Kilo-Instruction, Runahead and SMT Processors". M.Valero. Invited lecture Onasssis Foundation Summer School. Lectures on Computer Science. Heraklion, Crete, July 25th, 2008.

» "Supercomputing for the Future, Supercomputing from the Past". M.Valero. Keynote Lecture. ReCoSoC. Barcelona, July 9-11, 2008.

» "Performance Analysis with Paraver". J. Labarta. Invited talk. 2nd HLRS Parallel Tools for High-performance Computing Workshop. Stuttgart, July 2008

» "New techniques and integration efforts in the CEPBA-Tools environment". J. Labarta. Invited talk. Workshop on Performance Tools for Petascale Computing. Center for Scalable Application Development Software (CScADS), July 21-24, 2008. Salt Lake , Utah, USA

» "StarSs and CellSs: Dataflow programming for multicore systems". J. Labarta. Invited talk. 2nd Annual Georgia Tech, Sony/Toshiba/IBM Workshop on Software and Applications for the Cell/B.E. Processor, July 10-11, 2008 Atlanta, GA

» J. Ejarque, M. de Palol, I. Goiri, F. Julià, J. Guitart, J. Torres and R. M. Badia. Using Semantic Technologies for Resource Allocation in Computing Service Providers. 5th IEEE International Conference on Services Computing (SCC 2008), Honolulu, Hawaii, USA, pp. 583-587 (Work-in-Progress Paper), ISBN: 978-0-7695-3283-7, July 2008.

» Sebastian Isaza, Friman Sánchez, Georgi Gaydadjiev, Alex Ramirezi, Mateo Valero. Preliminary Analysis of the Cell BE Processor Limitations for Sequence Alignment Applications. Embedded Computer Systems: Architectures, Modeling, and Simulation (SAMOS'08), July 2008.

» M. Pericas, R. Gonzalez, F. J. Cazorla, A. Cristal, A. Veidenbaum, D. Jimenez and M.Valero. "A Two-level Load/Store Queue based on Execution Locality". IEEE-ACM International Symposium on Computer Architecture. Beijing, June 21-25, 2008.

» P. A. Castillo, J. J. Merelo, M. Moreto, F. J. Cazorla, M. Valero, A. M. Mora, L. J. L. Laredo and S. McKee. "Evolucionary System for Prediction and Optimization of Hardware Architecture Performance". IEEE Congress on Evolutionary Computation, CEC-2008. Hong Kong, June 1-6, 2008, pp. 1941-1948.

» M. Pericás, R. Chaves, G. N. Gaydadjiev, S. Vassiliadis and M. Valero. "Vectorized AES Core for High-Throughput Secure Environments". VECPAR-2008. 8th International Meeting High Performance Computing for Computational Science. Toulouse, France, 24-27 June 2008.

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» Marc Casas, Rosa M. Badia, Jesus Labarta. Automatic analysis of speedup of MPI applications. International Conference on Supercomputing 2008 (ICS 2008), June 2008.

» Javier Alonso, Jordi Torres, Rean Griffith, Gail Kaiser and Luis Silva. Towards Self-Adaptable monitoring framework for Self-healing. Procs. 3rd CoreGrid Workshop on Middleware, Barcelona, Spain. June 5-6, 2008., June 2008.

» Felix Hupfeld, Björn Kolbeck, Jan Stender, Mikael Högqvist, Toni Cortes, Jonathan Martí, Jesús Malo. FaTLease: Scalable Fault-Tolerant Lease Negotiation with Paxos. International Symposium on High-Performance Distributed Computing, Boston, MA, June 2008.

» David Carrera, Malgorzata Steinder, Ian Whalley, Jordi Torres and Eduard Ayguadé. Managing SLAs of heterogeneous workloads using dynamic application placement. 7th IEEE Symposium on High Performance Distributed Computing (HPDC 2008), Boston, MA, June 2008.

» Jordi Torres, David Carrera, Vicenc Beltran, Nicholas Poggi, Kevin Hogan, Josep Lluis Berral, Richard Gavaldà, Eduard Ayguade, Toni Moreno and Jordi Guitart. Tailoring resources: the energy-efficient consolidation strategy, goes beyond virtualization . 5th IEEE International Conference on Autonomic Computing (ICAC 2008), Chicago, IL, June 2008.

» Carlos Boneti, Francisco J. Cazorla, Roberto Gioiosa, Chen-Yong Cher, Alper Buyuktosunoglu and Mateo Valero. Software-Controlled Priority Characterization of POWER5 Processor . Beijing, China, June 2008. International Symposium on Computer Architecture

» Pedro A. Castillo, Juan Julian Merelo, Miquel Moreto, Francisco J. Cazorla, Mateo Valero, Antonio M. Mora, Juan Luis J. Laredo and Sally A. McKee. Evolutionary system for prediction and optimization of hardware architecture performance. IEEE Congress on Evolutionary Computation (CEC). Hong Kong, June 2008.

» "Barcelona Supercomputing Center: Mision, Research Lines and Microsoft Collaboration". M. Valero. Invited Lecture. Microsoft Research Latin America Academic Summit 2008. Panamá, May 13th -16th, 2008.

» "Supercomputing for the Future, Supercomputing from the Past". M. Valero. Invited Lecture. University of Chalmers. Göteborg, May 8th, 2008.

» Enric Tejedor and Rosa M. Badia.. COMP Superscalar: Bringing GRID superscalar and GCM Together. 8th IEEE International Symposium on Cluster Computing and the Grid 2008, Lyon, May 2008.

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» "Research on High Performance Computing at BSC and UPC". M. Valero. Keynote Lecture. First European-Mexican IT Workshop. LAEMI, Xalapa, April 9-11th, 2008.

» "Supercomputing for the Future, Supercomputing from the Past". M. Valero. Invited Lecture. CINVESTAV, Centro de Investigación y de Estudios Avanzados. Cuidad de México, April 7th, 2008

» Jordi Torres, David Carrera, Kevin Hogan, Ricard Gavaldà, Vicenç Beltran and Nicolas Poggi. Reducing wasted resources to help achieve green data centers. Workshop on High-Performance, Power-Aware Computing (HPPAC 2008), Miami, FL, April 2008.

» V. Beltran, J. Torres, and E. Ayguadé. Understanding tuning complexity in multithreaded and hybrid web servers. In IPDPS '08: Proceedings of the 22nd IEEE International Parallel and Distributed Processing Symposium, pages 56-64, Miami, FL, USA, 14-18 April 2008., April 2008.

» Carlos Boneti, Francisco J. Cazorla, Roberto Gioiosa, Julita Corbalan, Jesus Labarta and Mateo Valero. Balancing HPC Applications Through Smart Allocation of Resources in MT Processors. Miami, Florida, USA, April 2008. International Parallel & Distributed Processing Symposium (IPDPS)

» David Carrera, Malgorzata Steinder, Ian Whalley, Jordi Torres and Eduard Ayguadé. Utility-based Placement of Dynamic Web Applications with Fairness Goals. 11th IEEE/IFIP Network Operations and Management Symposium (NOMS 2008), Salvador Bahia, Brazil, April 2008.

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» "Research at the High Performance Computer Group in Barcelona". M. Valero. Birla Institute of Technology and Science. Pilani, India. March 14th 2008

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» C. Boneti, F, J. Cazorla, R. Giogiosa and M. Valero. " Soft Real-Time Scheduling on SMT Processors with Explicit resource Allocation". ARSC 2008, International Conference on Architecture and Computing Systems. Dresden, Germany, Feb. 25-28, 2008.

» A. Garcia, O. J. Santana, E. Fernandez, P. Medina, and M. Valero. "LPA: A First Approach to the Loop Processor Architecture". HiPEAC 2008 Conference. International Conference on High Performance Embedded Architectures and Compilers. Göteborg, Sweden, January 27-29, 2008

» "QoS on Multithreaded Processors". M. Valero. Invited lecture. University of Texas at Austin. February 13th, 2008.

» "Overcoming the Memory Wall: Kilo-Instruction, Runahead and SMT Processors". M. Valero. Invited lecture. University of Texas at Austin. February 13th, 2008.

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» "Back to Babel?". J. Labarta. Invited talk at MULTIPROG-2008 (1st workshop on Programmability issues for multi-core computers) Goteborg, Sweden, January 27, 2008

» Harald Servat, Xavier Aguilar, Cecilia Gonzalez, Daniel Cabrera, Daniel Jimenez. Drug Design Issues on the Cell BE. 3rd International Conference on High-Performance Embedded Architectures and Compilers (HiPEAC'08), January 2008.

» Miquel Moreto, Francisco J. Cazorla, Alex Ramirez and Mateo Valero. MLP-aware dynamic cache partitioning. International Conference on High Performance Embedded Architectures & Compilers, January 2008.

National Conferences

» "On the Future of Supercomputers". M. Valero. Invited Lecture. Open Research Day. Telefónica I+D. Barcelona, 3 de Noviembre de 2008.

» Pilar Gonález-Férez, Juan Piernas, and Toni Cortes . The RAM Enhanced Disk Cache Project (REDCAP). XIX Jornadas de Paralelismo, Castellón, Spain, September 2008.

» Josep L. Berral, Javier Alonso, Nicolas Poggi, Ricard Gavaldà, Manish Parashar, Jordi Torres. Distributed Learning Mechanism Against Flooding Network Attacks. XIX Jornadas de Paralelismo, Castelló, Spain, 17-19 of September, 2008., September 2008.

» "StarSs: Portable Programming for a Fuzzy Multicore Space", Jesus Labarta. Invited Talk Barcelona Multicore Workshop (BMW-2008), Barcelona, June 2008.

» "Researh at the Barcelona Supercomputing Center-Centro Nacional de Supercomputación". M. Valero. Invited Lecture. Joint Seminar on Information and Communication Technologies orhanized by the Chinese Academy of Engineering (CAE) and by the Spanish Royal Academy (RAI). Madrid, May 7th, 2008.

» "Supercomputing for the Future, Supercomputing from the Past". M. Valero. Invited Lecture. First Workshop on Supercomputing. Aeronautics School, Technical University of Madrid, March 26th, 2008.

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» M. Macías and J. Guitart. Influence of Reputation in Revenue of Grid Service Providers. 2nd International Workshop on High Performance Grid Middleware (HiPerGRID 2008), Bucharest, Romania, pp. 9-16, ISSN: 2065-0701, November 2008.

» F. Zyulkyarov, O. Unsal, A. Cristal, E. Ayguade, S. Cvijic, T. Harris and M. Valero. "WormBench: A Configurable Workload for Evaluating Transactional Memory Systems". MEDEA Workshop. TCPP-PhD- Forum'09 PACT, the IEEE Conference on Parallel Architectures and Compilation Techniques. Toronto, Canada, October 25-29, 2008.

» Roger Ferrer, Marc Gonzalez, Federico Silla, Xavier Martorell, Eduard Ayguade . Evaluation of Memory Performance on the Cell BE with the SARC Programming Model . Proceedings of the 9th Workshop on Memory Performance: Dealing with Applications, systems, and architecture (MEDEA'08), October 2008. Toronto, Canada

» Ferad Zyulkyarov, Sanja Cvijic, Osman Unsal, Adrian Cristal, Eduard Ayguade, Tim Harris, Mateo Valero. WormBench - A Configurable Workload for Evaluating Transactional Memory Systems. Workshop on MEmory performance: DEaling with Applications, systems and architecture (MEDEA), in conjunction with PACT, October 2008.

» C. Perfumo, N. Sonmez, O. Unsal, A. Cristal, T. Harris and M. Valero. "Dissecting Transactional Executions in Haskell". Second ACM Workshop on Transactional Computing TRANSACT - Aug 2008.

» M. Ejdys, U. Herman-Izycka, N. Lal, T. Kielmann, E. Tejedor and R. Badia,. Integrating Application and System Components with GCM. CoreGRID Symposium 2008, August 2008.

» Nikola Vujic, Marc Gonzalez, Xavier Martorell and Eduard Ayguade. Automatic Pre-Fetch and Modulo Scheduling Transformations for the Cell BE Architecture . Proceedings of the 21st Annual Workshop Languages and Compilers for Parallel Computing (LCPC'08), July 2008. Univ. of Alberta, Edmonton, Canada

» V. Cakarevic, P. Radojkovic, F. Cazorla, R. Gioiosa, A. Pajuelo, J. Verdu, M. Nemirosvky and M. Valero. " Understanding the Overhead of the Spin-lock Loop in CMT Architectures". WIOSCA, 2008. Workshop on Intearction Between Operating Systems and Computer Architecture". To be held in conjuction with ISCA 2008. Beijing, June 21-25, 2008.

» Jan Stender, Björn Kolbeck, Felix Hupfeld, Eugenio Cesario, Erich Focht, Matthias Hess, Jesús Malo, and Jonathan Martí. Striping without Sacrifices: Maintaining POSIX Semantics in a Parallel File System. 1st Workshop on Large Scale Computing Systems, Boston, MA, June 2008.

» Vladimir Cakarevic, Petar Radojkovic, Javier Verdu, Alejandro Pajuelo, Roberto Gioiosa, Francisco J. Cazorla, Mario Nemirovsky and Mateo Valero. Understanding the Overhead of the Spin-lock Loop in CMT Architectures. Bejing, China, In Workshop on the Interaction between Operating Systems and Computer Architecture (WIOSCA), June 2008.

» Carlos Villavieja, Isaac Gelado, Alex Ramirez, Nacho Navarro. Memory Management on Chip-MultiProcessors with on-chip Memories. Workshop on the Interaction between Operating Systems and Computer Architecture (WIOSCA'08), June 2008.

» Alex Duran, Josep M. Perez, Eduard Ayguade, Rosa M. Badia and Jesus Labarta. Extending the OpenMP Tasking Model to Allow Dependent Tasks. proceedings of International Workshop on OpenMP, May 2008.

» Alejandro Duran, Julita Corbalan and Eduard Ayguade. Evaluation of OpenMP Task scheduling strategies . Proceedings of the 4thInternational Workshop on OpenMP (IWOMP'08), May 2008. Purdue University, West Lafayette, IN, USA

» E. Vallejo, S. Sanyal, T. Harris, M. Valero, O. Unsal, A. Cristal, F. Vallejo and R. Beivide. "Towards fair, scalable, Locking". EPHAM-2008. Workshop on Exploiting Parallelism with Transactional Memory and other Hardware Assisted Methods. Held with CGO-2008. Boston USA, April 6-8, 2008.

» Attila Kertész, Ivan Rodero and Francesc Guim. Meta-Borkering Approaches in State-Of-The-Art Grid Resource Management. CoreGRID Integration Workshop. Integrated Research in Grid Computing, April 2008.

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» Pedro A. Castillo, Antonio M. Mora, Juan Julian Merelo, Juan Luis J. Laredo, Miquel Moreto, Francisco J. Cazorla, Mateo Valero and Sally A. McKee. Architecture performance prediction using evolutionary artificial neural networks. European Workshop on Hardware Optimization Techniques (EVOHot), March 2008.

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» V. Subotic, J. Labarta and M. Valero. "Overlapping MPI Computation and Communication by Enforcing Speculative Dataflow". INA-OCMC-08. Workshop on Interconnection Network Architectures On-Chip, Multi-Chip. To be held in conjuction with HiPEAC-2008, the +International Conference on High Performance Embedded Architectures and Compilers. Göteborg, Sweden, January 27-29, 2008

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Journals

» A. Folch, C. Cavazzoni, A. Costa, G. Macedonio. An automatic procedure to forecast tephra fallout . Journal of Volcanology and Geothermal Research, doi:10.1016/j.jvolgeores.2008.01.046, ISSN: 0377-0273, June 2008.

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» 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 system for the Iberian Peninsula, Balearic Islands and Canary Islands- First annual evaluation and ongoing developments . Advances in Science and Research, 2: 89-98, ISSN: 1992-0628, May 2008.

» Baldasano J.M., L. P. Güereca, E. López, S. Gassó, P. Jimenez-Guerrero. Development of a high-resolution (1 km x 1 km, 1 h) emission model for Spain: the High-Elective Resolution Modelling Emission System (HERMES) . Atmospheric Environment, 42 (31): 7215-7233, doi:10.1016/j.atmosenv.2008.07.026. ISSN: 1352-2310, October 2008.

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» Jorba, O., Loridan, T., Jiménez-Guerrero, P., Pérez, C., Baldasano, J.M., . Linking the advanced research WRF meteorological model with the CHIMERE chemistry-transport model . Environmental Modelling & Software, 23, 1092-1094, March 2008.

» María Gonçalves, Pedro Jiménez-Guerrero, Eugeni López and José M. Baldasano. Air quality models sensitivity to on-road traffic speed representation: Effects on air quality of 80 km h 1 speed limit in the Barcelona Metropolitan area . Atmospheric Environment, 42 (36): 8389-8402, doi:10.1016/j.atmosenv.2008.08.022. ISSN: 1352-2310, November 2008.

» Papayannis, A., Amiridis, V., Mona, L., Tsaknakis, G., Balis, D., Bösenberg, J., Chaikovski, A., Tomasi, F. De., Grigorov, I., Mattis, I., Mitev, V., Müller, D., Nickovic, S., Pérez, C., Pietruczuk, A., Pisani, G., Ravetta, F., Rizi, V., Sicard, M., Trickl, T., Wiegner, M., Gerding, M., Mamouri, R.E., D'Amico, G., Pappalardo,

» G.,. Systematic lidar observations of Saharan dust over Europe in the frame of EARLINET (2000-2002) . Journal of Geophysical Research VOL. 113, D10204, doi:10.1029/2007JD009028, May 2008.

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» M. C. Todd, D. Bou Karam, C. Cavazos, C. Bouet, B. Heinold, J. M. Baldasano, G. Cautenet, I. Koren, C. Perez, F. Solmon, I. Tegen, P. Tulet, R. Washington, and A. Zakey., Quantifying uncertainty in estimates of mineral dust flux: An intercomparison of model performance over the Bodélé Depression, northern Chad, Journal of Geophysical Research, 2008

» Cuevas E., J.M. Baldasano, C. Pérez, X. Querol, M.A. Martínez, S. Nickovic y L. Barrie, El Sistema de Alerta de Tormentas de Polvo y Arena para Europa, África y Oriente Próximo de la Organización Meteorológica Mundial, Boletín de la Asociación Meteorológica Española, 2008

Book Chapters

» Marras S., M. Vazquez, A. Aubry, O. Jorba, G. Houzeaux, J.M. Cela and J.M. Baldasano. A massively parallel Finite Element approach to the solution of non-hydrostatic compressible atmospheric flows. EMS8/ECAC7, EMS2008-A-00531, September 2008.

» Gonçalez 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. Air Pollution Modeling and its Application XIX., Editors: C. Borrego and A.I. Miranda. Springer: 54-62. 978-1-4020-8452-2., July 2008.

» Gonçalves, M., Jiménez-Guerrero, P., Baldasano, J.M., Air quality management strategies in urban areas: effects of introducing hybrid cars in Madrid and Barcelona Metropolitan Areas (Spain), Croatian Meteorological Journal. The 12th International Conference on Harmonization within Atmospheric Dispersion Modelling for Regulatory Purposes. Vol. 43, 119-123, 2008

» Martí, J., A. Geyer, A. Folch, J. Gottsmann. A review on collapse calderas modelling. Caldera Volcanism, Developments in Volcanology vol 10, Eds. Elsevier Science Title, ISBN: 978-0-444-53165-0, May 2008.

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» Baldasano J.M; Jiménez-Guerrero, P; Jorba, O; Martín, F; Querol, X; Diéguez, J.J, Caliope: Sistema de Calidad del Aire Operativo para España, Subvenciones de I+D+I en el ámbito de la prevención de la contaminación: balance 2004-2007, 2008

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» Alonso-Pérez S., E.Cuevas, C.Pérez, X.Querol y J.M.Baldasano. Tendencia positiva de las intrusiones de masas de aire africano sobre la región subtropical oriental del Atlántico Norte. XI Congreso de Ingeniería Ambiental, GEO2 2008, Bilbao (España), 4-6, November 2008.

» Baldasano J.M. P. Jiménez-Guerrero P., O. Jorba, E. López, S. Gassó, F. martin, M. García-Vivanco, I. Palomino, X. Querol, M. Pandolfi, J.J. Dieguez.. "A high-resolution system for air quality forecasting in Europe and the Iberian Peninsula: the CALIOPE project". Primeres Jornades de Meteorologia i Climatologiade la Mediterrània Occidental, Barcelona, 28, November 2008.

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» Jiménez-Guerrero P., M.T.Pay, O.Jorba, M.Piott, J.M.Baldasano. "Evaluating the annual performance of an air quality forecasting system (Caliope) with high resolution for Europe and Spain". ACCENT/GLOREAM Workshop, Antwerp (Belgium), 29-31, October 2008.

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» Baldasano J.M, "Earth Science Research at the Barcelona", 29th HPC Forum, Tucson, Arizona (USA), September 8-10, 2008

» Baldasano J.M., "Air Quality and Climate Simulations", International Workshop on Cyberinfrastructure-enabled Detection of & Response to Natural Disasters, Austin, Texas (USA), November 17, 2008

» Baldasano J.M., "Estimación del consumo de energía y de las", SOLVAY Indupa, Sao Paulo (Brasil, 14 Mayo y Buenos Aires (Argentina), 2008

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» Baldasano J.M., P. Jimenez-Guerrero, O. Jorba, C. Pérez, E. López, P. Güereca, F. Martin, M. García-Vivanco, I. Palomino, X. Querol, M. Pandolfi, M.J. Sanz y J.J. Diéguez. El proyecto CALIOPE: Sistema de Calidad del Aire Operativo para España. Objetivo y Estado Actual. XXX Jornadas Científicas de la AME (Asociación Española de Meteorología), Zaragoza (España), 6, May 2008.

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» Baldasano J.M., "Sostenibilidad ¿Para quién? ¿Para que?", Campus de Excelencia, Maspalomas (Gran Canaria), 26 Junio, 2008

» Baldasano J.M., "Aplicaciones HPC en Ciencias de la Tierra", Universidad Internacional Menenedez y Pelayo-UIMP, Santander, 9 Julio, 2008

» Baldasano J.M., "Nuevos retos en la gestión del agua", XXIX Edición de los Cursos de Verano de la Universidad de Cádiz en San Roque, 2008

» Baldasano J.M, "Ciudades y Medio Ambiente: impactos inevitables y sistemas eco-preventivos", Curso de Verano, Universidad Complutense de Madrid (UCM): Desarrollo Económico y Social y Grandes Ciudades en la España del Siglo XXI, 2008

» Baldasano J.M., "Supercomputadores: Herramientas de Futuro para el Modelado del Clima", Cambio Climático: Escenarios de Futuro, CaixaForum, Madrid, Octubre 15, 2008

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» Baldasano J.M., "Evaluación de la eficacia de las medidas de reducción del límite de velocidad a 80 km/h", CONAMA, Madrid, Diciembre 4, 2008

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» A.-C. Lesage and M. Araya-Polo and G Houzeaux. Wave acoustic propagation for geophysics imaging, Finite Difference vs Finite Element methods comparison and Boundary Condition treatment. 8th World Congress on Computational Mechanics (WCCM8) and 5th European Congress on Computational Methods in Applied Sciences and Engineering (ECCOMAS 2008). Venice (Italy), June 30 - July 5, 2008.

» A.-C. Lesage, H. Zhou, M. Araya, J.-M. Cela and F. Ortigosa. Hybrid Finite Difference-pseudospectral Method for 3D RTM in TTI Media. 70th EAGE Conference & Exhibition, Rome, Italy, June 2008.

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» M. Araya-Polo, F. Rubio, M. Hanzich, R. de la Cruz, J.-M. Cela, D.P. Scarpazza. 3D Seismic Imaging Through Reverse-Time Migration on Homogeneous and Heterogeneous Multi-Core Processors. Scientific Programming, Special Issue on the Cell Processor, Vol. 16, No. 4, December 2008, IOS Press, The Netherlands.

» M. Araya-Polo, F. Rubio, R. de la Cruz, M. Hanzich, J.-M. Cela and D.P. Scarpazza. High-Performance Seismic Acoustic Imaging by Reverse-Time Migration on the Cell/B.E. Architecture. ISCA2008 - WCSA2008 Beijing, China, June 21-26, 2008.

» R. Codina and H. Coppola-Owen and G. Houzeaux. The fixed mesh ALE approach: basic idea and two applications. Intern. Conference on Mathematics and Continuum mechanics. Porto (Portugal), 19-22 Febrary, 2008.

» R. de la Cruz, B.K. Muite, H. Servat. Strong linear scaling for spectral simulations of time dependent semilinear partial differential equations on Marenostrum. 8th World Congress on Computational Mechanics (WCCM8) and 5th European Congress on Computational Methods in Applied Sciences and Engineering (ECCOMAS 2008). Venice (Italy), June 30 - July 5, 2008.

» National Conferences

» D. Gil, J. Garcia-Barnés, F. Carreras, M. Ballester, M. Vázquez, R. Aris and G. Houzeaux. Un model 3D del ventricle esqerre integrant anatomia i funcionalitat. XX Congrès de la Societat Catalana de Cardiologia. Barcelona (Spain), 12-13 June, 2008.

» D. Taylor, D.J. Doorly, R.C. Schroter, J. Peiro, R. Almeyda, N. Tolley, G. Houzeaux and M. Vázquez. Computational modelling of nasal airflow. Grand Challenges in Computational Biology. Joint BSC-IRB Barcelona Conference. Barcelona (Spain), 2-4 June, 2008.

» M. Vázquez, R. Aris, G. Houzeaux, J.M. Cela, J.G Garcia-Barnes and D. Gil. Anatomical and Functional High Performance Computational Electrophysiology model of the Left Ventricle. Grand Challenges in Computational Biology. Joint BSC-IRB Barcelona Conference. Barcelona (Spain), 2-4 June, 2008.

» T. Pujol and M. Vázquez and G. Houzeaux and J.R. González and L. Montoro and M. Pelegri. Alya - Programa de Mecánica Computacional Avanzada Caso de Estudio: Aerodinámica Externa. XVII Congreso Nacional de Ingenieria Mecánica. Gij\'on (Spain), 14-15 Febrary, 2008.

2008 was a year of consolidation and development for the RES; new services were established to support users and the first training seminars were held for both users and technical staff. Demand for access to the network skyrocketed with requested time exceeding time available by over 300% by the end of the year.
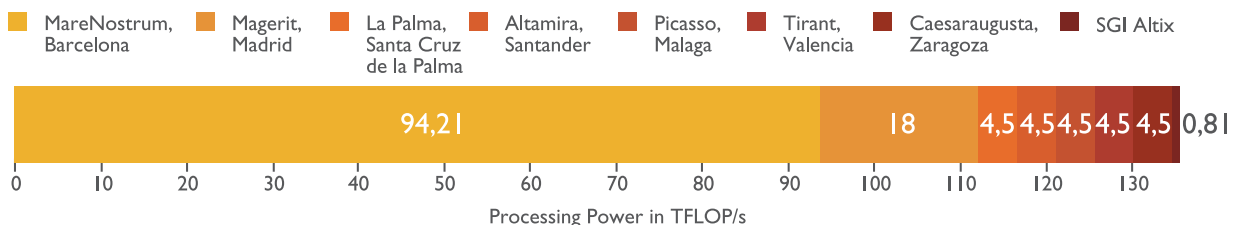

Nodes of the Spanish Supercomputing Network (RES)

What is the RES?

The Spanish Ministry of Science & Innovation (MICINN) created the Spanish Supercomputing Network (Red Española de Supercomputación - RES) in March 2007 as a response to the need of the Spanish scientific community for increased capacity and accessibility of calculation.

Processing Power of the RES

Colour	Site
▮	MareNostrum, Barcelona
▮	Magerit, Madrid
▮	La Palma, Santa Cruz de la Palma
▮	Altamira, Santander
▮	Picasso, Malaga
▮	Tirant, Valencia
▮	Caesaraugusta, Zaragoza
▮	SGI Altix

94,21   18   4,5 4,5 4,5 4,5 4,5 0,81

Processing Power in TFLOP/s

The RES consists of an infrastructure of supercomputers physically distributed in different sites in Spain, each of which contributes to the total processing power available to users. Each node reserves 20% of capacity for use by researchers at the host institute, and the other 80% is made available to the general scientific community via the Access Committee. The total processing capacity of the RES is 135,5 TFLOP/s (135,5 trillion floating point operations per second).

The RES is managed by the Operations Department of the BSC-CNS, which includes maintenance and upgrades, training of technicians, facilitation of access and all aspects of user support.

RES Usage 2008

All the nodes of RES are accessible for use by Spanish and international scientists via electronic application to a single Access Protocol.

Allocation of access to RES supercomputer facilities is based on criteria of efficacy, efficiency and transparency, mediated by a double filter system, with potential projects first being evaluated by the ANEP, followed by an evaluation by the Access Committee, composed of a **Core Team** and four **Expert Panels** of prestigious Spanish scientists external to the BSC-CNS, mainly managers of National Programs or of the ANEP.

The four Expert Panels are defined according to the classification established by the Spanish Foundation of Science and Technology (FECYT).

The Expert Panels:
▶ Astronomy, Space and Earth Sciences
▶ Biomedicine and Health Sciences
▶ Chemistry and Materials Science and Technology
▶ Physics and Engineering
Each of the above areas is chaired by a Group leader, who acts as a coordinator, an assistant, and eight experts in the area.

Access Committee Core Team 2008
▶ Ramón López de Arenosa, Ministerio de Educación y Ciencia
▶ Victoria Ley Vega de Seoane, Agencia Nacional de Evaluación y Prospectiva;
▶ Pedro de Miguel, Universidad Politécnica de Madrid
▶ José María Cela, BSC-CNS

The Access Committee allocates to both Spanish and international researchers more than 20 million computational work hours every four months. In addition to internal research groups, **over 270** external activities made use of the RES system in 2008.

It is important to note that many scientific projects often request numerous periods of access to the RES in order to perform different work activities (new activities or continuation activities). Each request is treated separately and must pass the evaluation procedure of the Access Committee. Thus the number of activities reported for the RES is greater than the number of projects registered for the year.

Access Requests 2008

Once the Access Committee has published its four monthly list of successful applicants and the number of computing hours each has been allocated, the Operations Department takes over the logistical processes of scheduling the users, preparing their software for loading, loading and running the software and ensuring the users have access to both the data results and statistics on the performance of their code, to facilitate future code improvements.

The graph shows the evolution of hours requested (blue), hours assigned (red) and hours used (green) over the last three years.

Hours Requested, Assigned and Used in the RES
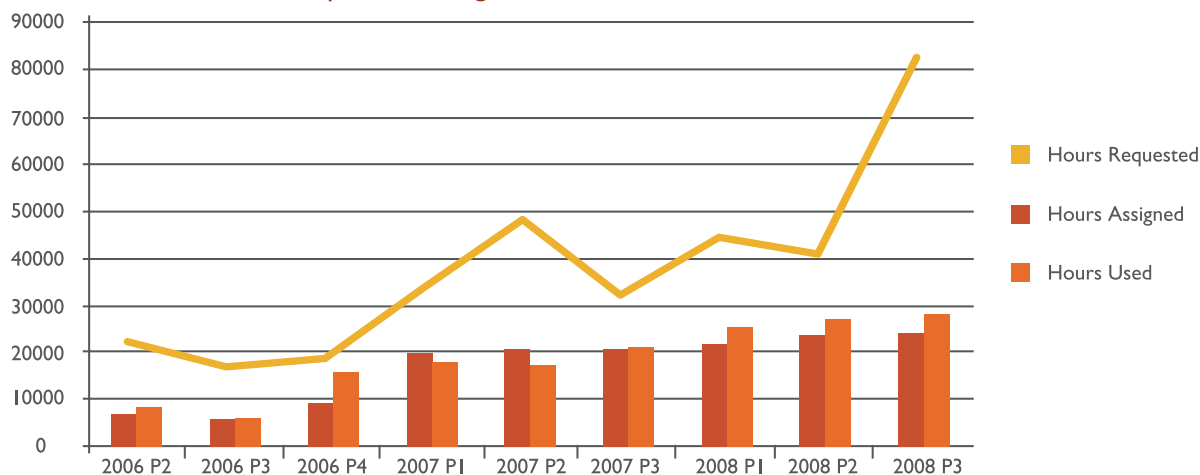
In the four years since the MareNostrum commenced operation, the MareNostrum and other RES nodes have collectively provided 193 million hours of computation. Over the same period 411 million hours were requested, indication that demand is more than double the hours that the RES can supply.

Broad Impact on Scientific Research

Despite the RES being only a few years old, awareness of the RES and the services it offers has spread quickly. More than 270 R&D activities took advantage of the RES infrastructure in 2008, led by researchers from institutions in over 30 cities in Spain, Europe and overseas.

Cities of Origin of RES Users, 2008

These activities were broadly distributed over many different scientific fields, ranging from climate simulations, to models of biological processes to the simulation of satellite missions. Results of these studies have been presented in conferences worldwide and published in leading scientific journals.

Importantly, many of these research activities could not have taken place if it were not for the extremely powerful computing capability offered by the RES, which enables calculations and simulations that would take years on ordinary PCs to be run in very short periods of time.

During 2008 the BSC-CNS began to hold seminars to educate potential users about the services available via the RES with the intention of further broadening access to the RES by sectors of the scientific community who have not been traditional users of supercomputers.

RES Hours Used in 2008 by Scientific Field
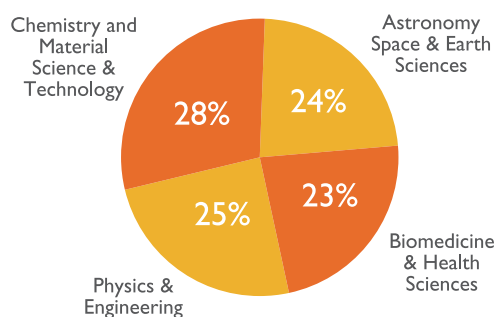
- Chemistry and Material Science & Technology — 28%
- Astronomy Space & Earth Sciences — 24%
- Biomedicine & Health Sciences — 23%
- Physics & Engineering — 25%

Overview
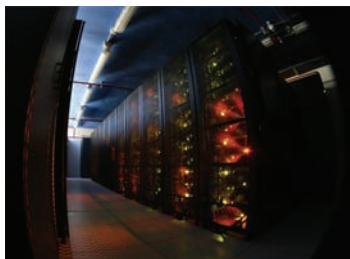
The MAGERIT Supercomputer

The Centro de Supercomputación y Visualización de Madrid (CeSViMA) located in the Montegancedo Science & Technology Park, centres its activities on the mass storage of data, high performance computing and advanced interactive visualisation.

Magerit, the name of CeSViMa´s supercomputer, is a cluster of 1204 nodes, of which 1036 are eServer BladeCenter JS20 with 4 GB of RAM and 168 are eServer BladeCenter JS21 with 8GB of RAM; in total 2744 CPUs with 5.5TB of RAM. All the nodes operate independently however utilise the same software configuration. Interconnection is via a high performance Myrinet fibre optic network with Gigabit connections for control and management. Total hard disk storage of 192TB is provided by a distributed and fault tolerant (GPFS) system.

At the time of its founding, Magerit was the 2nd most powerful Spanish supercomputer in history - in the November 2006 TOP500 listing it held 2nd in Spain, 9th in Europe and 34th in the world. In November 2007 it held 275th place in the GREEN500 list of most environmentally friendly supercomputers.

Organisational Structure
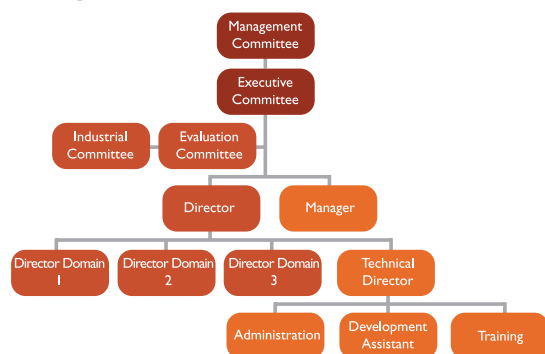
The Politechnic University of Madrid (UPM) is devolving the management of CeSViMa to the Faculty of Information Science so the centre is currently undergoing structural re-organisation. However the organisational structure which predominated in 2008 is shown in the diagram.

The team from left to right: Rubén Galeano, Oscar Cubo, Víctor Maestre, Fernando Limón, Borja Chocarro, Andrés Marín, Óscar Lozano

Technical and Scientific Highlights 2008

In 2008 the Magerit node achived an average uptime of 85% with 24x7 availability. This represents a provision of 20,6 million CPU hours.

Close to 6,6 million of these hours were used by local staff of the CeSViMa for various research projects, while the rest were made available to national and international users via the RES.

Key Publications 2008

S. González, L. Guerra, V. Robles, J. M. Peña and F. Famili, "CliDaPa: A new approach to combine clinical data with DNA microarrays", IDA Journal

K. Sánchez, P. Palacios, P. Wahnón, "Electronic structure of bulk- and Na-intercalated TiS2 determined from a GGA+U study with the Hubbard terms obtained ab initio ", Phys. Rev. Lett.

P. Palacios, I. Aguilera, K. Sánchez, J. C. Conesa, P. Wahnón, "Transition Metal Substituted Indium Thiospinels as Novel Intermediate Band Materials: Prediction and Understanding of their Electronic Properties", Phys. Rev. Lett.

P.L. G-Müller, F. Borondo, R. Hernández and R. M. Benito, Solvent Induced acceleration observed in an activated molecular reaction, Phys. Rev. Lett.

N. C. Karayiannis, and M. Laso, "Dense and nearly jammed random packings of freely jointed chains of tangent hard spheres", Phys. Rev. Lett.

M. Laso, and N. C. Karayiannis, "Flexible chain molecules in the marginal and concentrated regimes: Universal static scaling laws and cross-over predictions", J. Chem. Phys.

K. Foteinopoulou, N. C. Karayiannis, M. Laso, M. Kröger, and M. L. Mansfield, "Universal scaling, entanglements, and knots of model chain molecules", Phys. Rev. Lett.

K. Foteinopoulou, N. C. Karayiannis, M. Laso, and M. Kröger, "Structure, dimensions, and entanglement statistics of long linear polyethylene chains", J. Phys. Chem.

N. C. Karayiannis, K. Foteinopoulou, and M. Laso, "The characteristic crystallographic element norm: A descriptor of local structure in atomistic and particulate systems", J. Chem. Phys.

Rafael Borge, Vassil Alexandrov, Juan José del Vas, Julio Lumbreras, Encarnación Rodríguez

"A comprehensive sensitivity analysis of the WRF model for air quality applications over the Iberian Peninsula", Atmospheric Environment

M. Fontelos, U. Kindelan, O. Vantzos, "Evolution of neutral and charged droplets in an electric field", Physics of Fluids

M. Fontelos, U. Kindelan, "The shape of charged drops over a solid surface and symmetry-breaking instabilities", Siam Journal on Applied Mathematics

G. Otero, G. Biddau, C. Sánchez-Sánchez, R. Caillard, M. F. López, C. Rogero, F.J. Palomares, N. Cabello, M.A. Basanta, J. Ortega, J. Mendez, A.M. Echavarren, R. Pérez, B. Gómez-Lor y J.A. Martín-Gago, "Fullerenes from aromatic precursors by surface-catalysed cyclodehydrogenation.", Nature

Key Projects

The Magerit supercomputer, asides from supporting the projects of the RES users, provided support to numerous projects of the UPM, other universities in Madrid and those of other autonomous communities in Spain.

Listed below are the largest of these projects, which have generated a large number of articles and publications which are not detailed in this report.

Aero-Acústica computacional y experimental para predicción y control de ruido (ACE-PCOR), Eusebio Valero Sánchez Vassilis Theofilis, UPM

Algoritmos genéticos masivamente paralelos: Aplicaciones a problemas de ingenierí, José María Peña Sánchez, UPM

Arquitectura hardware/software para sistemas de alto rendimiento, Francisco Tirado Fernández, UCM

Criptoanálisis de algoritmos, Jorge Dávila Muro, UPM

CRP on Analytical and Experimental Benchmark Analyses of Accelerator Driven Systems (ADS), Alberto Abánades Velasco, UPM

Desarrollo de un modelo regional del clima con acoplamiento atmósfera-océano y optimización del código para computadores masivamente paralelos, Clemente Gallardo Andrés Fernando Cuartero Gómez, UCLM

Dinámica, compatibilidad molecular y nanoestructuras de poliolefinas de nueva generación, Javier Martínez de Salazar Bascuñana, CSIC

Estudio mecano-cuántico de la Fotoquímica y Control de moléculas en superficies de óxidos metálicos, María Pilar de Lara Castells, CSIC

Evolución y explosión de masas fluidas cargadas eléctricamente, Ultano Kindelán Bustelo, UPM

Experimentación con algoritmos evolutivos para optimizar tablas de datos, Juan Antonio Fernández del Pozo, UPM

Modelado estadístico de propiedades y actividades de moléculas con aplicación farmacológica, Gonzalo Fernando Colmenarejo Sánchez, UCM

Multiscale Modeling of Nanostructured Interfaces for Biological Sensors (MNIBS), Manuel Laso Carbajo, UPM

Nuevos materiales fotovoltaicos de banda intermedia, Perla Wahnón Benarroch, UPM

Optimización de técnicas de procesamiento y recuperación de información multimedia en sistemas computacionales paralelos y distribuidos, Ángel Rodríguez Martínez de Bartolomé, UPM

Protección radiológica y seguridad en aceleradores de alta intensidad tipo EVEDA/IF-MIF, Javier Sanz Gozalo, UNED

Simulación de burbujas transaccionales de separación en turbinas de baja presión, Javier Jiménez Sendín, UPM

Simulación de la dinámica de una reacción de isomerización en presencia de un fluido denso, Rosa María Benito Zafrilla, UPM

Simulaciones numéricas de la formación de estructuras en el universo, Gustavo Yepes Alonso, UAM

Sistema operacional de predicción de la calidad del aire para el continente europeo (MM5-CMAQEMIMO): Servicios de información regional, Roberto San José, UPM

Overview

The LaPalma Supercomputer

The LaPalma supercomputer, one of the seven nodes belonging to the RES and financed by the Ministry of Science and Innovation (MICINN), is located in the "Centro de Astrofísica de La Palma (CALP)", in Breña Baja.

The LaPalma supercomputer, along with four other "brother nodes" is formed from older processors derived from the MareNostrum which were relocated during its last upgrade, and the node is coordinated from the BSC-CNS.

The installation of the supercomputer at LaPalma was a strategic step whose objective is to boost the observation activities in the Observatorio del Roque de Los Muchachos – above all through the incorporation of the Gran Telescope CANARIAS (GTC) – and in this way reinforce the telecommunication development on the island.

Organisational Structure

For the administration and management of the supercomputer node, the Instituo de Astrofísica de Canarias (IAC) makes available its IT support team and has employed one engineer dedicated full-time to fulfill these functions.

The LaPalma Supercomputer Support Team
Carlos Martín Galán (Ingeniero Senior), Responsible Technician and the Manager of the Group.
Antonio Díaz Chinea (Ingeniero Senior), System Administrator.
Justo Luna López (Ingeniero), System Administrator.
Ubay Dorta Guerra (Ingeniero), System Administrator and UserSupport.
Ángel de Vicente (Ingeniero), User Support.

Technical and Scientific Highlights 2008

LaPalma´s maximum processing capacity is 4,5 teraflops (4,5 billion operations per second). Operations performed by LaPalma in one second would take more than 112 500 years for a person with a simple calculator.

LaPalma, installed in a controlled environment room of 32 square metres, has one terabyte of principal memory, (approximately equal to the memory of more than one million home PCs) and a further 14 terabytes of hard-disc data storage (equivalent to some 10 million books).

The various IAC installations on the islands and LaPalma communicate via a link of 10Gbps, of which the supercomputer can use up to 4Gbps.

Key Publications 2008

Moreno-Insertis, F. Invited Review lecture: Symposium 259 of the International Astronomical Union, Nov 2008. Title: Cosmic Magnetic Fields: from Planets, to Stars and Galaxies, Cambridge University Press, IAU Symposium Series (in press)

Moreno-Insertis, F., Galsgaard, K., Ugarte-Urra, I., Invited Lecture: Second Hinode Science Meeting, 29 September- 3 October 2008, Boulder, Colorado USA. Speaker: Moreno-Insertis, F. Title of invited lecture: X-Ray jets in coronal holes: numerical simulation and Hinode observations (in press)

"A nearly edge-on disk around the M5 ultracool dwarf Par-Lup3-4" by N. Huelamo, H. Bouy, C. Pinte, F. Menard, G. Duchene, F. Comeron6, M. Fernandez, D. Barrado y Navascues, and A. Bayo, submitted to Astronomy & Astrophysics

Olshevsky V., Khomenko E., Collados M. (2008) "Seismology of Sunspots: An Interplay between Temperature and Magnetic Field Structures" 12th European Solar Physics Meeting, Freiburg, Germany

Key Projects

Asides from the projects assigned by the RES, which utilise approximately 80% of LaPalma´s capacity, during 2008 the IAC executed its own scientific projects among which highlights are:

Propagation of Magnetoacustic Waves in Magnetic Structures Local helioseismology of solar active regions will be able to provide the information about the sub-surface magnetic fields to be used by magnetic dynamo models. For that, the physics of waves in magnetized regions has to be well understood. Forward numerical simulations have become a preferred approach in recent years to attack the complex non-linear physics of waves in non-trivial magnetic field configurations. The project aims to understand: (i) Mechanisms of excitation of waves in sunspots. (ii) Physics of umbral flashes and running penumbral waves. (iii) Identify wave types dominating helioseismological velocity signal detected in active regions. (iv) Analyse consequences of the strong magnetic field of sunspots onto helioseismology measurements and determination of sub-photospheric structure of solar active regions.
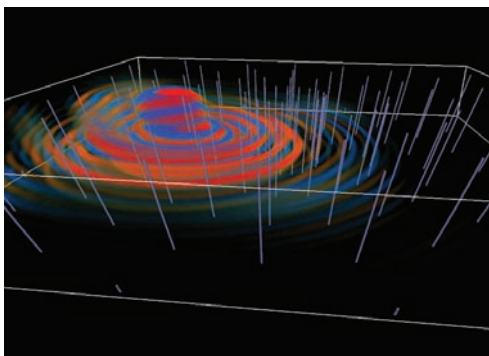
Magnetoacoustic Waves in a Sunspot

Galaxy Transformations Through Interactions, Mergers and Accretion About 8 billion years ago, rapid and violent growth of galaxies was largely complete, but galaxies still must have gone through important transformations to acquire their present-day morphologies, bulge-disk structure, and low star formation rates. This project addresses what types of transformations occur on a disk galaxy when it merges with a smaller galaxy, to determine the role of such minor mergers in galaxy evolution during the last half of the age of the Universe.

Image Reconstruction of Photometric and Spectropolarimetric Data by Means of the Multi-Object and Multi-Frame Blind Deconvolution Algorithm (MOMFBD) The investigation of the dynamics of the solar fine structure and its magnetic field. This project requires 2D photometric and spectropolarimetric data of the highest angular resolution (better than 0.1 arcsec) which can be only achieved by combining online and post-facto techniques, such as

Adaptive Optics and image reconstruction techniques, in order to reduce substantially the image distortions induced by the earth's atmosphere and to further improve the spatial resolution of the observed data sets.
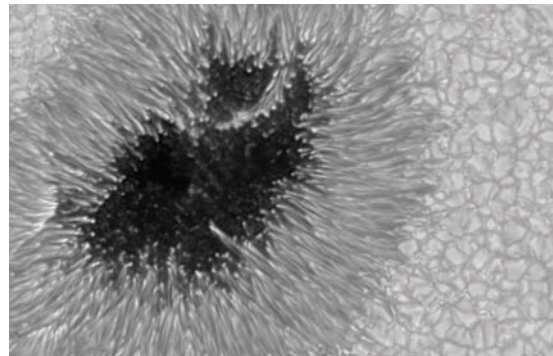
45 min Time Series of Reconstructed Broadband Images Harbouring a Large Sunspot

High Resolution in Solar Physics (Alta Resolucion en Fisica Solar) Understanding the physics of the Sun increasingly demands the resolution of small features in the solar surface, as those shown in the figure. To achieve this purpose complex and very time consuming computational techniques are required to compensate for the errors induced in the images by the telescope and atmospheric turbulence.
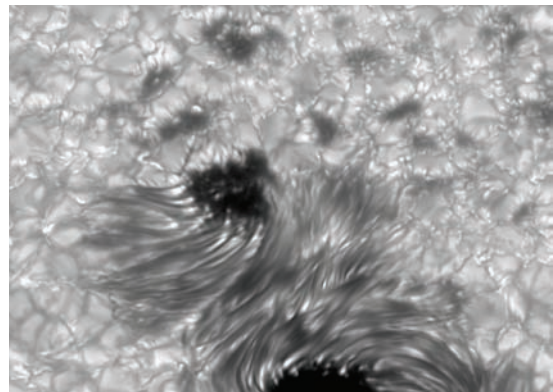
Sunspot Surrounded by Pores, Solar Granulation and "Bright Points"

Genetic Algorithm Analyses of Massive Stars Massive stars are key ingredients in the evolution of the Universe. Their short lifetimes, intense radiatio fields and strong stellar winds modify their surroundings on short time-scales. To understand the variety of processes taking place in these stars, a large number of analyses under different conditions are needed using state-of-the-art, realistic model atmospheres. To facilitate this task and concentrate resources on the inetrpretation of results, the team developped an automatic tool for the model calculation and analysis. During 2008 this tool was implemented and demonstrated to work well. The first application, the analysis of the V478 Cyg system, will be carried out during the first half of 2009.

Overview

The ALTAMIRA Supercomputer

The ALTAMIRA node of the RES at the University of Cantabria is located in the Juan Jorda Building and is jointly managed by the IFCA Distributed Computing Team and the Computer Architecture Group (ATC) of the University of Cantabria.

IFCA (Instituto de Fisica de Cantabria) is a joint center of the University of Cantabria and CSIC with research lines in astrophysics, high energy physics and distributed computing, and participates in several national and European computing projects (including the Spanish e-Science Network, and FP7 projects such as EUFORIA or DORII).

The main research areas of the Computer Architecture Group (ATC) of the University of Cantabria are the analysis, design, and evaluation of parallel computers, covering their principal aspects from programming to the lower hardware levels.

Organisational Structure
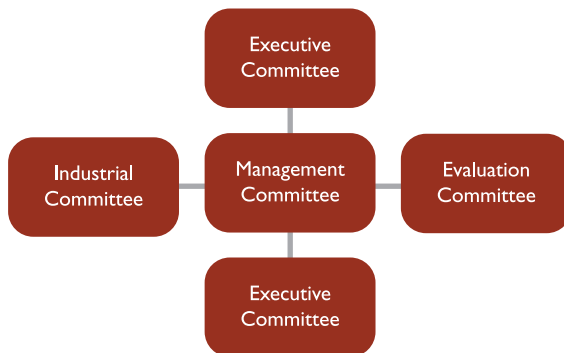
The ALTAMIRA node has dedicated technical support, with oversight by the scientific computing divisions of both IFCA and ATC. Also involved in managing the node are the managers of the computing research lines of IFCA and ATC.

The team from left to right: Luis Cabellos, Esteban Stafford, Rafael Marco, Ramon Beivide and Jesus Marco

Technical and Scientific Highlights 2008

In 2008 the Altamira node executed applications corresponding to local users at the University of Cantabria with a total of 1.2 million hours of CPU time.

Thanks to 360.000 hours of simulation in the Altamira node, UC researchers J. Junquera and P. Aguado published new results on the structure of ferroelectric ultrathin films (PRL 100, 177601).

The Ocean and Coastal Research Group of the University of Cantabria at the Environmental Hydraulics Institute used 320.000 hours to progress on studies like the application of the Cornell multi-grid coupled Tsunami model or the numerical modelling of wave interaction with low-mound breakwaters using a RANS model (Ocean Engineering 35(13), 1388-1400).

The astrophysics research Group at IFCA working on the study of Cosmic Microwave Background (CMB) advanced in the analysis of the non-gaussianity of CMB using different experimental results (Astronomy & Astrophysics 486, 383).

Key Publications 2008

Pablo Aguado-Puente and Javier Junquera, Ferromagnetic like Closure Domains in Ferroelectric Ultrathin Films: First-Principles Simulations, Physical Review Letters, 100, 177601 (2008)

Raul Guanche, Inigo J. Losada. Javier L. Lara, Numerical Analysis of Coastal

Structures Stability (2008). Coastal Engineering. ELSEVIER; An integrated approach to the analysis of coastal structures at prototype scale. Proceedings of the 31st International Conference on Coastal Engineering. ASCE (American Society of Civil Engineers).

I. Cabria, M. J. López and J. A. Alonso. "Shape of the Hydrogen Adsorption Regions of MOF-5 and its Impact on the Hydrogen Storage Capacity", Phys. Rev. B 78 (2008) 205432-205436.

A. Mañanes, F. Duque, A. Ayuela, M. J. López and J. A. Alonso, «Half-metallic finite zigzag single-walled carbon nanotubes from first principles", Phys. Rev. B, 78 (2008) 35432-35442.

Key Projects

Efficient density-functional calculations with atomic orbitals on nanosized ferroelectric nanostructures Led by Javier Junquera, a study of the behaviour of ferroelectric capacitors utilising the SIESTA program. The SIESTA program has been optimised for use in supercomputers by the BSC and its operation was trialled in the Altamira supercomputer. This activity has led to the authors publishing a number of articles and being invited to conferences in the field.

Storage of hydrogen in MOF-5 Led by Angel Mañanes Perez, a study on the storage of hydrogen in MOF-5. MOF-5 is highly porous and one of the most highly hydrogen absorptive substances. The DACAPO program was used in the Altamira to resolve DFT equations for solid materials.
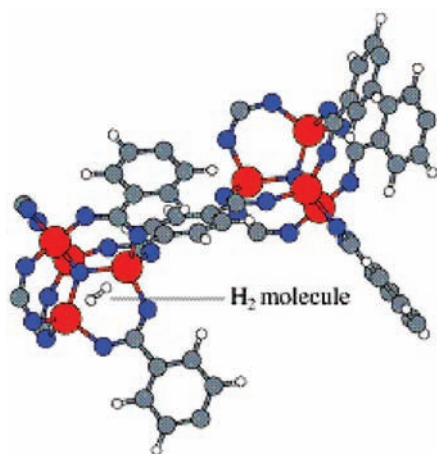
Molecular Scheme of the MOF-5 Material

Testing Gaussianity of CMB Maps Led by Enrique Martínez, the Group of Cosmic Microwave Background (CMB) of the Physics Institute of Cantabria undertook a number of different analysis projects. The Altamira was used in the analysis and detection of compact sources utilising data from the CMB Group. The project is financed by the National Research Plan.

Modelling of the structural mechanical response in high-rise buildings under real fire Led by Jorge A. Capote Abreu, a study and simulation of the propagation of fire in tall buildings, in order to predict the behaviour of fire in real situations. The Altamira supercomputer was used to resolve the fluid dynamic equations with which the fire was simulated. The project is financed by a Plan Nacional.
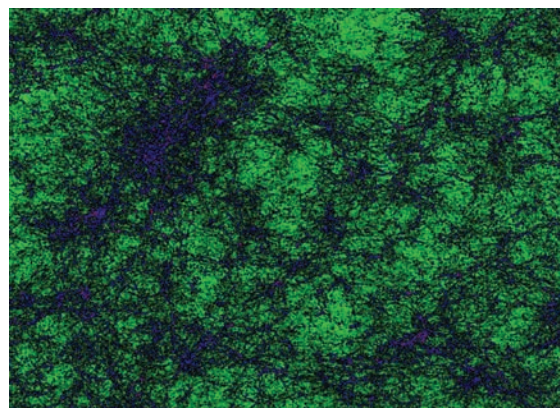
Simulated Maps of Structures in the Universe

Simulation at a Grand Scale of the N-body Universe Led by Jose María Diego, simulations of the universe utilising the Gadget-2 program. Gadget-2 is a highly parallelisable program and by using the Altamira it has been possible to run small simulations in reasonably short times, utilising up to 64 processor per execution. Larger simulations are planned for future execution periods.

Cornell Multi-grid Coupled Tsunami Model Led by Ernesto Mauricio Gonzalez Rodriguez, this activity is part of the European TRANSFER project (Tsunami Risk ANd Strategies For the European Region) which aims to improve understanding of tsunamis, in particular on European coastlines. Studies on floods of Cádiz and the Balearic Islands were run on Altamira.

Wave-structure interaction by the use of TRUCHAS Led by Iñigo Losada, a study in the 3-dimensional behaviour of wave structures using the TRUCHAS numerical method. The study also aims to validate the numerical results obtained by the Laboratory of the Oceanographic and Coastal Engineering Group (IH Cantabria).

Light scattering by micro-nano particles located on substrates Led by Pablo Alvella Echave, a study in the detection of defects in the micro structures of substrates used in the diffusion of light. The Altamira supercomputer was needed to advance from 2D calculations to 3D calculations and thereby enable the study of further situations. The project is financed by a Plan Nacional.

Overview

The Picasso Supercomputer

The Picasso node of the RES is located in the Bio-Innovation Building of the University of Málaga (UM) at the Technological Park of Andalusia (PTA), close to the city of Málaga. The computer is managed by the SCBI (Supercomputing and Bioinformatics Centre) of the UM, which runs several computational infrastructures supporting research activities within the University and in the Andalusian region, including the 512 CPU PowerPC-based cluster belonging to the RES, and a 128 CPU Itanium-based SMMP and a 80 CPU x86-based cluster belonging to the UM. All these resources share computer room, cooling, power and fire extinguishing systems.

Other remarkable resources include a virtualization infrastructure belonging to the Bioinformatics Platform of Andalusia, which hosts all its servers and the desktop systems as virtual machines running on a cluster of VMWare ESX servers.

Organisational Structure

SCBI team at Málaga (left to right):
Dario Guerrero Fernández (sysadmin)
Guillermo Pérez Trabado (manager)
Rafael Larrosa Jiménez (sysadmin)

The SCBI draws on 12 years of experience of the Computational Laboratory of the UM in running production supercomputers to support scientific research in several fields. It also incorporates a recently created research infrastructure, the Bioinformatics Platform of Andalusia, whose mission is to provide computational resources and commercial software licenses, and to transfer knowledge and experience on bioinformatics research to the scientific community in Andalusia.

The SCBI is an independent service with its own staff dedicated to administration of machines and user support, but also giving higher level support to researchers in the development of computational solutions for problems in several areas, especially biological research.

There is also strong cooperation with the Computer Architecture Department of the UM whose main research areas are analysis, design, and evaluation of high performance architectures, from the application level to the lower hardware levels.

Technical and Scientific Highlights 2008

After the initial test period, the Picasso node started offering service to its users at the beginning of February 2008.

On May 28th, SCBI and RES jointly organised a workshop for scientific users on applied supercomputing titled "Supercomputing Applied to Biology and Living Systems Simulation".

Key Publications 2008

L.F. Romero, Siham Tabika, Jesús M. Vías, Emilio L. Zapata, Fast clear-sky solar irradiation computation for very large digital elevation models, Computer Physics Communications, Vol. 178, Issue 11, June 2008, pp. 800-808

Key Projects

Parallel Programming Models and Compilers

Group on Parallel Programming Models and Compilers from the Computer Architecture Department of the University of Málaga.

In collaboration with George Almasi and Calin Cascaval and related with the project Parallel Programming and PGAS languages at IBM T.J. Watson Research Center, this Group has implemented an n-body algorithm (Barnes-Hut) using the IBM UPC compiler (xlupc). The Unified Parallel C (UPC) language is a parallel extension of the C language that provides a shared memory view of the physically distributed memory implemented in our IBM machine (pablo). This abstraction leads to a productive approach to the problem of exploiting an MPP architecture.

They are also exploring a library-based (STL-like) approach to provide a higher level of abstraction in order to more productively develop parallel codes based on recursive data structures for MPP architectures. This library will enhance the performance of the UPC run-time when dealing with pointer-based algorithms. Two important considerations will be to exploit the overlapping of communications and computations when possible and to also take advantage of that usually, in particular regions of the code, the traversed data structure is simpler than the real stored data structure.
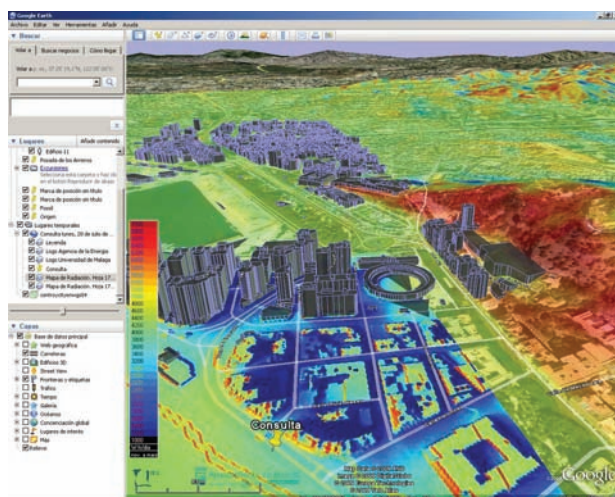
Projection of an Insolation Model on the Earth Surface, Using Google Earth.

High Precision Model of Solar Radiation

Luis F. Romero, researcher from the Parallel Applications Group of the Computer Architecture Group of the University of Málaga.

A high precision model of the incoming solar radiation was developed. This model has enabled the elaboration of an Insolation Atlas for Andalusia (with a precision of 10 metres) and a specific Insolation Atlas for Málaga (1 me-

tre precision). Merely analysing the shadows projected by tall buildings involves a large amount of CPU time (about 9700 hours for one map), however the high degree of parallelism obtained enabled the utilisation of up to 128 CPUs with efficiency close to 100%.

Andalusian Platform for Genomics, Proteomics, and Bioinformatics Research

Bioinformatics Platform of Andalusia

In collaboration with researchers of the Department of Molecular Biology and Biochemistry of the University of Málaga, three-dimensional folding models of enzymes and other proteins from conifers are being computed to study their structural and functional characteristics. The predicted characteristics represent a valuable resource to understand the function of this enzyme in plant amino acid metabolism.

The Group is also developing high performance computing workflows using its own tools to process data from genomics and proteomics projects which involve a large amount of input data which has to be analysed. These locally produced tools include SEQTRIM, FULL-LENGTHER and ALIGNMINER.
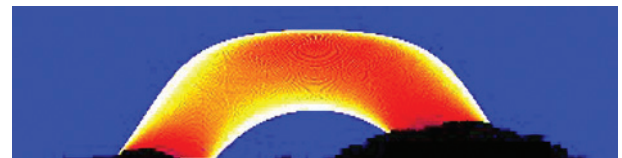
Integration of Energy Received Rrom Sun for an Specific Location on Earth Taking Into Account Horizon Elevation.

Overview

The TIRANT Supercomputer

The RES node located at the University of Valencia was inaugurated in January 2008. The supercomputer is called Tirant, in reference to the main character of the book "Tirant lo blanc", written in the Valencian language in 1490 by Joanot Martorell. The node is installed on a data center specially designed to host it and is managed by technicians of the Servei d'Informàtica de la Universidad de Valencia (SIUV). The SIUV has a long tradition in managing supercomputers: since 1978, the service has been central to the university's efforts in the field of scientific computation. The SIUV also hosts the RedIris PoP of the Valencian region, the network infrastructure of the university, the central database, the university web page, e-mail services, application services, etc.

Organisational Structure

Tirant is managed by technicians from SIUV, an IT Group led by its director. Three technicians are responsible for the system management (dealing with hardware problems, installation and configuration of software) and user support (compiling scientific programs, managing the system queue, solving other users' problems). The access committee is responsible for assigning the CPU hours among Tirant users by evaluating new projects.
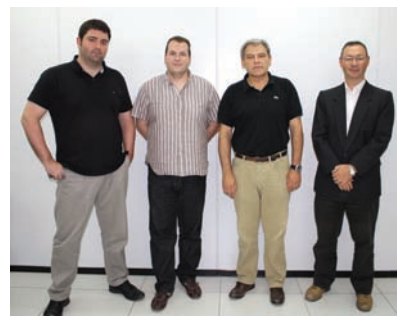
From the left: Gabriel Aparicio - System Analyst, Alejandro Soriano - System Analyst, Salvador Roca - IT Group Director, Jose María Gonzalez - Operator

Technical and Scientific Highlights 2008

In 2008, Tirant offered 1.1 million CPU hours of which some 80% was made available to the RES and the rest was made available to all the scientific community of the Valencia region, including researchers at the University of Valencia.

Key Publications 2008

R. Casasús, E. Climent, M.D. Marcos, R. Martínez-Máñez, F. Sancenón, J. Soto, P. Amorós, J. Cano, E. Ruiz, "Dual aperture control on pH- and anion-driven supramolecular nanoscopic hybrid gate-like ensembles", J. Am. Chem. Soc., 2008, 130, 1903-1917.

P. Hernandez, M. Laine, C. Pena, E. Torro, J. Wennekers, H. Wittig, Determination of the Delta S = 1 weak Hamiltonian in the SU(4) chiral limit through topological zero-mode wave functions, JHEP 0805 (2008) 043.

L. Giusti, P. Hernandez, S. Necco, C. Pena, J. Wennekers, H. Wittig, Testing chiral effective theory with quenched lattice QCD, JHEP 0805 (2008) 024.

B. Blossier et al. (ETM Collaboration), Light quark masses and pseudoscalar decay constants from N(f)=2 Lattice QCD with twisted mass fermions, JHEP 0804:020,2008

Aloy, M.A., Mimica, P., Observational Effects of Anomalous Boundary Layers in Relativistic Jets, ApJ, 681, 84 (2008)

Giannios, D.; Mimica, P.; Aloy, M. A., On the existence of a reverse shock in magnetized gamma-ray burst ejecta, A&A, 478, 747 (2008)

Mimica, P.; Giannios, D.; Aloy, M.-A., An RMHD study of transition between prompt and afterglow GRB phases, (2008), arXiv0801.1325

Key Projects
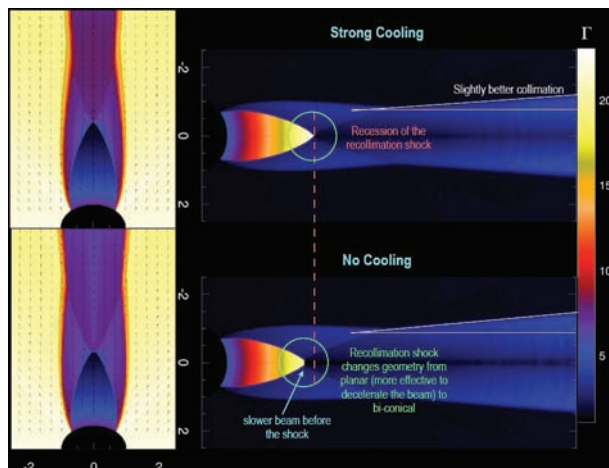
Cooling & Collimation of Subpcscale Jets

Explaining blazars and gamma-ray bursts with numerical relativistic magneto-hydro-dynamics
Led by Miguel Ángel Aloy Torás, this project is related to coupling relativistic plasma (magneto-)hydro-dynamics to non-thermal emission in order to provide synthetic models that explain the observed electromagnetic patterns of some astrophysical sources (blazers, gamma-ray bursts and relativistic jets).
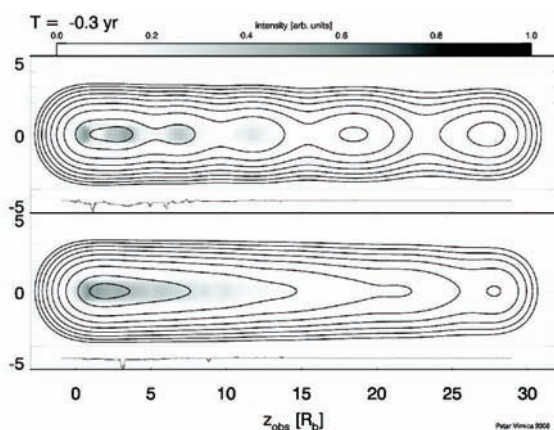
Radio Imaging of a PC-Scale Jet

Numerical simulations of hadron properties
This is a project led by Vicent Giménez Gómez and the main goal is to quantitatively describe and predict, using numerical simulations of the Quantum Chromodynamics (QCD), the properties of hadrons, mesons and baryons, like the proton and the neutron which form the nucleus of all the atoms.

Coupling of gold catalyzed hydrogenation of nitroaromatics with selective alcohol oxidation
This project is led by Mercedes Boronat Zaragozá and its general objective is to prepare hybrid organic-inorganic nanoporous and mesoporous materials and use them as sensors, catalysts and for H2 storage.

Analysis of CRISPR Sequences present in Metagenomes
Led by Francisco Rodríguez-Valera, this project contains one research line of exploratory metagenomics concentrating mostly on the microbiota of the Mediterranean Sea, producing archives, in the form of metagenomic libraries and gene sequences in databases. It represents an invaluable genetic heritage useful for specialized studies.

Enzymatic hydrolysis of phosphoesters. A free energy surface exploration
Understanding the mechanism of the enzymatic catalysis is a way to allow us to create artificial catalysts with industry oriented purposes. Led by Ignacio Tuñón, this project tries to elucidate the mechanism of one of them: the hydrolysis of phosphoesters done by an alkaline Phosphatase.

Flavour Physics from Mixed-action Lattice QCD
The final goal of the project led by Pilar Hernández is to determine the low-energy couplings of the Chiral Lagrangian that are relevant in flavour physics, beyond the quenched approximation.

Long-term simulations of kiloparsec scale jets: Evolution, morphology and feed-back
The aim of the project led by Manuel Perucho Pla is to study the impact of the jets in the galactic and cluster gas in detail in order to use this result as information for cosmological simulations.
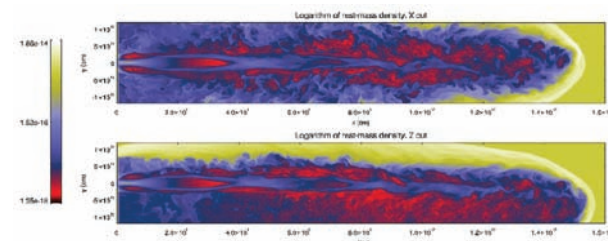
Microquasar Jets With RATPENAT (3D Simulations)

Overview
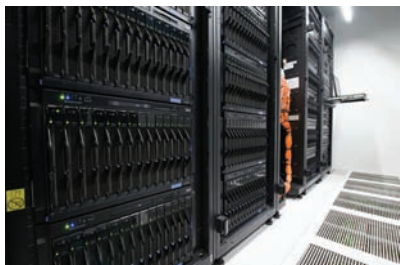
The CAESARAUGUSTA Supercomputer

Located at the Faculty of Science of the University of Zaragoza, the CAESARAUGUSTA supercomputer was one of the initial seven founding nodes of the RES. It is managed by the Supercomputing Area of the Institute for Biocomputation and Physics of Complex Systems (BIFI).
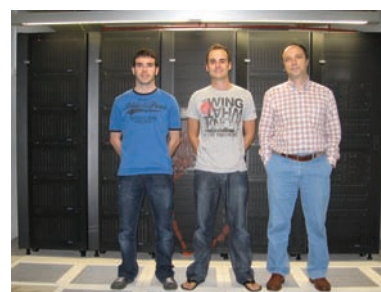
BIFI is a research institute that promotes interdisciplinarity to develop competitive research in computation applied to physics of complex systems and biological systems. Despite its youth, the Institute has already developed intensive research activity in several fields of computation: cluster, grid computing, dedicated computers (FPGAs) and volunteer computing.

Organisational Structure

CAESARAUGUSTA is maintained by technical staff of the Supercomputing Area at BIFI. This includes hardware and software administration as well as first level user support, all of which is coordinated with the BSC-CNS operations department.

There is also a local Access Committee which manages the 20% of the CPU time which is at the disposal of the University of Zaragoza. This time is assigned by the Committee after evaluating the applications received for each four-month period (coinciding with RES schedule). During 2008, the members of the local Access Committee were:

CAESARAUGUSTA Operations Team
Arturo Giner (BIFI's sysadmin),
Guillermo Losilla
(BIFI's computing manager),
Alfonso Tarancón (BIFI's secretary professor
& Head of the Computing Area)

▶ Pablo Ibáñez Marín. Professor at Departamento de Informática e Ingeniería de Sistemas and member of Grupo de Arquitectura de Computadores UZ (gaZ)

▶ Luis Rández García. Professor at Departamento de Matemática Aplicada and member of Instituto Universitario de Matemáticas y Aplicaciones UZ (IUMA)

▶ Alfonso Tarancón Lafita. Professor at Departamento de Física Teórica and secretary professor at Instituto de Biocomputación y Física de Sistemas Complejos UZ (BIFI)

Technical and Scientific Highlights 2008

Although the CAESARAUGUSTA supercomputer commenced operating in November 2007, the node was officially inaugurated on 13 February 2008 in the presence of Aragón's President, the Rector of the University of Zaragoza, the BSC Associate Director and BIFI's Director, among others.

2008 was a year of consolidation for CAESARAUGUSTA with a total of 14 local projects accepted by the local Access Committee, utilising 1.200.000 hours of CPU time. These activities have produced numerous scientific results and publications.

Key Publications 2008

A detailed account of scientific results can be found in Los Alamos' preprint server: http://arxiv.org/abs/0905.0322 (currently under peer review in a Physics journal)

Angarica, V.E., Cuesta-Lopez, S., Estrada, J. and Sancho, J. (2008). Conformational Changes of the LDL-r LA5 Module Upon Mutation: a Computational Approach. XXXI Congress of the Spanish Society for Biochemistry and Molecular Biology, Bilbao, Spain (Poster Presentation)

Ciegis, R.; Gaspar, F.J., Rodrigo C. *On the parallel multiblock geometric multigrid algorithm.* CMAM 8 (2008) 223-236

Introducing Chaos in Economic Gas-Like Models Carmen Pellicer-Lostao and Ricardo López-Ruiz Proceedings of the 2nd Chaotic Modeling and Simulation International Conference MAICh Conference Centre, Chania, Crete, Greece

Key Projects

Heisenberg Spin Glasses: Large Lattices at Low Temperatu res Led by Víctor Martín Mayor, a study of the glass transition for Heisenberg spin glasses. This is a major computational challenge, requiring thermal equilibrium at very low temperatures for a large number of samples. The results suggest that Heisenberg spin glasses order at a low (but finite) temperature, and show ordering both in the spin and chiral sectors.
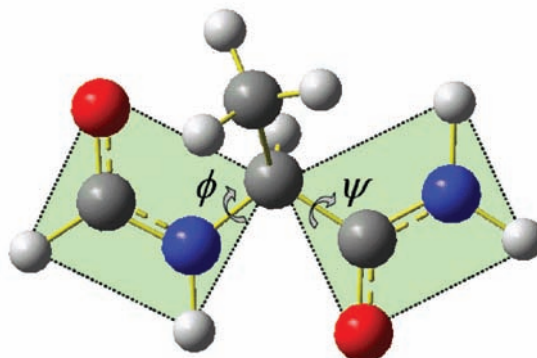
The search for efficient Quantum Chemistry methods to study the conformational preferences of peptides Led by Pablo Echenique, (BIFI, Theoretical Physics Department UZ), this project searches for a quantum chemical potential energy function that is accurate enough to describe the relevant processes in the simulation of biological molecules such as peptides and proteins, yet presenting the lowest possible numerical cost.

Quantum mechanics modeling of support-enhanced enantioselective heterogeneous catalytic reactions Led by José Antonio Mayoral Murillo, a study of the nature of a catalyst, (bisoxazoline-copper complexes) attached to an inorganic support. The project modeled the stability and association mechanisms of the organometallic complexes to the surfaces, involving intensive parallel DFT calculations to optimize the geometries of the reactants and their characterization by frequency calculations.

Prediction of conformational diseases from simulation Led by Javier Sancho Sanz (BIFI, Department of Biochemistry and Molecular and Cellular Biology UZ), a study of mutations in the gene encoding the low-density lipoprotein receptor, which is linked to the conformational disease familial hypercholesterolemia. Simulations were run of mutations to develop an anticipated computational diagnosis strategy to assess the structural implications and probability to give rise to disease. This analysis identified a Group of SNPs which have not been previously described that could be related to the disease.
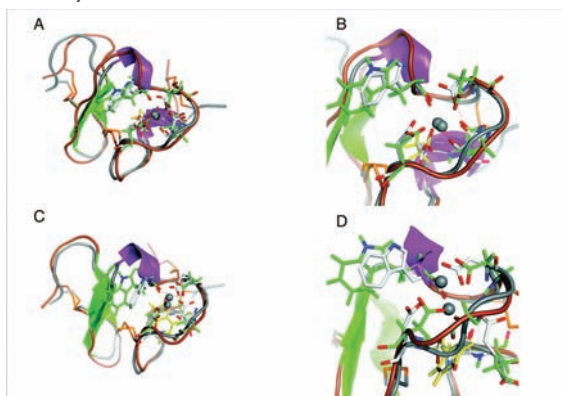
Dipeptide Formil-Alanina-Amida

Many-body expansion of the quantum chemical energy surface of biological molecules. Towards a new type of force fields Led by Pablo Echenique (BIFI, Theoretical Physics Department UZ), this project pursues the application of the many-body expansion of potential energy functions to the reduction of the cost in the calculation of the conformational preferences of biological molecules with quantum chemical methods. The project is still in progress.

Parallel geometric multigrid Led by Francisco José Gaspar Lorenz a study of a parallel multiblock geometric multigrid that was applied to solve a two-dimensional poroelastic model. A new strategy for the solution of the discrete problem on the coarsest grid was proposed and the efficiency of the obtained algorithm was investigated.

Application of chaotic systems to cryptography and other statistical problems Led by Ricardo López Ruiz, this project had two objectives, the generation of random and chaotic sequences of binary numbers based on nonlinear dynamical systems, and secondly its application to produce simulation scenarios in the field of Econophysics.

Simulation-based estimation of peer group effects in the decision of participating in drugs markets Led by José Julián Escario & Rosa Duarte, the estimation of a structural econometric model of peer effects in binary choice by simulated maximum likelihood. The model uses the joint distribution of all the binary decision of the Group as a multivariate normal distribution. Thus, the estimation of the model requires the evaluation of a complex multidimensional integral.

Global and Coordinating Site Structural Fluctuations of the LDL-A Module Upon Mutation

Assimilation of High Resolution Precipitation Estimates in an Ensemble of Numerical Models, Francisco J. Tapiador, Universidad de Castilla-La Mancha en Toledo
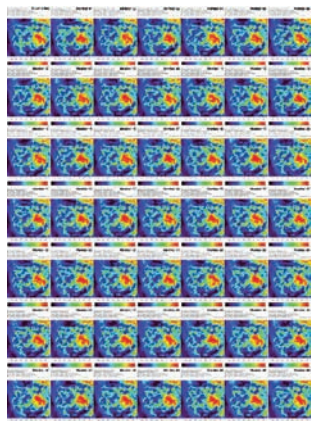
High-resolution forecast of accumulated daily precipitation in the Iberian MareNostrum in 2008

Abstract The aim of this project is to evaluate the performance of a standard NWP when three-dimensional high-resolution satellite-derived rainfall estimates are assimilated using variational methods. The working hypothesis is that the assimilation of the satellite rainfall estimates will improve the forecasts of extreme events, including hurricanes. To validate this idea, the project will use an extensive set of physical parameterizations accounting for microphysical processes in clouds. This activity is supported by the CICYT project ASPRES and is done in collaboration with NASA's ground validation GPM activities.

Results The results show that large differences appear depending on the physical parameterization used. The future perspectives will be to investigate the effects of perturbed initial conditions in the ensemble, and to compare those with the physical ensemble results.

Gaia: Simulation of Telemetry Stream, Jordi Torra i Roca, Universitat de Barcelona

Abstract The Gaia mission will provide positional, kinematical and physical data with unprecedented accuracy of about one billion stars in our Galaxy and throughout the local Group. The design and data management system must be implemented as an integral and critical part of the mission. The project has developed simulators of the mission, GASS and GOG, which include physical models of the objects that will be observed by the satellite, as well as of the on-board instrumentation and the operation mode of the satellite. The data generated are used in the development and testing of the data management system and the reduction processes which are the goals of the DPAC consortium of over 300 researchers throughout Europe.
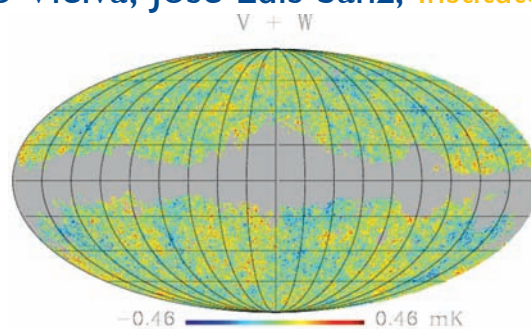
Errors in the Star Position Determination as a Function of Star Brightness, Obtained From Radiation-Damaged (left) and Undamaged (right) Simulations.

The Intermediate Data Updating module is the most demanding process in the whole Gaia data reduction pipeline; its implementation in MareNostrum is a key goal of mission development. One of the main features of IDU will be the mitigation of radiation effects on the data reduction pipeline.

Results Due to the complex models used by GASS, GOG and IDU, the processing requirements are huge. E.g., the generation with GASS of 3 seconds of realistic data in a very crowded area of the Galaxy would require 10 hours in a home PC. The GOG simulator similarly has massive processing requirements. IDU is the most demanding process of the Gaia data reduction, with a simulation run scheduled every 6 months. Each run is incrementally more complex, both in the universe and instrument models, and generates increasingly larger amounts of data, progressively approaching the actual volume to be generated by Gaia. Only the use of the MareNostrum supercomputer allows the periodic generation of these amounts of data in such short, recurrent periods and with increasing realism and data volumes.

Gaia photometry and spectroscopy. Highlights of Spanish Astrophysics V: Y. Isasi, X. Luri, A. Robin et al., Gaia Universe Model Snapshot. Highlights of Spanish Astrophysics V: J. Portell, J. Castañeda, Y. Isasi, C. Fabricius, X. Luri, J. Torra, D. Vicente, Massive parallelization of a space mission simulator and data processing system. Highlights of Spanish Astrophysics V: E. Masana, Y. Isasi, X. Luri, J. Peralta, El simulador de la misión GAIA: diseño y resultados. Highlights of Spanish Astrophysics V: X. Luri et al., Preparación del procesado de datos de Gaia: primeros resultados.

Study of the non-Gaussianity of the CMB, Enrique Martínez González, Andrés Curto, R. Belén Barreiro, Patricio Vielva, José Luis Sanz, Instituto de Física de Cantabria

V + W

-0.46 0.46 mK

Map of the Cosmic Microwave Background Temperature

Abstract The Cosmic Microwave Background Radiation (CMB) has become an important research tool in Modern Cosmology with a large number of on ground, balloon-borne and satellite experiments currently operating and/or planned for the near future. The existence of the CMB is a proof of the primordial explosion widely-known as Big-Bang. The anisotropies of the black body radiation temperature measured in different directions of the sky provide valuable information about the primordial times of the universe and its evolution. The standard inflation theory, developed in the 1980's and nowadays widely accepted, predicts that these anisotropies follow very closely a Gaussian random field. The detection of non-Gaussian deviations in the CMB would have far-reaching consequences for our understanding of the universe.

Results Several tests were run to study the statistical distribution of the CMB anisotropies, based on cubic statistics of spherical wavelets, Minkowski functionals and the n-point distribution function. Consistency with the Gaussian hypothesis was found for both Archeops and WMAP data. In addition, strong constraints have been imposed on the non-linear coupling parameter fnl characterizing non-standard models of inflation. The algorithms applied in these activities were developed by the Observational Cosmology and Instrumentation Group at the Instituto de Física de Cantabria, and will be applied to the data that will soon be measured by the ESA Planck mission.

Publications "Constraints on the non-linear coupling parameter fnl with Archeops data", A. Curto et al., Astronomy and Astrophysics, 2008, vol 486, pag 383.

The MareNostrum Numerical Cosmology Project: Grand Challenge simulations of structure formation in the Universe, Gustavo Yepes Alonso, Universidad Autónoma de Madrid
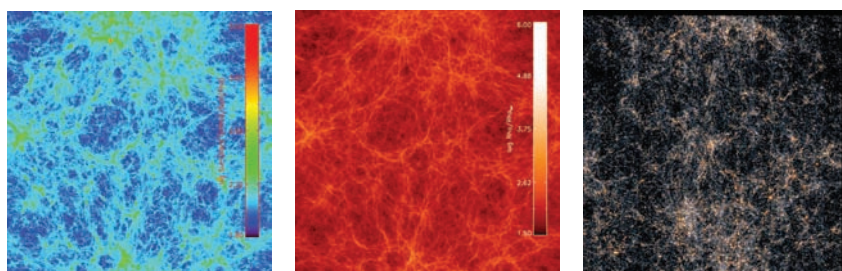
Left: A Slice Cut Through the 50 Mpc Box Showing the Temperaure of the Gas at z=5.4
Middle: A Slice Cut Through the 50 Mpc Box Showing the Gas Density at z=5.4
Right: Mock CCD Image of the Galaxies in the 50 Mpc Box Simulation

Abstract The aim of this project is to test the capability 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.

Results Several world-record simulations were successfully completed - the MareNostrum Universe: The largest SPH simulation of Large Scale Structure formation, and the MareNostrum Galaxy Formation Simulation: The largest simulation of galaxy formation at high redshift.

Thanks to the large number of processors available in MareNostrum the project was able to solve problems in a manner not possible only a few years ago.

Publications A list of publications and presentations in international meetings can be found at the home page of the MNCP project http://astro.ft.uam.es/marenostrum

Scavenging Properties of Truncated Hemoglobin N from M. Smegmatis, Enrique F. J. Luque, Universidad de Barcelona
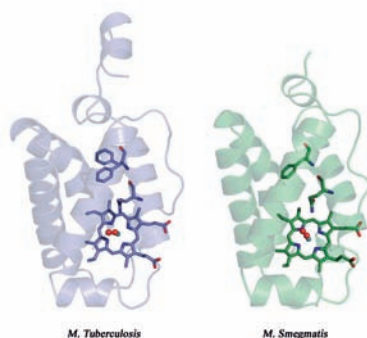
Abstract Nitric oxide is a signalling and defense molecule of major importance, but the basis of resistance to NO and nitrosative stress is poorly understood in many microbes. In the case of M. tuberculosis, it appears to be associated with the truncated hemoglobin N, which would convert NO into the harmless nitrate anion. In order to verify the suitability of this mechanism, the project used molecular dynamics simulations to compare the structural, dynamical and functional properties of the truncated hemoglobins N from M. tuberculosis and M. smegmatis.

Results Extended molecular dynamics (MD) simulations enabled the project to unravel the molecular mechanisms that control diatomic ligand diffusion through the apolar tunnel system detected in the protein matrix. Our studies suggest a ligand-induced dynamical regulation mechanism, by which binding of O2 to the heme triggers the opening of the gate that would regulate the access of NO through the long branch of the tunnel. 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 coordination to Fe(III). In addition, a new eggresion pathway to the bulk solvent has been identified. Finally, our studies also highlight the unsuspected crucial role played by pre-A segment, which affects the dynamical interplay that modulates opening of the tunnel gate. Overall, the results suggest a delicate relationship between the structural and dynamical features of the protein, and the functional role played by truncated hemoglobin N in NO detoxification.

Use of TBLASTX to Find Regions of Homology Among Multiple Large-size Full Genomes, Roderic Guigó, Centro de Regulación Genética, Barcelona

Abstract In this project, the MareNostrum was used to run the computationally intensive algorithm TBLASTX to find regions of homology between two full genomes (Mouse vs. Human). MareNostrum´s processing speed enables the execution of TBLASTX to find homologies among many different genomes at the same time and in a reasonable time frame.

Results A MareNostrum-optimized version of the TblastX algorithm was used to look for orthologous regions between different assemblies of Human and Mouse genomes, to compare versions of the Bovine genome against previous assemblies of these species, to look for matches between the Rat genome and older assemblies of the Human genome, to analyze assemblies of the several other mammals of interest, and to annotate the Bovine genome. SPG homology-based annotations of the Mouse, Rat, Human, Cow and Chicken, many of which were obtained with the help of MareNostrum, can be seen at the golden path (UCSC- genome.ucsc.edu) genome browser.
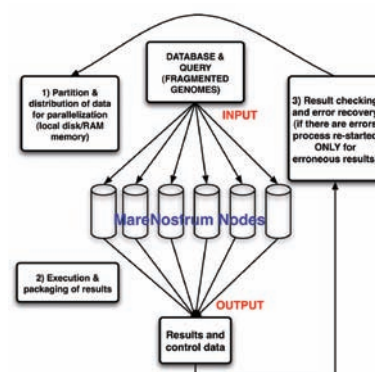
Tblastx MN Pipeline

Maximum-Likelihood Refinement of Electron Microscopy Data, Jose Maria Carazo & Sjors Scheres, Centro Nacional de Biotecnologia - CSIC

Abstract The co-existence of macromolecular complexes in distinct conformational states is a major problem in 3D electron microscopy, as the inability to separate them limits the resolution obtained and, more importantly, loses information about the instinct functional states of the molecules under study. The Group developed a series of novel algorithms based on maximum-likelihood principles that allow separation of structurally heterogeneous data sets into distinct homogeneous subsets, improving on the statistical description of the abundant experimental noise in cryo-electron microscopy data and allowing classification of data sets without the necessity for a priori information about the structural variability.

Results A novel statistical model for electron microscopy data was formulated and corresponding maximum-likelihood algorithms were proposed, implemented and tested on several simulated and experimental data sets. A standardized workflow and graphical user interface was designed for image processing in the Group´s freely available scientific software package Xmipp. Also the ML3D classification was successfully applied to obtain new biological insights from various data sets, including the 70S ribosome, molecular chaperonin CCT and the 26S proteasome.

Publications S.H.W. Scheres, R. Nuñez-Ramirez, C.O.S. Sorzano, J.M. Carazo & R. Marabini, "Standardized image processing of electron microscopy data using Xmipp", Nat. Protoc., 3, 977-990, (2008). J. Cuellar, J. Martin-Benito, S.H.W. Scheres, R. Sousa, F. Moro, E. Lopez-Viñas, P. Gomez-Puertas, A. Muga, J.L. Carrascosa & J.M. Valpuesta, "The structure of a CCT:Hsc70NBD complex suggests a mechanism for Hsp70 delivery of substrates to the chaperonin", Nat. Struct. Mol. Biol., 15, 858-864, (2008). P. Julian, A.L. Konevega, S.H.W. Scheres, M. Lazaro, D. Gil, W. Wintermeyer, M.V. Rodnina & M. Valle, "Structure of Ratcheted Ribosomes with tRNAs in Hybrid States", Proc. Natl. Acad. Sci. U S A, 105, 16924-16927, (2008).
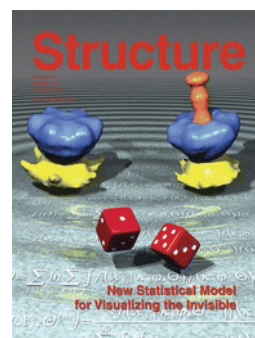
Scanned Cover of October Issue of Structure

Molecular Modeling of Enzyme-substrate Interactions and Reaction Mechanisms in Carbohydrate-bound Enzymes and Aldo-keto Reductases, Miquel Carme Rovira, Parc Científic de Barcelona

Abstract The project aims to decipher the mechanisms of substrate specificity in aldo-keto reductases (AKRs), glycoside hydrolases (GHs), and glycosyl transferases (GTs) by means of ab initio QM/MM simulations. Aldo-keto reductases (AKRs) are responsible for a wide variety of biological functions and have recently been recognized to have activity with retinoic acids. The project investigates the structural factors for this specificity.

Results (a) Kinetic measurements of the activity of the enzyme with different substrates show that the AKR1B10 enzyme has a high activity with all-trans-retinaldehyde (a precursor of retinoic acid, an anticancer agent). Simulations show that the Lys125 at the entrance of the binding pocket is responsible for the specificity (it induces a change of loop conformation when the substrate binds). This was confirmed by site-directed mutagenesis. These results should facilitate the design of specific inhibitors, with potential use in cancer and diabetes treatments.

Glycoside hydrolases are the enzymes that break the glycosidic bond in carbohydrates. In collaboration with the Group of A. Planas (Biochemistry Lab. IQS) the way the substrate changes shape during catalysis was determined at the atomic level. The results are important for the design of specific inhibitors for these enzymes.
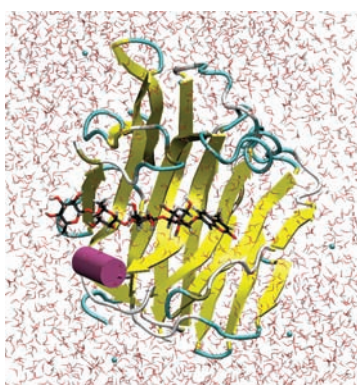
Setup of the E•S Complex of 1,3-1,4-Beta-Glucanase
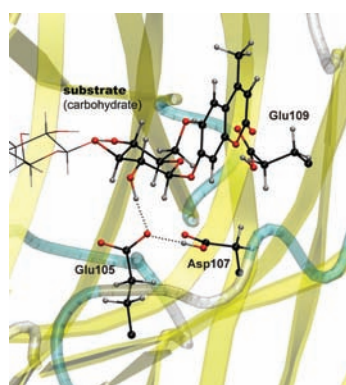
Elis Complex of 1,3-1,4-Beta-Glucanase
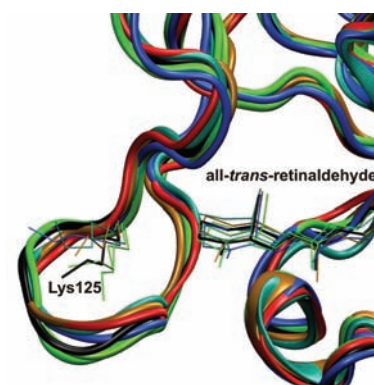
Conformational Free Energy Landscape of Beta-D-Glucopyranose

Publications O. Gallego, F. X. Ruiz, A. Ardèvol, M. Domínguez, R. Àlvarez, A. R. de Lera, C. Rovira, J. Farrés, I. Fita, X. Parés. "Structural basis for the high all-trans-retinaldehyde reductase activity of the tumor marker AKR1B10". Proceedings of the National Acadademy of Sciences USA. 104, 20764-20769 (2007); F. Xavier Ruiz, O. Gallego, A. Ardèvol, A. Moro, M. Domínguez, R. Alvarez, A. R. de Lera, C. Rovira, I. Fita, X. Parés, J. Farrés. "Ring-oxidized retinoid specificity and retinoic acid signaling of aldo-keto reductase AKR1B10". Chemico-Biological Interactions. Accepted; 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". Journal of the American Chemical Society. 129, 10686-10693 (2007); X. Biarnés, J. Nieto, A. Planas, C. Rovira. "Substrate distortion in the Michaelis complex of Bacillus 1,3-1,4-beta-glucanase. Insight from first principles molecular dynamics simulations". Journal of Biological Chemistry. 281, 1432-1441 (2006).

➤ Computational design of new catalysts based on nanoparticles, Francesc Illas, Universitat de Barcelona
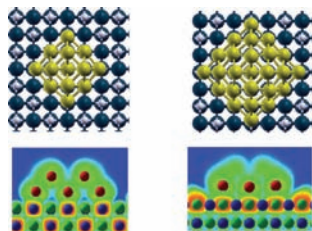
A New Catalysts Based on Au Nanoparticles Supported on TiC

Abstract Catalytic performance of supported metals can be dramatically improved either by changing the nature of the support (e.g. carbides instead of oxides) or when the support is in the form of nanoparticles rather than bulky samples. This work addresses two issues: on one hand, catalytic performance of Au nanoparticles supported on TiC and, on the other, the focus is on determining smallest ceria nanoparticles, for which adsorption parameters become almost independent of the particle size. For the former experiments DFT calculations have been carried out whereas for the latter, adsorption of a CO probe molecule on a particular surface site of series of model nanoparticles containing ~ 50-230 atoms was calculated using the DFT+U approach.
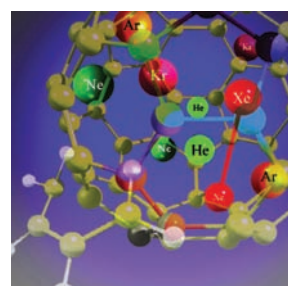
Results First, it was found that isolated Au nanoparticles have a critical size towards molecular oxygen. It was also shown that Au nanoparticles supported in TiC have enhanced catalytic properties over more current systems where the particles are supported on oxides. The main reason for this catalytic effect is the strong polarization of the metal nanoparticle. For the ceria nanoparticles and, in line with results of previous cluster-size convergence studies for other substrates, geometric parameters of adsorption complexes of the probe CO adsorbate on (CeO2-x)n clusters vary only very slightly with the particle size, whereas the calculated adsorption energy Ead exhibits a rather strong dependence on the size. These results enable the usage of model (CeO2-x)n clusters with n larger than 40 in future electronic structure calculations of interactions with nanostructured ceria species that take place in recently proposed catalysts.

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➤ Endohedral fullerene chemistry: exohedral reactivity of Ng2@C60 (Ng= He, Ne, Ar and Kr), Miquel Solà Puig, Universitat de Girona

Abstract The aim of this activity is to study the exohedral reactivity of the endohedral compounds Ng2@C60, Ng= He, Ne, Ar and Kr. In particular, measuring and comparing the thermodynamics and kinetics of the [4+2] Diels-Alder cycloaddition for all different reactive bonds of the noble gas endohedral fullerenes. This is of interest due to the possible application of these materials in the fields of biology, nano-technology, and medicine.

Non-Equivalent Bonds of Fullerene Containing Noble Gas Dimers

Results It was shown that the exohedral reactivity of He2@C60 or Ne2@C60 is similar to that of free C60, while for the other Ng dimers a more reactive fullerene cage is observed. Similar to C60, the most reactive bonds are the pyracylenic [6,6] bonds. The reactivity of Xe2@C60 is substantially different and becomes extremely exothermic and highly unselective. This unexpected finding is attributed to the encapsulation of larger noble gas atoms inside C60 which leads to a highly reactive strained fullerene. The reaction induces pyramidalization of the attacked carbon atoms and breaks the C-C bonds giving additional space to accommodate the noble gas dimer.
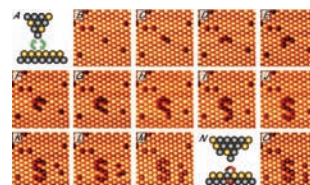
Publications S. Osuna, M. Swart and M. Solà. "Study of the Diels-Alder reaction on the noble gas endohedral fullerenes Ng2@C60 (Ng= He, Ne, Ar, Kr, and Xe)". In preparation.

➤ Interaction of Atoms and Molecules with metals and metallic oxides characterized by first-principles calculations and simulations of surface imaging techniques, Rubén Pérez, Departamento de Física Teórica de la Materia Condensada, Universidad Autónoma de Madrid

Abstract The Group performed first-principles simulations (working in close collaboration with experimental Groups) to gain insight into the interaction of atoms and molecules with metal and oxide surfaces. The work focused on the development of imaging and manipulation tools for Nanotechnology, such as Atomic Force Microscopy (AFM), and the possibility to induce controlled chemical reactions at the nanoscale (Nanochemistry).


Creation of atomic patterns displaying the symbol of silicon by vertical interchange atom manipulation with AFM at room temperature.

Results In collaboration with Seizo Morita in Osaka University (Japan), an efficient method was developed to produce atomic-scale surface patterns based on the interchange of atoms between the AFM tip and the substrate: atomic "dip-pen" nanolithography (Science 2008). The first-principles calculations with simplified tip-models were designed to understand the interplay between purely mechanical and thermally-activated processes driving these vertical atomic interchanges. These simulations covered the characterization of key atomic structures and the magnitude of the energy barriers between the relevant atomic configurations leading to vertical manipulation. As part of a multidisciplinary team including also the Institute of Materials Science of Madrid, the Center for Astrobiology and the Catalan Institute of Chemical Research, a new method was developed for the controlled synthesis of closed heterofullerenes from planar precursors (Nature 2008).

Publications Y. Sugimoto, P. Pou, O. Custance, P. Jelinek, M. Abe, R. Perez and S. Morita "Complex patterning by vertical interchange atom manipulation using atomic force microscopy." SCIENCE 322, 413-417 (2008); G. Otero, G. Biddau, C. Sánchez-Sánchez, R. Caillard, M. F. López, C. Rogero, F.J. Palomares, N. Cabello, M.A. Basanta, J. Ortega, J. Mendez, A.M. Echavarren, R. Pérez, B. Gómez-Lor and J.A. Martín-Gago "Fullerenes from aromatic precursors by surface-catalysed cyclodehydrogenation." NATURE 454, 865-868 (2008); P. Jelinek, R. Perez, J. Ortega and F Flores "Ab-initio study of the evolution of the mechanical and transport properties of clean and contaminated Au nanowires along the deformation path." Physical Review B 77, 115447 (2008); P. L. de Andres, R. Ramirez and J.A. Verges, "Strong covalent bonding between two graphene layers" Physical Review B 77, 045403 (2008); M. Blanco-Rey, K Heinz & P.L. de Andres, "Quantitative LEED analysis using a simultaneous optimisation algorithm.", J. of Phys: Cond. Matt. 20, 304201 (2008); J. Sanchez, J. Fullea, C. Andrade and P.L. de Andres, "Hydrogen in alpha-iron: stress and diffusion", Phys. Rev. B. 78, 014113 (2008); N. Rey, A Munoz, P. Rodriguez-Hernandez and A.San Miguel, "First-principles study of lithium-doped carbon clathrates under pressure" J. of Phys.: Cond. Matt. 20, 215218 (2008).

## Properties of the Metal/Metal-Oxide Interface. First-Principles Computational Simulations, Miquel Javier Fernandez Sanz
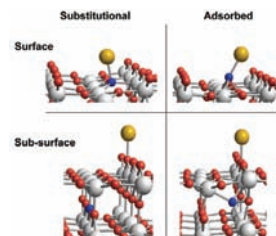
Optimized structures of Au atom deposited on N doped TiO2(110) rutile surface

Abstract An exhaustive investigation of the electronic properties of Au deposited atoms and clusters on doped TiO2(110) surfaces was performed using a realistic model and density functional periodic calculations. N and C doping induces the appearance of in gap states, shrinking of the band gap, and other electronic features in the band structure. Oxygen vacancies were found to cooperatively interact with C and N implanted atoms. Preadsorbed Au clusters stabilize implanted N atoms showing a synergistic effect. Au/N-TiO2 system was found to be a highly active catalyst in the WGS reaction.

Results The calculations show the appearance of localized in-gap states that could be responsible for an enhancement of photo activity under visible light. The stability of different sites, as well as the possible formation of diatomic species preadsorbed on the surface (NO, CO) was clarified. Au preadsorption on TiO2 surfaces significantly increases the reachable amount of N implanted in the oxide. An outstanding consequence of this new method for N-doping is that by controlling the N:V ratio the strength of the metal-support interaction and the oxidation state of the supported gold atoms in contact with the surface could be controlled. Moreover the Au/TiNxO2-y system was found to be active in two main processes for the production of H2: the dissociation of water and the water-gas shift (WGS) reaction. Both processes play a key role as a source of clean hydrogen to be used in fuel cells. For water splitting, the experiments showed the Au/TiNxO2-y system to be more active than both stoichiometric and reduced TiO2 surfaces, and even better than Au/TiO2. In the WGS reaction, the Au/TiNxO2-y surfaces were able to catalyze the production of hydrogen at elevated temperatures (575-625 K) displaying a catalytic activity superior to that of pure copper or supported Cu nanoparticles, the current standard in industrial applications. Co-adsorption with Au is therefore an attractive approach for facilitating the embedding of N in oxide photocatalysts and for enhancing the adhesion of Au clusters on the surface. In addition to N doped surfaces, catalysts based on Cu/TiO2 and CeOx/TiO2 systems were found to display a high activity in the WGS process.

Publications J. Graciani, A. Nambu, J. Evans, J.A. Rodriguez, and J. F. Sanz, "Au-N Synergy and N-Doping of Metal Oxide-Based Photocatalysts", J. Am. Chem. Soc. 2008, 130, 12056, J. Oviedo, R. Sánchez-de-Armas, M.A. San Miguel J. F. Sanz, "Methanol and water dissociation on TiO2 (110): the role of surface oxygen", J. Phys. Chem. C 2008, 112, 17737. J. Graciani, L. J. Álvarez, J. A. Rodriguez and J. F. Sanz, "N- doping (110) TiO2 surface: a Theoretical DFT Study", J. Phys. Chem. C 2008, 112, 2624. A. B. Mukhopadhyay, C. B. Musgrave and J. F. Sanz, "Atomic Layer Deposition of Hafnium Oxide from Hafnium Chloride and Water", J. Am. Chem. Soc. 2008, 130, 11996.

Towards Large Eddy Simulation of an industrial gas turbine, Thierry Poinsot, CERFACS
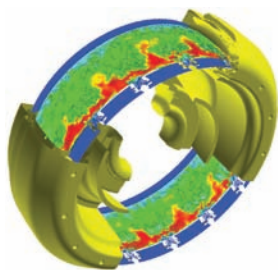
A Temperature File for a Full Helicopter Combustion Chamber Simulation.

Abstract The CFD Team at CERFACS specializes in ground breaking massively parallel simulations of combustion processes. The use of numerical approaches to replace or add to the knowledge of experimental test cases of gas turbines is limited by the realistic modeling of these devices. Using the MareNostrum the Group performed the first full chamber Large Eddy simulation taking into account all possible geometric elements (casing, swirler, dilution films, etc.)

Results The Large Eddy Simulation approach enables the investigation of little known phenomena which take place in helicopter and airplane engines and that are quite difficult to study in real setups. By further improving upon these results, real engine tests may be replaced by numerical ones thus allowing a wide variety of modifications to be examined to improve safety, consumption and pollution. Th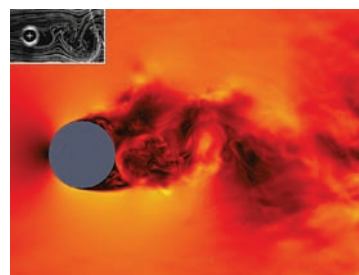e simulation required enormous CPU time. The full chamber LES would have required 16 years on a single CPU computer and was performed on a little less than two months. Also the enormous data sets (over 2.5 Gb per data file) required a lot of time to be written and MareNostrums GPFS system is among the most efficient, reducing data I/O from 2,5 hours to 8 min per file. The MareNostrum therefore presents a giant leap in making possible advanced studies of very complex cases within reasonable timeframes.

Direct Numerical Simulation of turbulent flows in complex geometries using unstructured meshes. Flow around a circular cylinder, Assensi Oliva Llena, UPC, CTTC (Centre Tecnològic de Transferència de Calor)

Abstract Direct numerical simulation (DNS) is an important area of contemporary fluid dynamics, for understanding the physics of turbulence and the development of better turbulence models. The study of flow around cylindrical structures and of flow related to unsteady loading of such structures is crucial for hydro and aerodynamic control and design. The MareNostrum enabled DNS simulation of flow around circular cylinder was performed at very high Reynolds numbers up to 10000.

Instantaneous Velocity Magnitude in the Near Wake, Comparison Between Experimental Visualization From Norverg et al.

Results The computational domain that has been simulated is a rectangular box of dimensions [-4D, 20D],[-4D, 4D],[0,PiD] with a circular cylinder of a diameter D at (0,0,0). At the inflow, velocity (u,v,w) = (1,0,0) has been prescribed. Periodic boundary conditions are used for the spanwise direction that allow to use a Fourier diagonalisation to solve the Poisson equation [1,2]. At the other boundaries, pressure based conditions are used. Three different meshes have been used to evaluate the impact of the geometrical discretisation, a coarse grid of 1.5 million Control Volumes (CV), a medium sized grid of 8 million of CV and a final mesh of 16 million of CV (chosen to perform the complete DNS at Re=10000). The simulations required 240 CPU of MareNostrum over two months divided in different jobs.

Study of SubAtomic Interactions through Lattice Quantum Chromo Dynamics on Mare Nostrum (SAIL), Assumpta Parreño Garcia, University of Barcelona

Abstract Quantum Chromodynamics (QCD) is the underlying theory governing the interaction between quarks and gluons, the strong force, and therefore, responsible for all the states of matter in the Universe. Analytical solutions of QCD in the low energy regime cannot be obtained due to the complexity of the quark-gluon dynamics. The only known non-perturbative method that systematically implements QCD from first principles is its formulation on a dis-

cretized space-time, lattice QCD. This numerical simulation of the theory consists in a Monte Carlo evaluation of a functional integral. The goal is to extract information on hadronic interactions through Lattice QCD using the enormous computing capabilities of the MareNostrum, especially on those sectors where experiments are difficult to perform.

Results Hadron-hadron scattering at different values of the light quark masses and at different lattice spacings were explored. This enabled the extraction of low energy effective range parameters for the pion-pion, kaon-kaon, pion-kaon, nucleon-nucleon, hyperon-nucleon, multipion and multikaon sectors and the reduction of both the statistical and systematic errors in the evaluation of scattering parameters. Also simulated were multi-pion states, required for future calculations of nuclear systems, and the first LQCD investigation of kaon condensation obtained by studying systems containing up to twelve negatively charged kaons, related to studies of the physics of the interior of neutron stars.

Publications William Detmold, Kostas Orginos, Martin J. Savage, Andre Walker-Loud, "Kaon Condensation with Lattice QCD", Phys. Rev. D78, 054514, 2008; Silas R. Beane, Kostas Orginos, Martin J. Savage, "Hadronic Interactions from Lattice QCD", Int. J. Mod. Phys. E17, 1157-1218, 2008; William Detmold, Martin J. Savage, Aaron Torok, Silas R. Beane, Thomas C. Luu, Kostas Orginos, Assumpta Parreño, " Multi-Pion States in Lattice QCD and the Charged-Pion Condensate", Phys. Rev. D78, 014507, 2008; William Detmold, Martin J. Savage, "The Energy of n Identical Bosons in a Finite Volume at O(L^{-7})", Phys. Rev. D77, 057502, 2008; Silas R. Beane, William Detmold, Thomas C. Luu, Kostas Orginos, Martin J. Savage, Aaron Torok, "Multi-Pion Systems in Lattice QCD and the Three-Pion Interaction", Phys. Rev. Lett. 100, 082004, 2008; Silas Beane, Thomas Luu, Kostas Orginos, Assumpta Parreño, Martin Savage, Aaron Torok, Andre Walker-Loud, "The K+K+ Scattering Length from Lattice QCD", Phys. Rev. D77, 094507, 2008; Silas R. Beane, Thomas C. Luu, Kostas Orginos, Assumpta Parreño, Martin J. Savage, Aaron Torok, Andre Walker-Loud, "Precise Determination of the I=2 Scattering Length from Mixed-Action Lattice QCD", Phys. Rev. D77, 014505, 2008; Assumpta Parreño, " Extracting low-energy hadron-hadron physics from lattice QCD", Few Body Syst. 43, 149-154, 2008.
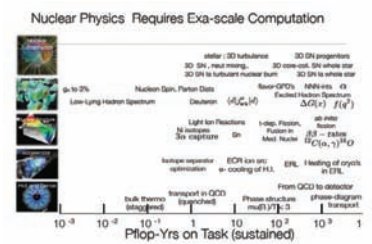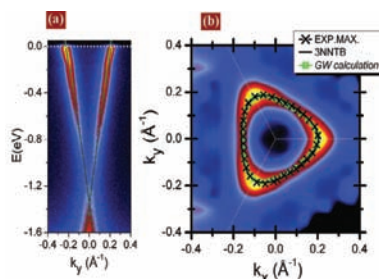

Martin J. Savage, Dept of Physics, U of Washington, US
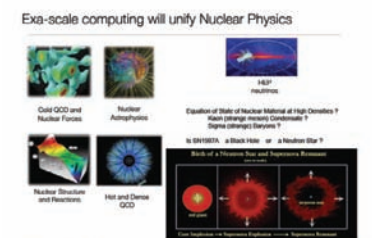
Martin J. Savage, Dept of Physics, U of Washington, US

☞ Optical Properties of BN Nanotubes and Hexagonal BN (ETSF activity), Angel Rubio, Dpto. Física de Materiales, Facultad de Químicas, Universidad del País Vasco

(a) ARPES Scan Measured Close to the Key Direction Along With the TB Fit of the Bare-Band Dispersion (black) and the GW Calculation for Electrostatically Doped Graphene (blue) and Undoped Graphene (Green Circles). (b) Symmetrized Equi–Energy Contour for E=0.24 eV and Maxima (Crosses) Along With the TB Fit and the GW AB–Initio Calculations.

Abstract The progressing trend towards smaller and smaller structures in electronics will lead to the demand of components in the nanometer range. Possible candidates for the construction of nanoelectronics are nanotubes/nanowires. In particular, the interaction with light is of fundamental importance both for the characterization and for the design of light harvesting and emitting nanostructures. This project studied the effect of reduced dimensionality, defects and external field on the optical properties of different nanostructure relevant for electronics applications.

Results The electronic structure of graphene-based compounds were studied to unravel the electronic structure of pure graphite and KC$_8$ intercalated graphite using using ab-initio calculations, and the results were compared with recent ARPES experiments. In the study of optical properties of low dimensional nanostructures, excitonic confinement in one-dimensional molecular chains was identified as the main driving force for the saturation of the chain polarizability as a function of the number of molecular units. This conclusion is based on first principles time-dependent density functional theory calculations. Finally, a new "on the fly" method was introduced to perform Born-Oppenheimer ab-initio molecular dynamics (AIMD) inspired by Ehrenfest dynamics in time-dependent density functional theory.

Publications Efficient Formalism for Large-Scale Ab Initio Molecular Dynamics based on Time-Dependent Density Functional Theory J. L. Alonso, X. Andrade, P. Echenique, F. Falceto, D. Prada-Gracia, and A. Rubio Physical Review Letters 101, 96403 (2008) Optical saturation driven by exciton confinement in molecular-chains: a TDDFT study D. Varsano, A. Marini and A. Rubio Physical Review Letters 101, 133002 (2008) Electron-Electron Correlation in Graphite: A Combined Angle-Resolved Photoemission and First-Principles Study A. Grüneis, C. Attaccalite, T. Pichler, V. Zabolotnyy, H. Shiozawa, S.L. Molodtsov, D. Inosov, A. Koitzsch, M. Knupfer, J. Schiessling, R. Follath, R. Weber, P. Rudolf, L. Wirtz and A. Rubio Physical Review Letters 100, 37601 (2008) A time-dependent approach to electron pumping in open quantum systems G. Stefanucci, S. Kurth, A. Rubio, and E. K. U. Gross Physical Review B 77, 75339 - 14 (2008) Optimal Laser-Control of Double Quantum Dots E. Räsänen, A. Castro, J. Werschnik, A. Rubio, E. K. U. Gross Physical Review B 77, 85324 - 5 (2008) Conserving GW scheme for non-equilibrium quantum transport in molecular contacts K.S. Thygesen and A. Rubio Physical Review B 77, 115333 - 22 (2008) Ultrafast Electron-Phonon Decoupling in Graphite K.Ishioka, M. Hase, M. Kitajima, L. Wirtz, A. Rubio and H. Petek Physical Review B 77, 121402 - 4 (2008).

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» Computational Study of the Molecular Bass of Allosteric Mechanisms and its Conservation Amongst Species – Francisco Javier de la Cruz Montserrat, Institut de Recerca Biomédica (IRB)

» De-novo protein folding and structure prediction with free-energy forcefields – Wolfgang Wenzel, Research Center Karlsruhe

» Detecting evolutionary novelties generated by frameshift translation in several genomes – Arcadi Navarro i Cuartiellas, ICREA and Departament de Ciéncies Experimentals i de la Salut. Universitat Pompeu Fabra

» Determination of native ensembles for proteins using ensemble restrained simulations – Xavier Salvatella, Institut de Recerca Biomedica

» Effect of selective mutations in Pre-A region on the NO detoxification activity of truncated hemoglobin HbN – F J Luque, Univ. Barcelona

» Evolutionary algorithms and de novo peptide design – Ernest Giralt, Institut de Recerca Biomédica

» Exploring enzyme promiscuity of IPL: bi-dimensional QM/MM free energy surfaces – Vicent Moliner, Universitat Jaume I

» Finding new non-coding RNAs in the human genome with homology search – Cédric Notredame, Centre de Regulació Genómica

» Free Energy profile of benzocaine across an asymmetric lipid bilayer: A molecular dynamics simulation study – Jose Javier López Cascales, Universidad Politécnica de Cartagena

» Genomic Distribution of Ancestral Natural Selection in Human Introns – Arcadi Navarro i Cuartiellas, ICREA and Departament de Ciéncies Experimentals i de la Salut. Universitat Pompeu Fabra

» High Performance Parallel Genetic Algorithms for Biomarkers Selections – José María Peña, Universidad Politécnica de Madrid

» Large-scale phylogenetics of the fungal pathogens – Toni Gabaldón, Centro de Investigación Príncipe Felipe

» Ligand migration in truncated hemoglobin O from M. tuberculosis – F J Luque, Univ. Barcelona

» maximum-likelihood refinement of electron microscopy data – Jose Maria Carazo, Centro Nacional de Biotecnologia - CSIC

» MDmix: a new druggability index based on first principles – Xavier Barril Alonso, ICREA & Universitat de Barcelona

» Modelling the Thermal Stability of a Triple Helical Peptide – Natalia Díaz Fernández, Universidad de Oviedo

» Epistatic model of the complete genome in rheumatoid arthritis with MDR by means of parallel computation. Study of combinations associated with diagnosis and disease progression – Dra Sara Marsal Barril, Institut Recerca Hospital Vall Hebron

» Molecular Dynamics Simulation of Self-assembling Cyclopeptide Nanotubes – Juan R. Granja Guillán, Universidad de Santiago de Compostela

» Molecular Dynamics Simulation of the Folding/Unfolding Mechanism of Apoflavodoxin Francisco – Javier de la Cruz Montserrat, Institut de Recerca Biomédica (IRB)

» Molecular modeling of enzyme-substrate interactions and reaction mechanisms in carbohydrate-bound enzymes and aldo-keto reductases – Carme Rovira, Parc Científic de Barcelona

» NO scavenging properties of truncated hemoglobin N from M. smegmatis – F J Luque, Univ. Barcelona

» Optimization and Applications of MDmix, a druggability index based on first principles – Xavier Barril Alonso, ICREA & Universitat de Barcelona

» Parameter estimation and optimal design in computational systems biology – Jordi Villa i Freixa, University Pompeu Fabra

» Prediction of conformational diseases from simulation – Javier Sancho Sanz, Universidad de Zaragoza. Dept. Bioquimica, Biologia Molecular y Celular de Zaragoza.

» RAS superfamily and the interactions with their effectors: functional specificity – Gloria Fuentes, Centro Nacional de Investigaciones Oncológicas

» Rigid chiral dendronized systems based on proline with a thermally stable right-handed helical conformation – Carlos Alemán Llansó, Universitat Politécnica de Catalunya

» Rigid Polyelectrolytes Formed by Chiral Dendronized Polymers Based on Proline – Carlos Enrique Alemán Llansó, Universitat Politécnica de Catalunya

» Simulation of peptide folding induced by inorganic materials (II) – Piero Ugliengo, University of Torino

» Study of domain-induced membrane curvature by means of MD – Manuel Palacín Prieto, Universidad de Barcelona y Institute of Research in Biomedicine

» Study of Protein-membrane interactions of the pore-forming-toxin Sticholysin II by Molecular Dynamics simulation – Tirso Pons, Centro Nacional de Investigaciones Oncológicas

» Synthetic residues in tumor treatment experiments – Carlos Enrique Alemán Llansó, Universitat Politécnica de Catalunya

» The 3D code of DNA: understanding apparition of curvature from atomic detail to gene scale – Agnes Noy Freixa, IRB-BSC/University of Sheffield

» Unraveling the reaction and drug activation mechanisms in catalase-peroxidases by means of QM/MM Car-Parrinello simulations – Carme Rovira, Parc Científic de Barcelona

» Use of TBLASTX to find regions of homology among multiple large-size full genomes – Roderic Guigó, Centro de Regulación Genética

» VSDMIP: Virtual Screening Data Management on an Integrated Platform – Antonio Morreale, Centro de biologia molecular Severo Ochoa

Chemistry and Material Sciences

» Ab Initio Based Polarizable Force Fields Parametrization for Ion-Water Interactions – Elvira Guardia, Universitat Politecnica de Catalunya

» Ab initio simulation of amorphous silica surface and its interaction with biological molecules – Mariona Sodupe, Universitat Autonoma de Barcelona

» Ab-initio phase behaviour of light alkali metals – Eduardo R. Hernandez, Institut de Ciencia de Materials de Barcelona (ICMAB-CSIC)

» Accurate methods for the theoretical prediction of polymorphic crystalline materials of technological interest – Juan J. Novoa, Univ. Barcelona

» Alternative energy resources - computational studies of metal organic framework materials for hydrogen storage – Michele Parrinello, Department of Chemistry and Applied Biosciences, ETH Zurich

» Atomistic simulations of atactic polystyrene in the glassy state, extension to beta relaxation – Doros N. Theodorou, National Technical University of Athens

» Atomistic simulations of atactic polystyrene in the glassy state, Stress relaxation experiments – Doros N. Theodorou, National Technical University of Athens

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- » Computational design of enzymes with targeted specificity for glucaric acid production in E. coli – Alfonso Jaramillo, Ecole Polytechnique (France)

- » Computational design of new catalysts based on nanoparticles – Francesc Illas, Universitat de Barcelona

- » Computational modeling of enantioselective hydrogenation – Feliu Maseras, Instituto Catalán de Investigación Química (ICIQ)

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- » Cubic Molecular Nano-Containers as Selective Fullerene Hosts – Josep M. Luis, Institute of Computational Chemistry, University of Girona.

- » Design of fullerene-based materials for photonic applications – Manthos G. Papadopoulos, National Hellenic Research Foundation

- » Development of force fields for simulations of substrates and reaction intermediates-photocatalyst-zeolite interactions – Sofia Calero, Universidad Pablo Olavide

- » DFT calculation of defects, electronic structure and reactivity in redox-active oxide catalysts – José Carlos Conesa Cegarra, Instituto de Catálisis y Petroleoquímica, CSIC

- » Effect of the total angular momentum on the dynamics of the H_2+H_2 system – Ernesto García Para, Universidad del País Vasco

- » Effects of Cholesterol and headgroup on the structural properties of cell membranes (continuation) – Ramon Reigada Sanz, Physical Chemistry Department of the University of Barcelona

- » Endohedral Fullerene Chemistry: Exohedral Reactivity of $M_3N@C_{78}$ (M=Sc and Y) as Compared to that of C_{78} – Miquel Solà Puig, Universitat de Girona

- » Endohedral fullerene chemistry: exohedral reactivity of $Ng_2@C_{60}$ (Ng= He, Ne, Ar and Kr) – Miquel Solà Puig, Universitat de Girona

- » Exploring complex catalytic sytems by first principle methods using realistic models – Francesc Illas i Riera, Universtitat de Barcelona (Dept. Quimica Fisica & IQTCUB)

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- » Large scale simulations of solvation effects in the structure and dynamics of weakly bound clusters – Alberto García Vela, Instituto de Matemáticas y Física Fundamental

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- » MD study of Protein Protein modification triggered by Al(III) – Jesus Mari Ugalde Uribe-txeberria, Universidad del País Vasco

- » Metal clusters on oxide ultra-thin films: the way towards new materials with unprecedented properties – Gianfranco Pacchioni, Universita di Milano-Bicocca

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- » Model bottom-up nanotechnology for the development of Silicon nanowires aimed for nanodevices – Albert Cirera Hernández, Universitat de Barcelona

- » Modelization of the chemical transport, storage and anion detection functions of modified mesoporous solids – Joan Cano Boquera, ICREA-Universitat de Barcelona

- » Molecular Dynamics Applied to model bottom-up nanotechnology for the development of Silicon nanowires aimed for nanodevices – Albert Cirera Hernández, Universitat de Barcelona

- » Molecular dynamics study of the CO_2, CH_4, and H_2 clathrates – Sergey Vy, Universitat de Girona

- » Montmorillonite clay catalyzed synthesis of RNA oligomers – Mariona Sodupe Roure, Universitat Autónoma Barcelona

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- » On the understanding of the key factors controlling the deactivation pathways of the very efficient for olefin metathesis silica supported Schrock type alkylidene complex es – Xavier Solans-Monfort, Universitat Autónoma Barcelona

- » Phase Change Materials from First Principles – Marco Bernasconi, Department of Material Science, University of Milano-Bicocca

» Photoreactivity, reactivity, and control of molecules adsorbed on metal and metal-oxide surfaces from first principles – Pilar de Lara Castells, Consejo Superior de Investigaciones Científicas (CSIC)

» Properties of the metal/metal oxide interface. First-principles computational simulations. – Javier Fernandez Sanz, Universidad de Sevilla

» Quantum and non-adiabatic reaction dynamics – Octavio Roncero, Instituto de Física Fundamental Blas Cabrera

» Quantum Chemical Study of Self Assembled Monolayers of Mixed Thiols on Noble Metal and Metal Oxide Surfaces – Frederik Tielens, Universite Pierre et Marie Curie-Paris6

» Quantum rate coefficients for the N+N2 reaction – Ernesto García Para, Universidad del País Vasco

» Reactivity of organic and organometallic molecules inside nano-sized molecular vessels – Carles Bo Jane, Instituto Catalán de Investigación Química (ICIQ)

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» Super-lattices in membranes induced by cholesterol: Importance of cholesterol structure to modulate membrane properties – Ramon Reigada Sanz, Universitat de Barcelona

» Supported metal nanoparticles as chemoselective hydrogenation catalysts – Avelino Corma Canós, Instituto de Tecnología Química UPV-CSIC

» Synthesis of new high-pore-volume zeolitic topologies – German Sastre Navarro, Instituto de Tecnologia Quimica UPV-CSIC

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» Theoretical investigation of metal-exchanged zeolites – Petr Nachtigall, Institute of Organic Chemistry and Biochemistry

» Theoretical Study of Magnetic Properties of Single Molecule Magnets and Molecular Magnets – Eliseo Ruiz Sabín, Universitat de Barcelona

» Understanding the Shilov reaction: alkane C-H activation in aqueous solution – Gregori Ujaque, Universitat Autónoma Barcelona

» Unraveling the molecular mechanisms of heterogeneous catalysis by combination of computational modeling and controlled experiment in model systems – Francesc Illas Riera, Universitat de Barcelona

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Physics and Engineering

» Atomistic simulations of colloidal micelles used as drug-delivery agents – Christian D. Lorenz, Kings College London

» Computer simulations of the adsorption of molecules on the surface of nanostructures – María J. López, University of Valladolid/Dpto. Física Teórica

» Determination of the exchange coupling in FeCu multilayers – Jaime Ferrer, Universidad de Oviedo

» Dimensionality and quantum confinement in p-type and n-type semiconductor nanomaterials: a first-principles study based on the PARSEC code – Manuel Maria Gonzalez Alemany, Departamento de Fisica de la Materia Condensada, Facultad de Fisica, Universidad de Santiago de Compostela

» Direct Numerical Simulation of Turbulent Flow Around a Wall-Mounted Cube at Re-NUMBER up to 10000 – Assensi Oliva Llena, UPC, CTTC (Centre Tecnológic de Transferéncia de Calor)

» Direct Numerical Simulation of Turbulent Flows in Complex Geometries – Assensi Oliva Llena, UPC, CTTC (Centre Tecnológic de Transferéncia de Calor)

» Disorder-Induced Order in Continuous Symmetry Systems – Maciej Lewenstein, ICFO - Institut de Ciencies Fotoniques, Barcelona

» DNS of the logarithmic layer on turbulent channels – Javier Jiménez Sendín, School of Aeronautics, Universidad Politecnica Madrid

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» Exploring new avenues towards giant magnetoelectric effects – Jorge Íñiguez, Instituto de Ciencia de Materiales de Barcelona (ICMAB-CSIC)

» First-principles calculations of excitations and optical properties of spin-polarized electronic systems – Frank Fuchs, Institut für Festkörpertheorie und -optik and European Theoretical Spectroscopy Facility (ETSF)

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» Global instability analysis of the trailing vortex system in the wake of commercial aircraft – Vassilis Theofilis, Universidad Politecnica de Madrid

» Interfacial phenomena in multifunctional thin films and superlattices – Jorge Íñiguez González, Instituto de Ciencia de Materiales de Barcelona (ICMAB-CSIC)

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- » Lattice-Boltzmann Simulations of Complex Fluids – Ignacio Pagonabarraga Mora, Department de Fisica Fonamental, Universitat de Barcelona
- » Market Efficiency and Accounting Data – José M. Marín, IMDEA Social Sciences (Madrid), IE Business School (Madrid)
- » Monte Carlo numerical computations of the properties of hadrons – Vicent Gimenez Gomez, Dept. Fisica Teorica Universitat de Valencia and IFIC
- » Monte Carlo simulation of disordered electronic systems – Matteo Palassini, Departament de Fisica Fonamental, Universitat de Barcelona
- » Nondiffusive transport in plasma turbulence – Luis Garcia Gonzalo, Universidad Carlos III
- » Nuclear and Electronic Dynamics in One- and Multi-photon Ionization of Atoms and Molecules by Ultrashort Pulses and Synchrotron Radiation – Fernando Martín, Departamento de Química, C-9. Universidad Autónoma de Madrid
- » Numerical simulation of airframe noise – Frank Thiele, Institut fuer Stroemungsmechanik und Technische Akustik (Tech. Universitaet Berlin)
- » Optical Properties of BN Nanotubes and Hexagonal BN (ETSF activity) – Angel Rubio, "Dpto. Fisica de Materiales, Facultad de Quimicas, Universidad del Pais Vasco, Unidad de Fisica de Quimicas, Universidad del Pais Vasco, Unidad de Fisica deMateriales"
- » PASTRAMY: Persistent and Highly Available Software Transactional Memory – António Rito Silva, Instituto de Engenharia de Sistemas e Computadores, ESC ID/INESC/IST/UTL)
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- » Towards Large Eddy Simulation of an industrial gas turbine – Thierry Poinsot, European Centre for Research and Advanced Training in Scientific Computation (CERFACS)
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